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Physically based multiscale-viscoplastic model for metals and steel alloys: theory and computation

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PHYSICALLY BASED MULTISCALE-VISCOPLASTIC MODEL FOR METALS AND STEEL ALLOYS: THEORY AND COMPUTATION

A Dissertation
Submitted to the Graduate Faculty of the Louisiana State University and Agricultural and Mechanical College in partial fulfillment of the requirements for the degree of Doctor of Philosophy
in
The Department of Civil & Environmental Engineering

by
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August 2005
TO MY BELOVED MOTHER & FATHER

MAY ALLAH ENLIGHTEN YOUR GRAVES AND BLESS YOU IN THE DAY AFTER
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The completion of this dissertation has been a monumental accomplishment in my academic career. I am grateful for this opportunity to acknowledge and thank those that have helped me throughout this process. If it were not for my wife, kids, brothers and sisters who have supported me throughout all of my different interests, I would not have finished.

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ABSTRACT

The main requirement of large deformation problems such as high-speed machining, impact, and various primarily metal forming, is to develop constitutive relations which are widely applicable and capable of accounting for complex paths of deformation. Achieving such desirable goals for material like metals and steel alloys involves a comprehensive study of their microstructures and experimental observations under different loading conditions. In general, metal structures display a strong rate- and temperature-dependence when deformed non-uniformly into the inelastic range. This effect has important implications for an increasing number of applications in structural and engineering mechanics. The mechanical behavior of these applications cannot be characterized by classical (rate-independent) continuum theories because they incorporate no ‘material length scales’. It is therefore necessary to develop a rate-dependent (viscoplasticity) continuum theory bridging the gap between the classical continuum theories and the microstructure simulations.

Physically based viscoplasticity models for different types of metals (body centered cubic, face centered cubic and hexagonal close-packed) and steel alloys are derived in this work for this purpose. We adopt a multi-scale, hierarchical thermodynamic consistent framework to construct the material constitutive relations for the rate-dependent behavior. The concept of thermal activation energy, dislocations interactions mechanisms and the role of dislocations dynamics in crystals are used in the derivation process taking into consideration the contribution of the plastic strain evolution of dislocation density to the flow stress of polycrystalline metals. Material length scales are implicitly introduced into the governing equations through material rate-dependency (viscosity).

The proposed framework is implemented into the commercially well-known finite element software ABAQUS. The finite element simulations of material instability problems converge to meaningful results upon further refinement of the finite element mesh due to the successful incorporation of the material length scale in the model formulations. It is shown that the model predicted results compare very well with different experimental data over a wide range of temperatures (77K°-1000K°) and strain rates (10^-3-10^4s^-1). It is also concluded from this dissertation that the width of localization zone (shear band) exhibits tremendous changes with different initial temperatures (i.e., different initial viscosities and accordingly different length scales).
CHAPTER 1
INTRODUCTION

Plastic/viscoplastic deformation in metals is a very complex phenomenon originating from highly nonlinear dynamical processes associated with microscopic defects, such as dislocations which tend to self-organize in the form of patterns, resulting into a heterogeneous field of deformation at the microscale although the overall macroscopic field is thought to be homogeneous. Although there has been a tremendous effort to understand work hardening/strain softening and associated material instability phenomena, this research area is still in a parlous state, and rife with controversy. This is due to the difficulty of carrying out truly definitive experiments on critical aspects of the evolution of the dislocation structure. But more important have been the immense theoretical difficulties of dealing with large numbers of dislocations and defects. Nevertheless, it is well understood that plastic deformation and strengthening in metals can be related to a number of heterogeneous patterns, such as dislocation cells, slip bands, microshear bands, persistent slip bands and dislocation tangles, which are critical for material properties. For example, localized deformation, shear banding and dislocation cell structures play a significant role in determining the flow properties of heterogeneous materials, such as MMCs, even at small macroscopic strains (Zbib et al., 2002).

The understanding of high-strain-rate behavior of metals is essential for the modeling and analysis of numerous processes including high-speed machining, impact, penetration and shear localization. Thus, a desirable goal in constitutive modeling is to develop models which are widely applicable and capable of accounting for complex paths of deformation, temperature and strain rate which represent the main requirements of large deformation problems. The intended applications of the model as well as the availability and ease in obtaining experimental data specify the degree of complexity of the constitutive model. Moreover, the degree of success of the model mainly depends on the flexibility and simplicity of determining material constants from a limited set of experimental data and capturing the important aspects of static and/or dynamic behavior besides being mathematically and computationally accurate. In dynamic problems that introduce high strain rates, the dynamic yield stress is considered the most important expression needed to characterize the material behavior and is also used in finite element codes. Although we are concerned with the macroscopic response of the plastic flow, investigating the grain and atomic level of the material deformation will help us understand the failure mechanisms for different material structures. Accordingly, the definition of dynamic yield (flow) stress differs from metal to metal depending on their internal crystal structure; body centered cubic (bcc), face centered cubic (fcc), hexagonal close packing (hcp), and others. These crystal structure differences affect differently the dislocations movement during the plastic deformation process under high strain rates loading. Each of these three crystal structures exhibits a characteristic thermomechanical behavior which is associated with the available slip systems and symmetries as well as the nature of dislocation cores. The viscoplastic deformation of steel alloys is generally controlled by the dislocation mechanisms attributed to the content of their compositions. The percentage of carbon in steel plays a crucial role in determining the phase behavior (Ferrite and Austenite) of the material over a wide range of temperatures.
Generally, the plastic flow is characterized macroscopically as a visible distortion, microscopically as the appearance of slip systems, and atomically as a movement of dislocations. Microscopic plasticity in metals is primarily the result of dislocation moving through the crystal lattice. The interaction of these dislocations (see Figure 1.1) with the lattice and the various obstacles encountered through the lattice determine the flow strength of the material. The motion of a dislocation through the lattice or past an obstacle requires the surmounting of an energy barrier by a combination of applied stress and thermal activation. The result is that the effective shear stress required to generate an overall plastic strain rate is intimately tied to the temperature at which the deformation occurs. Competing thermal activation effects will influence deformations that occur at both high temperature and high strain rates. The coupling of rate and temperature through dislocation kinematics indicates that the rate of thermal softening of metals should be related to the rate of deformation. These considerations are particularly important in the development of material models for use within simulation of high-rate phenomena, which generally involve high temperatures because of adiabatic heating.

The question is: What are the microscopic quantities of interest and how do they relate to the macroscopic quantities. As macroscopic plasticity theories are usually based on a yield condition, we have to identify this feature within the microscopic theory. This dissertation address the need of consistent physically based definitions for the yield surface that is required for dynamic localizations (see Figure 1.2).
In inelastic deformation, the localization of deformation into narrow bands of intense straining is considered one of the characteristic features in metals and steel alloys. Localization for the case of rate-independent formulation is associated with a change in the character of the governing equations. That is, under quasi-static loading conditions the equations governing incremental equilibrium lose ellipticity, while under dynamic loading conditions wave speeds become imaginary. Standard boundary value problems are then ill posed; one manifestation of this is that the width of the band of localized deformation is arbitrary narrow. As a consequence numerical solutions to localization problems for rate-independent solids exhibit inherent mesh dependence. The minimum width of the band of localized deformation is set by the mesh spacing (see Figure 1.3). Furthermore, global quantities such as the overall stiffness characteristics of the body depend on the mesh size used to resolve the band of localized deformations. The inelastic response of materials is perhaps inevitably rate dependent. When material rate dependence is accounted for, there is no loss for ellipticity in quasi static problems and wave speed remains real, as long as stress levels remain small compared to elastic stiffness. Even though the phenomenology of localization can be the same for both rate-dependent and rate-independent material behavior, pathological mesh dependence does not occur in numerical solutions for rate-dependent solids because boundary value problems remain well posed. The rate independent solid does emerge as the appropriate limit of the rate-dependent solid, although the limiting case is a singular one (Needleman, 1988).

Under both quasi static and dynamic loading conditions, the solutions to localization problems for rate-independent solids permit arbitrary narrow bands of intense deformation. There is nothing in the formulation to set a minimum width to such bands. On the other hand, in numerical solutions the minimum width is set by the mesh spacing and key features of the solutions can be a consequence of the discretization. This is clearly an undesirable state of affairs and stems from the character of the continuum problem. One approach to remedying this situation is to explicitly introduce a length scale into the material characterization by using a nonlocal constitutive relation. In this dissertation, we will show that material rate dependence, no matter how small, leads to well posed boundary value problems with unique solutions. This can be viewed in terms of material rate dependence implicitly introducing a
length scale into the boundary value problem formulation. Of course, in any particular circumstance, the question remains as to whether or not this is the relevant length scale.

Figure 1.3 (a) Mesh-dependent results for dynamic localization (shear bands) using classical plasticity theory. (b) Mesh-independent results using rate-dependent (viscoplasticity) theory.

Since modern structures exhibit a strong rate dependency especially at elevated temperatures, the constitutive relations which have been developed to describe the behavior of different
types of metals must be able to reproduce these facts. Processes related with high velocities therefore must be described by a rate-dependent viscoplasticity whereas the same constitutive relations for vanishing velocities must turn over to a rate-independent plasticity. Prior to establishing constitutive relations that can fulfill these conditions, a proper physical interpretation of the phenomena observed during inelastic deformation is needed. This means that the different mechanisms that can explain the dissipation implied by internal changes of the material are to be analyzed. It is known from appropriate microscopic investigations that in a temperature, strain rate spectrum in general different regions can be observed reflecting different mechanisms of inelastic deformation. These are; (1) athermal mechanisms characterized by a yield stress (e.g., fcc metals) or hardening stress (e.g., bcc metals) relatively insensitive to the strain rate; (2) thermally activated dislocation motion characterized by a more markedly, temperature and rate sensitivity of the yield and hardening stresses.

### 1.1 Review and Background

The problem of developing a continuum micromechanical-based theory which could be used as an engineering tool both in analysis and in computer-aided design of materials, is a topical and still unsolved material science problem. Attempts to construct such a theory are faced with the difficulties in describing the microscopic structure of materials in terms of continuum mechanics. When load is applied, the elastic and inelastic deformation of materials occurs in most cases not homogeneously, but reveals fluctuations on various space scales. This heterogeneity plays a key role in determining the mechanical properties of materials.

Many researchers extensively investigated the subject of modeling the dynamic flow stress of the material plastic flow at high strain rates and elevated temperatures. Studies were made in characterizing material behavior through both phenomenological and physically based models. Empirical equations were initially developed with simple uniaxial stress-strain models (Campbell et al., 1977; Nicholas, 1982a) and one-dimensional stress wave propagation models (Nicholas, 1982b) by describing the effect of temperature and strain hardening as well as strain rate on the flow stress. However, for the von Mises type material, the one-dimensional models that express flow stress as a function of strain and strain rate can be converted into the equivalent three-dimensional material models by replacing stresses, strains, and strain rates by their equivalent invariant three-dimensional forms (Zukas, 1990). Johnson and Cock (1983) proposed a phenomenological model that is widely used in most computer codes for static and dynamic analyses in order to predict the behavior of the material flow stress at different strain rates ($10^{-4} \, s^{-1} - 10^5 \, s^{-1}$) and temperatures. The main advantage of this model is that it is relatively easy to calibrate with a minimum of experimental data in the form of stress-strain curves at different strain rates and temperatures. This model is given as:

$$
\sigma_{eq} = [A + B \dot{\varepsilon}_p^n][1 + C \ln \left(\frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_{po}}\right)][1 - T^* m]
$$

(1.1)

where $A$, $B$, $C$, $n$, and $m$ are material constants, $T^* = (T - T_r)/(T_m - T_r)$ is the homologous temperature, where $T_r$ is the room temperature, $T_m$ is the melting temperature, and $\dot{\varepsilon}_{po}$ is the user-defined reference accumulative plastic strain rate. In this model, however, the difference
in the deformation behavior between different types of metal structures is not considered. Moreover, the strain rate and temperature effects on the flow stress are uncoupled which implies that the strain rate sensitivity is independent of temperature. This is not the case as observed in most metals. It is rather found that the rate sensitivity increases with increasing temperature while the flow stress decreases. The Johnson-Cook model is an empirical equation of state (Johnson, 1988) designed for ease in computational implementation. This approach, however, does not represent any thermal or strain rate history effects. In general, strain rate and thermal history effects can be taken into account by introducing internal state variables, which are necessary to represent the material behavior (Mecking and Kocks, 1981; Follansbee and Kocks, 1988; Bammann, 1990; Bammann et al., 1990a). Quite recently, Milella (2001) presented a constitutive equation based on the experimental results obtained by him and those available at the open literature for different temperatures and strain rates. He observed from the experimental evidence that for bcc metals, the trend of the yield strength is linear, when plotted in the log scale versus the reciprocal of the temperature, independently of the strain rate applied. Moreover, he showed that all these linear trends at different strain rates point towards a lower common value that represents the athermal component of the yield strength.

The understanding of high-strain-rate behavior of metals is essential for the modeling and analysis of numerous processes including high-speed machining, impact, penetration and shear localization. Recently, considerable progress has been made in understanding the role of rate controlling dislocation mechanisms on the temperature and strain rate dependence of the flow stress for metals and alloys. Hoge and Mukherjee (1977) studied the effect of both temperature and strain rates on the lower yield stress of Tantalum and proposed a model incorporating the combined operation of the Peierls’ mechanism and dislocation drag process. They concluded from the stress-temperature relationship and the variation of the activation volume with stress and strain that the rate controlling mechanism for deformation could be rationalized in terms of Peierls mechanism. This behavior is mainly attributed to the specific crystal structure of body cubic centered metals. Steinberg and co-workers (see for example, Steinberg et al., 1980; Steinberg and Sharp, 1981; Steinberg and Lund, 1989) described a constitutive model for use with hydrodynamic codes to account for the dependence of shear modulus and yield strength on high strain rates, temperature, and pressure-dependent melting. Although their model is intended to be used at high strain rates, their formulation did not specifically include strain rate effects.

Zerilli and Armstrong (1987) used dislocation mechanics concepts to develop a flow stress model that accounts for strain, strain rate and temperature in a coupled manner, which can be incorporated in dynamics related computer codes. Their model considers two different forms for two different classes of metals;

body centered cubic (bcc):

\[ \sigma_{eq} = Y e^{-\beta_1 T + \beta_2 T \ln \dot{\varepsilon}} + Be^\dot{\varepsilon} + Y_a \]  \hspace{1cm} (1.2)

and face centered cubic (fcc):

\[ \sigma_{eq} = B e^{0.5 \dot{\varepsilon}^{-\beta_1 T + \beta_2 T \ln \dot{\varepsilon}}} + Y_a \]  \hspace{1cm} (1.3)
where $\beta_1$ and $\beta_2$ are material parameters, $B$ and $n$ are the hardening constants, $Y_a$ is the athermal part of the yield stress and $\hat{Y}$ is the threshold yield stress. The rational for the differences in the two forms mainly depends on the dislocation characteristics for each particular structure. Bcc metals show stronger dependence of yield stress on temperature and strain rate while in the case of fcc metals the yield stress is mainly affected by strain hardening. In other words, the cutting of dislocation forests is the principal mechanism in fcc metals, while in bcc metals; the overcoming of Peierls-Nabarro barriers is the principal mechanism. These two different dislocation mechanisms of the two different metal classes will be further investigated in this dissertation. Zerilli-Armstrong model has been derived based on the concept of thermal activation analysis for overcoming local obstacles to dislocation motion. This model has been widely used in many computer codes from which its material parameters are physically interpreted. In fact, this physical interpretation of material constants becomes meaningless if one tries to identify them from the experimental data by using a very small reference strain rate rather than using the one corresponding to the reference dislocation velocity as been derived in the model. It has been shown that the Zerilli-Armstrong model as compared to the Johnson-Cook model gives slightly better correlation with experimental results; however, none of these two models is very accurate in describing the behavior of metals at elevated temperatures (Johnson and Holmquist, 1988; Abed and Voyiadjis, 2005).

Nemat-Nasser and his co-workers (e.g., Nemat-Nasser and Isaacs, 1997, Nemat-Nasser & Li, 1998, Nemat-Nasser et al., 1999, and Nemat-Nasser & Guo, 2000) developed an experimental technique measuring the flow stress of different bcc, fcc and hcp metals and alloys over a broad range of strains, strain rate, and temperatures in uniaxial compression. Some of their experimental results are, actually, used in this work for models evaluation and comparisons. They also presented a constitutive model that characterizes the plastic deformation of different metals and alloys using the thermal activation concept and assuming constant dislocation density throughout the deformation process. That is neither the plastic strain evolution of dislocation density nor the rate multiplication of the dislocation density evolution is considered.

There has been a significant progress made over the years in the development theories of plasticity and viscoplasticity for the phenomenological representation of inelastic constitutive properties. In particular, mathematical modeling of metal viscoplasticity developed based on the so-called internal state variable formalism in the thermodynamics of irreversible processes. A large number of specialized forms of these modern unified viscoplastic models (e.g., isotropic or anisotropic, fully associative or non-associative, isothermal or non-isothermal, etc.) have been successfully applied to different metals with different crystal structures (Coleman and Gurtin, 1967; Lubliner, 1973; Germain et al., 1983; Lemaitre and Chaboche, 1990; Chaboche, 1989; Arnold and Saleeb, 1994; Robinson and Duffy, 1990; Arnold et al., 1995, 1996; Robinson et al., 1987; Freed and Walker, 1993; Simo and Taylor, 1985, 1986).

Generally, the additive decomposition of the total strain rate into elastic and plastic components is generally assumed in plasticity/viscoplasticity constitutive modeling for small elastic strains. Various viscoplastic material models have been proposed. Some of them are physically based and others are phenomenological. A widely used viscoplastic formulation is the Perzyna model (Perzyna, 1963; 1966; 1986, 1988, 1998). The main feature of Perzyna
model is the dynamic yield surface which is used in describing the viscoplastic strain. This dynamic yield surface can be larger than zero, and is known as the “overstress”. In other words, the overstress is defined as the difference between the dynamic stress and its static counterpart and it is the common notion of viscoplasticity, which implies that an inelastic process can only take place if, and only if, the overstress is positive.

On the other hand, viscoplasticity can be modeled by incorporation of the time dependency in a yield function, which, together with the consistency parameter, obeys the classical Kuhn-Tucker relations. In Wang et al. (1997) and Wang (1997), a so-called Consistency model has been proposed, in which the time-derivative of a rate-dependent yield surface governs the irreversible viscous deformation behavior. Furthermore, Mahnken et al. (1998) and Johansson et al. (1999) have considered a rate-dependent yield formulation in combination with coupling to damage. Very recently, Ristinmaa and Ottosen (2000) have given a thorough discussion on the main features and implications of modeling rate-dependency within a yield surface concept.

Large-scale finite element numerical simulations provide a feasible approach for assessing the performance of inelastic structural components operating under complex thermomechanical and multiaxial loading conditions. The global solutions for any discretized finite element model are typically achieved, from the computational point of view, by an increment iterative procedure (e.g., Newton-Raphson technique). The mathematical forms, accuracy and stability properties of a selected integration procedure will directly affect the accuracy and efficiency of the overall finite element solution. The development of stress integration algorithms with improved performance has received considerable attention in the recent literature on computational plasticity and viscoplasticity. In this regard, due to their stability and wide range of applicability, a number of well-established implicit schemes of time integration have attracted the attention of many authors for plasticity and viscoplasticity (Simo and Taylor, 1985, 1986; Simo, 1991; Ju, 1990; Loret et al, 1992; Lush et al., 1987; Caddemi and Martin, 1991; Hornberger and Stamm, 1989; Auricchio and Taylor, 1994; Freed and Walker, 1992; Saleeb, 1993; Kojic and Bathe, 1987; Bathe, 1996).

1.2 Objectives and Fundamental Concepts

The main objective of this work is to introduce physically based multiscale constitutive relations that are thermodynamically consistent and able to characterize the deformation behavior of metals under low and high strain rates and temperatures. Moreover, these constitutive models should be able to capture (1) the softening effects associated with high strain rate inelastic deformations and high temperatures, (2) strain-rate and temperature sensitivity, and (3) dynamic localizations of different initial boundary value problems for several types of metals and steel alloys subjected to different loading conditions. Research in this dissertation focuses on several areas of multi-scale constitutive and computational modeling and mathematical characterization of material response under various static and dynamic loading conditions. The framework of this dissertation is summarized as follows:
1. Developing microstructural physically based relations for modeling the flow stress of metals based on their crystal structures using the activation energy concept as well as the dislocation interaction mechanisms. These material models should be first tested by experimental comparisons before using them in the thermodynamical formulation of the multiscale constitutive model.

Dislocations play a main role in determining the inelastic behavior of a metal and its flow stress under different load conditions (temperature, strain rate etc.). Loading of a material in the inelastic range causes dislocations to be generated, moved and stored. Motion of dislocations, however, indicates that the metal has exceeded its elastic limit or yield strength $Y$ and hence plastic strains are generated inside the material. In this regard, Orwan’s equation (Orwan, 1948), which relates the plastic shear strain $\gamma^p$ to the density of the mobile dislocations, $\rho_m$, is utilized:

$$\gamma^p = \rho_m b l$$

where $b$ is the magnitude of the Burgers vector and $l$ is the dislocation displacement or it can be interpreted as the free path of trapped dislocations. In general, the dislocation mechanisms and the activation energy principle are utilized in developing microstructural physically based material models that characterize the plastic deformation behavior. These models, however, will have different forms depending on the internal crystal structure of metals and steel alloys.

In the case of fcc metals, like copper and aluminum, the emergence and evolution of a heterogeneous microstructure of dislocations as well as the long-range intersections between dislocations dominates and controls the mechanisms of thermal activation analysis behavior. Thus, the thermal activation is strongly dependent on the plastic strain. That is, the increase in the yield point with a decrease in temperature is highly dependent on the strain-hardened states for fcc metals. In contrast, the behavior of bcc metals shows a strong dependence of the thermal yield stress on the strain rate and temperature. The thermal stress is attributed to the resistance of the dislocation motion by the Peierls barriers (short-range barriers) provided by the lattice itself. Moreover, the plastic hardening of most bcc metals, like pure iron, tantalum, molybdenum, and niobium, is hardly influenced by both strain rate and temperature and therefore, it contributes to the athermal part of the flow stress besides the small percentage of the yield stress. The difference of the mechanical behavior of bcc metals to fcc metals may be ascribed to the dislocation size and the corresponding concentration of Cottrell’s atmosphere. During their movement, dislocations displaced across the lattice and accordingly their atmosphere of interstitial atoms will be moved. Atoms movement results in a drag force that opposes these atom clouds. Drag-force increases as the concentration mismatch between the Cottrel’s atmosphere and the solute atoms in the lattice increases and, therefore, the thermal yield stress increases (Milella, 1998). The yield strength produced by these effects depends on both temperature and strain rate since the solute atoms concentration does so.

The mechanical behavior of hcp metals, like titanium and zirconium, can be determined by addressing the structure and energies of dislocation cores and planer defects, including twin boundaries and stacking faults. However, different hcp materials have dramatically different mechanical properties which make the modeling of the plastic flow of hcp metals very
complicated and not unique over broad temperature and strain rate ranges. In fact, hcp materials often show strong temperature dependent behavior, often associated with changes in deformation modes which, in turn, affect both the polycrystalline ductility and dynamic recrystallization. Although the crystal structure of hcp metals is close-packed like fcc metals, it shows plastic anisotropy and lacks the symmetry needed to be sufficient in satisfying, for instance, the von Mises criterion (Yoo et al., 2002). Since each hcp metal has its own mechanical behavior depending on the internal structure (a/c ratio) and slip plane and direction, the authors choose to concentrate in this study only on the thermal plastic deformation behavior of titanium. Its alloys are considered to be the most increasingly used hcp metals in structural applications at low and high strain rate of loading.

As explained earlier, the microstructure of steel alloys mainly consists of components that have several types of crystal structures; bcc, fcc, and hcp. The experimental observations of steel alloys reveal some characteristics that need to be addressed in the plastic deformation modeling. The first characteristic is that both the hardening and the yield stress depend on the temperature and the strain rate and their corresponding history. Second characteristic is that the microstructure of the material evolves mainly with the temperature history. Third characteristic is that the long-rang obstacles are related to the plastic strain as well as the initial yield stress.

2. Deriving thermodynamically consistent evolution for the internal state variables used in the multiscale formulation based on the thermodynamics equilibrium (first and second laws. This constitutive model, however, should take into consideration small and large deformation analyses and will be applicable for both low and high strain rates at different elevated temperatures.

It is generally assumed that the rate of deformation can be additively decomposed into an elastic (reversible) part and an inelastic (irreversible) part (Nemat-Nasser, 1983; Khan, 1995; Lubliner, 1990). ‘Non-instantaneously reversible’ deformation is a more general description of the inelastic deformation since it is corresponding to the following set of physical phenomena: instantaneous plasticity and viscoplasticity. The first type of inelastic deformation is a time-independent mechanism, which is generally considered in the rate-independent plasticity theories. While the viscoplastic deformation, which is sometimes qualified as creep, is a rate-dependent mechanism. Both of those two mechanisms are generally sufficient to describe the set of experimental observations under high strain rates. The underlying objective here is to efficiently incorporate material length scales in the classical continuum plasticity theories through the development of viscoplastic formulation by relating the viscosity parameter to the microstructure physical quantities. This development will allow us to investigate a range of phenomena that cannot be well addressed by the conventional continuum plasticity theories such as the size-dependent of material behavior and localization in softening media.

Thermodynamics with internal variables offers a good framework to introduce constitutive equations. It offers both a guideline and some constraints for the choice of thermodynamically consistent evolution equations. A special form uses the notion of a standard generalized material, where the complete thermo-elastic-inelastic behavior is defined from the knowledge of two potentials; the thermodynamic potential to describe the present state and the dissipative
potential for the irreversible evolutions, is proposed. Introducing mechanical constitutive models into a thermodynamic framework allows the partition of the plastic work into the energy stored by the material and the one dissipated away as heat. The constitutive equations are derived from the first and second laws of thermodynamics, the expression of Helmholtz free energy, the additive decomposition of the total strain rate into elastic and viscoplastic, the Clasius-Duhem inequality, the maximum dissipation principle, generalized normality, and the thermomechanical heat equation. The viscoplastic yield criterion adopted in this work is of a von Mises type, but it needs to be modified to account for high-strain rates and temperature dependency. This is done by replacing the yield strength, the hardening function, and the viscous stress by the physically based flow stress model that will be developed in the first part of this work. The irreversible thermodynamic process can be characterized by a time incremental approach allowing for the equilibrium thermodynamic characterization. The irreversible thermodynamic is compensated for by introducing internal state variables such that they are implicitly non-equilibrated by a set of fictitious thermodynamic conjugate forces. Thus, the internal energy is defined as a function of the thermomechanical variables of the material which are of the Eulerian total elastic strain tensor, \( e^E_{ij} \), absolute temperature, \( T \), the rate of loading, \( \dot{p} \), and certain numbers of phenomenological internal state variables, \( N_i \). Thus, the Helmholtz free energy density at the current state of deformation within the thermodynamic framework and considering the assumption of small elastic strains can be written as follows:

\[
\Psi = \Psi \left( e^E_{ij}, \dot{p}, T; N_i \right) \tag{1.5}
\]

where \( N_i \) represents either a scalar or a tensorial variable and are introduced to represent the material microstructure and deformation processes when subjected to high strain rate loadings. Hence, the internal energy is defined as a function of the thermomechanical variables of the material which are the elastic strain, the temperature, the deformation gradient.

3. Developing a consistent algorithmic treatment for the developed viscoplasticity constitutive relations within the context of small strain deformation. The algorithm is then extended to account for the objectivity of stress integration in finite strain viscoplasticity. Implementing the developed thermo-viscoplastic models in two- and three-dimensional finite element codes. Finally, testing the numerical implementation of the proposed model for different strain rates and temperatures related problems by numerical comparison to the available experimental data in the literature.

The development of stress integration algorithms with improved performance has received considerable attention in the recent literature on computational plasticity and viscoplasticity. The very efficient implementations of the implicit integration using the radial return schemes for metals corresponding to the special case of full isotropy (both elastic and inelastic responses), enabled by the complete reductions of the rate tensor equations to a final single/scalar nonlinear equation; e.g. in terms of the effective stress, or equivalently the plastic multiplier or the “magnitude” of the inelastic strain vector. In order to achieve a strong algorithmic treatment for any complex viscoplasticity constitutive models used for large-scale deformation, the following three tasks are required (Saleeb et al., 2000); (1) detailed study of
the mathematical structure of the viscoplastic equations, and the corresponding integrated field of stress and internal state variables, (2) development and implementation of the implicit backward-Euler stress-updating algorithm, and the associated nonlinear iteration equation solver (e.g., Newton Raphson technique), (3) testing the convergence, stability, and accuracy properties of the algorithms.

On the theoretical side, the general framework is developed in the specific context of the fully implicit (backward Euler) difference scheme which is known to exhibit excellent convergence and accuracy characteristics in large scale computations that involve large time steps, particularly with complex anisotropic inelastic models (Ortiz and Popov, 1985). Radial return algorithm which is a special case of the backward-Euler method is used to introduce a nonlinear scalar equation in terms of the viscoplastic multiplier for the case of the Consistency viscoplastic model and in terms of the equivalent stress for the case of Perzyna viscoplastic model. Consistent algorithmic tangent stiffness matrices are derived for both small and finite strain viscoplastic models.

The extension of a small strain constitutive relation to finite strains requires the consideration of finite rotations. The development of objective rates has been studied extensively in the literature in introducing stress update algorithms (e.g., Simo and Marsden, 1984; Simo and Ortiz, 1985; Cuitino and Ortiz, 1982; Rodriguez-Ferran et al., 1997). In this study, we will adopt a stress integration methodology that is called “local rotated representation” explained later at which the problem can be reduced to the numerical integration of an initial value problem that generates a one-parameter subgroup of proper orthogonal transformation.

Numerical simulations using finite element codes for modeling the high deformation rates behavior and failure of these materials require an accurate description of strain, strain rate, loading history, temperature, internal damage, and deformation. The proposed frameworks are implemented in the well-known explicit commercial finite element software ABAQUS (2003) by using the material subroutines VUMAT. This implementation is utilized in investigating different deformation phenomena like for example a thin shear band region of finite width that undergoes significant deformation and temperature rise. This, however, requires an appropriate identification procedure for the constitutive parameters which is based on the experimental observations. Finally, several numerical examples are introduced to test the proposed algorithm and its implementation in the ABAQUS FE Code and also to study the initiation and growth of shear bands and necking in tensile plane strain problems.

1.3 Outline

This dissertation is divided into six primary chapters (Chapters 2 - 7), each with a series of objectives directed towards addressing the issues of developing consistent and physically based constitutive relations for low and high strain rate and temperature-related problems. This research is a necessary step in understanding the microstructure behavior of different metals and alloys with different types of crystal structures. It should be mentioned here that the
materials presented in chapters 2, 3, 4, and 5 are already published in four separated journal papers.

In chapter 2, two physically based flow stress models for both bcc and fcc metals are derived based on the concept of thermal activation analysis as well as dislocation interaction mechanisms. The models address the effect of dislocation density multiplications on the thermal component of the material flow stress through a consistent formulation based on the characterization of the dislocation microstructure. Comparisons between the results predicted by the developed models with the experimental results for the one-dimensional case are also presented for Niobium, Vanadium, Tantalum, Molybdenum, and OFHC Copper.

Chapter 3 presents the characterization and modeling of the viscoplastic deformation behavior of AL-6Xn Stainless steel using a combination of the two bcc and fcc constitutive models. The experimental results provided by Nemat-Nasser et al. (2001) are utilized in determining the material parameters for the proposed viscoplastic deformation modeling of AL-6XN. Moreover, the classical secant modulus method is utilized here in modeling the true stress strain curves for different temperatures and strain rates. Comparisons are made between the predicted results and the experimental data for different strain rates and temperatures.

The purpose of the study presented in Chapter 4 is to investigate the physical basis of the Z-A constitutive relations and to modify the physical interpretation of the model parameters by introducing validated constitutive relations with material parameters that are related accurately to the nano-/micro-physical quantities. A detailed discussion about the physical basis as well as the procedure used in deriving the Z-A relations is also given. The physical interpretation of the Z-A model parameters is investigated and consequently modified relations are proposed. Applications of the proposed modified model for different metals at low and high strain rates and temperatures are performed. Comparisons are also made of the proposed model with both the Z-A model and the experimental results.

Chapter 5 presents further modification of the work presented in chapter 2 after considering the effect of plastic strain evolution of dislocation density in determining the flow stress of three major categories of metal structures; body centered cubic (bcc), face centered cubic (fcc), and hexagonal close packed (hcp) over a wide range of temperatures and strain rates. The proposed constitutive models are derived based on the concept of thermal activation analysis, dislocation interaction mechanisms, experimental observations, and the additive decomposition of flow stress to thermal and athermal components. The role of dislocation dynamics inside the crystal lattice in determining the general form of the thermal plastic stress is investigated using the well-known Orowans relation that considers the plastic deformation as a dynamic process obtained by the motion of dislocations with an average velocity. In turn, the plastic shear strain rate at the microscale is related to the plastic strain rate tensor at the macroscale using the expression postulated by Bamman and Aifantis (1982). Moreover, the evolution of dislocation density with plastic strain given by Klepaczko (1987) is also utilized in the derivation process of the proposed modeling. Both the thermal and athermal components of the flow stress are physically derived and all the models parameters are related to the nano and micro-structure quantities. The hardening stresses are characterized using two different definitions of hardening parameters for each metal structure. Finally, the dynamic strain aging
and the twinning phenomena encountered in some polycrystalline metals at certain range of strain rates and temperatures are briefly discussed.

Chapter 6 presents the derivation of a thermodynamically consistent framework for introducing solid constitutive equations to describe the viscoplastic behavior of polycrystalline bcc and fcc metals. A special form uses the notion of a standard generalized material, where the complete thermo-elastic-inelastic behavior is defined from the knowledge of two potentials; the thermodynamic potential to describe the present state and the dissipative potential for the irreversible evolutions, is proposed. Introducing mechanical constitutive models into a thermodynamic framework allows the partition of the plastic work into the energy stored by the material and the one dissipated away as heat. An explicit definition of a length scale parameter is introduced through the definition of the viscosity parameter as related to the material temperature as well as the microstructure quantities such as; initial dislocation density (distance between dislocation, grain size (distance between the obstacles), and the average waiting time of dislocations at obstacles. The definition of the viscoplastic multiplier is determined using both the Perzyna viscoplastic model and the Consistency model. New definition for the Gibbs free energy function is proposed in terms of the proposed internal state variables taking into consideration both the temperature and strain rate.

Chapter 7 presents the incremental equations and numerical algorithms used in the numerical simulations by ABAQUS (2003). The radial return algorithm which is a special case of the backward-Euler method is used to introduce a nonlinear scalar equation in terms of the viscoplastic multiplier for the case of the Consistency viscoplastic model and in terms of the equivalent stress for the case of Perzyna viscoplastic model. Consistent algorithmic tangent stiffness matrices are derived for both small and finite strain viscoplastic models. The classical elastic predictor-plastic corrector concept is followed with extensions to rate-dependent problems. Finite deformation numerical framework for direct extensions of small deformation constitutive relations to finite deformations is proposed. Stress integration methodology that is called a “local rotated representation” is adopted in which the problem may be reduced to the numerical integration of an initial value problem that generates a one-parameter subgroup of proper orthogonal transformation. Finally, several numerical examples are introduced to test the proposed algorithm and its implementation in the ABAQUS finite element code and also to study the initiation and growth of shear bands using the previous bcc and fcc metals with their material parameters. Of particular interest is solving the mesh-sensitivity in two-dimensional material instability problems.

Finally, valuable conclusions and future interests are presented in Chapter 8.
CHAPTER 2
MICROSTRUCTURAL BASED MODELS FOR BCC AND FCC METALS WITH TEMPERATURE AND STRAIN RATE DEPENDENCY

2.1 Introduction

A desirable goal in constitutive modeling is to develop models which are widely applicable and capable of accounting for complex paths of deformation, temperature and strain rate which represent the main requirements of large deformation problems such as high speed machining, impact, and various primarily metal forming operations. The intended applications of the model as well as the availability and ease in obtaining experimental data specify the degree of complexity of the constitutive model. Moreover, the degree of success of the model mainly depends on the flexibility and simplicity of determining material constants from a limited set of experimental data and capturing the important aspects of static and/or dynamic behavior besides being mathematically and computationally accurate. In dynamic problems that introduce high strain rates, the dynamic yield stress is considered the most important expression needed to characterize the material behavior and is also used in finite element codes.

The subject of modeling the material behavior at high strain rates and elevated temperatures was extensively investigated by many researchers. Studies were made in characterizing material behavior through both phenomenological and physically based models. Empirical equations were initially developed with simple uniaxial stress-strain models (Campbell et al., 1977; Nicholas, 1982a) and one-dimensional stress wave propagation models (Nicholas, 1982b) by describing the effect of temperature and strain hardening as well as strain rate on the flow stress. However, for the von Mises type material, the one-dimensional models that express flow stress as a function of strain and strain rate can be converted into the equivalent three-dimensional material models by replacing stresses, strains, and strain rates by their equivalent invariant three-dimensional forms (Zukas, 1990). Johnson and Cock (1983) proposed a phenomenological model that is widely used in most computer codes for static and dynamic analysis in order to predict the behavior of the material flow stress at different strain rates and temperatures. The main advantage of this model is that it is relatively easy to calibrate with a minimum of experimental data in the form of stress-strain curves at different strain rates and temperatures. However, the strain rate and temperature effects on the flow stress are uncoupled which implies that the strain rate sensitivity is independent of temperature. This is not the case as observed in most metals. It is rather found that the rate sensitivity increases with increasing temperature while the flow stress decreases. The Johnson-Cook model is an empirical equation of state (Johnson, 1988) designed for ease of computational implementation. This approach, however, does not represent any thermal or strain rate history effects. In general, strain rate and thermal history effects can be taken into account by introducing internal state variables, which are necessary to represent the material behavior (Mecking and Kocks, 1981; Follansbee and Kocks, 1988; Bammann, 1990; Bammann et al., 1990a). Quite recently, Milella (2001) presented a constitutive equation based on the experimental results obtained by Milella and those available at the open literature for different temperatures and strain rates. He observed from the experimental evidence that for
BCC metals, the trend of the yield strength is linear, when plotted in the logarithmic scale versus the reciprocal of the temperature, independently of the strain rate applied. Moreover, he showed that all these linear trends at different strain rates point towards a lower common value that represents the athermal component of the yield strength.

The understanding of high-strain-rate behavior of metals is essential for the modeling and analysis of numerous processes including high-speed machining, impact, penetration and shear localization. Recently, considerable progress has been made in understanding the role of rate controlling dislocation mechanisms on the temperature and strain rate dependence of the flow stress for metals and alloys. Hoge and Murkherjee (1977) studied the effect of both temperature and strain rates on the lower yield stress of Tantalum and proposed a model incorporating the combined operation of the Peierls’ mechanism and dislocation drag process. They concluded from the stress-temperature relationship and the variation of the activation volume with stress and strain that the rate controlling mechanism for deformation could be rationalized in terms of Peierls’ mechanism. This behavior is mainly attributed to the specific crystal structure of body cubic centered metals. Steinberg and co-workers (see for example, Steinberg et al., 1980; Steinberg and Sharp, 1981; Steinberg and Lund, 1989) described a constitutive model for use with hydrodynamic codes to account for the dependence of shear modulus and yield strength on high strain rates, temperature, and pressure-dependent melting. Although their model is intended for use at high strain rates, their formulation did not specifically include strain rate effects.

Zerilli and Armstrong (1987) used the dislocation mechanics concept to develop a constitutive model that accounts for strain, strain rate and temperature dependence in a coupled manner, which can be incorporated in high rates of loading related computer codes. Their model considers two different forms for the two different classes of metals; body centered cubic (bcc) and face centered cubic (fcc). The rational for the differences in the two forms mainly depends on the dislocation characteristics for each this particular structure. Bcc metals show stronger dependence of the yield stress on temperature and strain rate while in the case of fcc metals the yield stress is mainly affected by strain hardening. In other words, the cutting of dislocation forests is the principal mechanism in fcc metals, while in bcc metals; the overcoming of Peierls-Nabarro barriers is the principal mechanism. These two different dislocation mechanisms of the two different metal classes will be further investigated in the following sections. The Zerilli-Armstrong model has been derived based on the concept of thermal activation analysis for overcoming local obstacles to dislocation motion. This model has been widely used in many computer codes from which its material parameters are physically interpreted. In fact, this physical interpretation of material constants becomes meaningless if one tries to identify them from the experimental data by using a very small reference strain rate rather than using the one corresponding to the reference dislocation velocity as been derived in the their model. Moreover, their material parameters lose their physical meaning when they are used for high temperature and strain rate applications which will be discussed in the following sections. It has been shown that the Zerilli-Armstrong model as compared to the Johnson-Cook model gives slightly better correlation with experimental results; however, none of these two models is very accurate in describing the behavior of metals at very large strains (Johnson and Holmquist, 1988).
Meyers et al (2002) used the Zerilli-Armstrong model in describing the response of metals at high-strain-rate deformation by incorporating dislocation dynamics, twining, grain-size, stacking fault, and solution hardening effects. They presented a mechanism for dislocation generation that provided a constitutive description of plastic deformation based on the theory of thermally activated processes. Nemat-Nasser and Isaacs (1997) developed an experimental technique measuring the flow stress of Ta and Ta-W alloys over a broad range of strains, strain rates, and various temperatures in uniaxial compression. Their experimental results showed that the flow stress of these materials was controlled by a simple long range plastic-strain-dependent barrier, and a short range thermally activated Peirels mechanism. They also presented a constitutive model that properly fits the experimental data up to 100% strain, 40,000/s strain rates, and from -200 to 1000°C. Moreover, they interpreted the material constants physically and succeeded in introducing physical definitions for the material constants derived in their model. Nemat-Nasser and his co-workers (see for example, Nemat-Nasser & Li, 1998; Nemat-Nasser et al., 1999; Nemat-Nasser & Guo, 2000; Nemat-Nasser & Guo, 2000; Nemat-Nasser et al., 2001; and Cheng et al., 2001) extended their experimental techniques and model applications to different bcc and fcc metals and alloys (Molybdenum, Niobium, Vanadium, OFHC Copper, and AL-6XN stainless steel) at very high strain rates and elevated temperatures. Moreover, they introduced a model that characterizes the deformation mechanisms of commercially pure Titanium (Ti) (an hcp metal) for experimentally-observed high strain rate dynamic strain aging (Nemat-Nasser et al., 1999 and Cheng & Nemat-Nasser, 2000).

The objective of this chapter is to derive physically based constitutive relations based on the concept of thermal activation analysis for two different material structures; bcc and fcc metals. We start the formulation with Orowan’s Equation (Orowan, 1948) taking into consideration the effect of dislocation density rate which has been ignored by most previous authors. Most recently, the evolution of dislocation densities has been extensively investigated by many authors. For example, Kubin and Estrin (1990) proposed a system of differential equations to describe both forest and mobile dislocation density evolution. They introduced through this system of differential equations terms that account for the immobilization of mobile dislocations that trap each other and the generation of constant dislocations. Bammann (2001) developed a crystal plasticity model which is embedded with a natural length scale. He related the evolution of the statistical stored dislocations to the plastic strain rate as a function of both statistically stored dislocations and geometrically necessary dislocations. Bammann (2001) assumed that the statistically stored dislocations are stored proportionally to their mean free path. The relation is initially proportional to the inverse of the square root of the density of statistically stored dislocations. The models described in the following sections address the effect of dislocation densities on the thermal component of the material flow stress through a consistent formulation based on the characterization of the dislocation microstructure.

In section 2.2, the formulation of dislocation microstructure as related to activation energy using Orowan’s definition and based on the concept of thermal activation analysis is given. Sections 2.3 and 2.4 present two different forms of the thermal and athermal components of the flow stress for bcc and fcc metals respectively. Moreover, the physical basis as well as the derivation procedure of the Zerilli Armstrong (Z-A) model is investigated and few modifications for the model parameters are presented. Section 2.5 explains the procedure used
to obtain flow stress coefficients and shows applications on both bcc and fcc metals. In section 2.6, Conclusions are given and ideas for future work are suggested.

2.2 Micro Structural Basis in Constitutive Modeling

Dislocations play a main role in determining the inelastic behavior of a metal and its flow stress under different load conditions (temperature, strain rate etc.). Loading of a material in the inelastic range causes dislocations to be generated, moved and stored. Motion of dislocations, however, indicates that the metal has exceeded its elastic limit or yield strength $Y$ and hence plastic strains are generated inside the material. Orowan’s equation relates the equivalent plastic strain rate $\dot{\varepsilon}_p = (2\mathbf{\dot{e}}_{ij} \mathbf{\dot{e}}_{ij} / 3)^{0.5}$ to the density of the mobile dislocations, $\rho_m$, dislocation speed $v$, and the magnitude of the Burgers vector $b$ as follows:

$$\dot{\varepsilon}_p = \dot{m}b\rho_mv$$

(2.1)

where $\dot{m}$ can be interpreted as the Schmidt orientation factor.

Generally, dislocations are mainly classified into two types; statistically stored dislocations which are stored by trapping each other in a random way, and geometrically necessary dislocations which are stored in order to maintain the continuity (compatibility) of various components of the material. However, movement of these dislocations controls the material behavior under different strain rates and temperature loadings as is related to the plastic strain.

Recently, great efforts were made in order to obtain an evolution equation for the dislocation densities in terms of strain rate and temperature. Kubin and Estrin (1990) have proposed the following equation to describe the mobile dislocation density evolution:

$$\dot{\rho}_m = \left(\lambda_1 / b^2 - \lambda_2 \rho_m - \lambda_3 \sqrt{\rho_f / b}\right)\dot{\varepsilon}_p$$

(2.2)

where the constant coefficients $\lambda_i$ are related to the multiplication of mobile dislocations ($\lambda_1$), their mutual annihilation and trapping ($\lambda_2$), and their immobilization through interaction with forest dislocations ($\lambda_3$). Along with Eq.(2.2) Kubin and Estrin (1990) also presented another equation that characterizes the evolution of the forest dislocation density ($\rho_f$) which describes hardening. Bammann (2001) presented an evolution equation for the statistically stored dislocation density in terms of both the statistically stored dislocation density $\rho_{ss}$ and the geometrically stored dislocation density, $\rho_{gn}$ as a function of plastic shear strain rate such that:

$$\dot{\rho}_{ss} = \left[c_1 \left(\rho_{gn} + \sqrt{\rho_{ss}}\right) - c_2 \rho_{ss}\right]\dot{\gamma}_p$$

(2.3)

where $c_1$ and $c_2$ are constant coefficients. Originally, Eq.(2.3) was written for the case of a single crystal and it is generalized here for polycrystalline plasticity by taking the summation as well as the mean value of the dislocation densities.
The average dislocation velocity $v$ can be determined through thermal activation by overcoming local obstacles to dislocation motion. Many authors have introduced velocity expressions for thermally activated dislocation glides (Li, 1968; Conrad and Weidersich, 1960; Hirth and Nix, 1969). However, the following general expression is postulated (Bammann and Aifantis, 1982)

$$v = v_o \exp\left(-\frac{G(\tau)}{kT}\right)$$  \hspace{1cm} (2.4)

where $v_o = d / t_w$ is the reference dislocation velocity, $t_w$ is the time that a dislocation waits at an obstacle, $d$ is the average distance the dislocation moves between the obstacles, $G$ is the shear stress-dependent free energy of activation which may depend not only on stress but also on temperature and the internal structure, $k$ is Boltzmann’s constant, and $T$ is the absolute temperature.

In conservative glide, the plastic flow rate clearly depends on both dislocation production $\dot{\rho}$ and dislocation speed $v$ as follows (Aifantis (1987) and Bammann and Aifantis (1987):

$$\dot{\rho}_p = x_1 v + x_2 \dot{\rho}_m = \left(\frac{\partial \gamma^p}{\partial l}\right) v + \left(\frac{\partial \gamma^p}{\partial \rho}\right) \dot{\rho}_m$$  \hspace{1cm} (2.5)

where, after making use of Orowans equation, the scalar coefficient $(x_1 \sim b \rho_m)$ is related to the magnitude of the Burgers vector and the mobile dislocation density and consequently, one can relate the coefficient $(x_2 \sim bl)$ to the same microstructural physical components with the dislocation distance instead of the mobile dislocation density.

Utilizing Eq.(2.1) through Eq.(2.5) and solving for $G$, one can obtain the following relation:

$$G = \left[\ln\left(\frac{\tilde{m} \rho_m v_o}{\tilde{m} \lambda_2 \rho_m + \tilde{m} l \lambda_3 \sqrt{\rho_f - \tilde{m} l \lambda_3 / b + 1}}\right) - \ln \dot{\rho}_p\right] kT$$  \hspace{1cm} (2.6)

It should be noted that the reference dislocation velocity $v_o$ is much greater than any other dislocation velocity $v$. Thus, in the case of higher strain values, the dislocation density evolution becomes the crucial aspect in determining the flow stress of the deformed material. In other words, the behavior of the flow stress is governed by temperature effects while the strain rate effect is neglected.

Many authors using different forms have related the activation energy $G$ to the thermal flow stress $\sigma_t$; for example, Kocks et al. (1975) suggested the following definition:

$$G = G_o \left[1 - \left(\frac{\sigma_t}{\sigma}\right)^p\right]^q$$  \hspace{1cm} (2.7)
where \( G_0 \) is the reference Gibbs energy at \( T=0 \), \( \hat{\sigma} \) is the threshold stress at which the dislocations can overcome the barriers without the assistance of thermal activation, and \( p \) and \( q \) are constants defining the shape of the short-range barrier. According to Kocks, (2001), the typical values of the constant \( q \) are 1.5 and 2 whereas the typical values of the constant \( p \) are less than 1.0.

Hoge and Mukherjee (1977) and Zerilli and Armstrong (1987) related the thermal component of the flow stress to both the energy activation and the activation volume \( V^* \). A generalization of their work can be given in the following form:

\[
G = G_0 - \tau_{th} V
\]  

(2.8)

where \( \tau_{th} \) is the thermal component of the shear stress and \( V \) is the mean value of the activation volume and its units are of the order \( b^3 \).

Many researchers have investigated the temperature and strain rate dependence of the activation volume. For example, Roberts (1977) showed that the activation volume was approximately independent of temperature and strain rate, while Hoge and Mukherjee (1977) concluded that this dependency existed. Zerilli and Armstrong (1987), however, considered the dependency of temperature only and they assumed that the activation volume is not affected by the strain rate. All these conclusions will be discussed in the following formulations showing the effect of each one on the final formulae of the thermal stress.

On the other hand, everyone agrees that in face centered cubic (fcc) materials, the activation volume decreases as plastic strain increases while it is constant in the case of body centered cubic (bcc) materials. Therefore, the thermal stresses will take two different forms based on the geometry of the crystal inside the material (bcc or fcc).

In order to understand quantitatively the deformation behavior of metals, a constitutive description is required. As we mentioned earlier, to deform a metal beyond the elastic limit means to activate and move its dislocations through the crystal. Once the dislocations start moving through the crystal, two types of obstacles are encountered that try to prevent dislocation movements through the lattice; long range and short-range barriers. The long-range obstacles are due to the structure of the material and cannot be overcome by introducing thermal energy through the crystal. Therefore they contribute to the flow stress \( \sigma \) with a component that is non-thermally activated (athermal stress). In the other hand, the short-range barriers can be overcome by thermal energy (Bonora and Milella, 2001). Therefore, the flow stress of a material \( \sigma = \left(3\sigma_{ij}\sigma_{ij} / 2\right)^{1/2} \) on the Von Mises base) can be additionally decomposed into equivalent athermal stress \( \sigma_a \) and equivalent thermal stress \( \sigma_{th} \) as follows:

\[
\sigma = \sigma_a + \sigma_{th}
\]  

(2.9)

The above assumption of additional decomposition for the formulation of the flow stress has been proven experimentally and is used by several authors (see for example, Zerilli and Armstrong, 1987; Nemat-Nasser and Isaacs, 1997; Nemat-Nasser et al., 1999).
2.3 Body Centered Cubic Metals (BCC)

The behavior of bcc metals shows a strong dependence of the thermal yield stress on the strain rate and temperature. The thermal stress is attributed to the resistance of the dislocation motion by the Peierls barriers (short-range barriers) provided by the lattice itself. Moreover, the plastic hardening of most bcc metals, like pure iron, tantalum, molybdenum, and niobium, is hardly influenced by both strain rate and temperature and therefore, it contributes to the athermal part of the flow stress besides the small percentage of the yield stress. Thus, the athermal component of flow stress can now be defined as:

\[ \sigma_a = B \varepsilon_p^n + Y_a \]  

(2.10)

where \( B \) and \( n \) are the plastic hardening constants and \( Y_a \) represents the temperature-independent stress.

The difference of the mechanical behavior of bcc metals to fcc metals may be ascribed to the dislocation size and the corresponding concentration of Cottrell’s atmosphere. During their movement, dislocations displaced across the lattice and accordingly their atmosphere of interstitial atoms will be moved. Atoms movement results in a drag force that opposes these atom clouds. Drag-force increases as the concentration mismatch between the Cottrel’s atmosphere and the solute atoms in the lattice increases and, therefore, the thermal yield stress increases (Milella, 1998). The yield strength produced by these effects depends on both temperature and strain rate since the solute atoms concentration does so.

Following the formulation used in the previous section, the thermal component of the flow stress may be obtained in two ways:

2.3.1 Model 1

By equating both Eq.(2.6) and Eq.(2.7), the thermal yield stress is obtained as follows:

\[ \sigma_{th} = \hat{Y} \left( 1 - \left( \beta T \right)^{1/q} \right)^{1/p} \]  

(2.11)

where \( \hat{Y} \) is the threshold yield stress of the Peierls barrier to the dislocation motion. The constant \( \beta \) is related to the strain rate as follows:

\[ \beta = \beta_1 - \beta_2 \ln \dot{\varepsilon}_p \]  

(2.12)

where the parameters \( \beta_1 \) and \( \beta_2 \) are defined as follows:

\[ \beta_1 = \frac{K}{G_o} \ln \left( \frac{\bar{m}b \rho_{m \nu}}{1 - \bar{m}l \lambda_3 / b + \bar{m}b l \lambda_2 \rho_m + \bar{m}l \lambda_3 \sqrt{\rho_f}} \right) \]  

(2.13)
and
\[ \beta_2 = \frac{K}{G_0} \quad (2.14) \]

It is obvious that parameter \( \beta_i \) plays the major component in controlling the behavior of the material by characterizing the effect of both dislocations densities and the length scale through the evolution of hardening at large strains.

The final constitutive relation is obtained by substituting Eq.(2.10) and Eq.(2.11) into Eq.(2.9) and utilizing Eq.(2.12), such that:
\[ \sigma = \dot{\gamma} \left( 1 - \left( \beta_1 T - \beta_2 T \ln \dot{\varepsilon}_p \right)^{1/q} \right)^{1/p} + B \varepsilon^n + Y_a \quad (2.15) \]

As it was mentioned earlier \( p \) and \( q \) are constants that range between 0 to 1.0 for the former and 1 to 2 for the latter. Moreover, Ono (1968) and Kocks et al (1975) suggested that in most cases these two fitting constants provide an acceptable description of the profile of the energy barrier.

In the adiabatic case of deformation, heat inside the material increases as plastic strain increases and therefore, the temperature \( T \) is calculated incrementally by assuming that the majority of the plastic work is converted to heat:
\[ T = \frac{\chi}{c_p \rho} \int_{0}^{\varepsilon_p} \sigma d\varepsilon_p \quad (2.16) \]

here \( c_p \) is the specific heat at constant pressure and \( \rho \) is the material density. The Taylor-Quinney empirical constant \( \chi \) is often assigned the value of 0.9. However, recent tests have indicated that this parameter may vary with plastic strain (for more details see the work of Kapoor and Nemat-Nasser, 1998). Eq.(2.16) may be solved numerically or can be integrated without introducing any noticeable errors by either using the mean value theorem or the simple Euler method.

2.3.2 Model 2; (Modification of Material Parameters of the Z-A Model)

An alternative approach for determining the thermal stresses as a function of both strain rate and temperature can be obtained by assuming that the activation volume is independent of the strain rate and temperature. Substituting Eq.(2.6) into Eq.(2.8) one obtains:
\[ \sigma_{th} = \dot{\gamma} e^{-\beta T} \quad (2.17) \]

where
\[ \hat{Y} = \frac{mG}{V_o} \]  

(2.18)

The constant \( m \) represents the Taylor factor that relates the shear stress to the normal stress and can be defined the same way as \( \hat{m} \) is defined. As in the case of Model 1, \( \hat{Y} \) is the threshold yield stress. The activation volume \( V_o \) is independent of both the temperature and the strain rate. Thus, the slope \( \beta \) takes the following expression which is confirmed experimentally:

\[ \beta = (-1/T) \ln \left( 1 + \left( \beta_2 T \ln \dot{\varepsilon}_p - \beta_1 T \right) \right) \]  

(2.19)

where the physical interpretation of constants \( \beta_1 \) and \( \beta_2 \) are similar to those given in Eq.(2.13) and Eq.(2.14) respectively.

If one considers the dependence of the activation volume on temperature, no major changes will appear to the thermal stress relation, given by Eq.(2.17), except that an additional term will be added to the \( \beta \) constant as follows:

\[ \beta = (1/T) \ln \left( V'/V_o \right) - (1/T) \ln \left( 1 + \left( \beta_2 T \ln \dot{\varepsilon}_p - \beta_1 T \right) \right) \]  

(2.20)

where \( V' = V(T) \) is the temperature dependent activation volume. Substituting Eqs.(2.10) and (2.17) into Eq.(2.9) and utilizing Eq.(2.19), the final constitutive relation is obtained after making use of the expansion \( \ln(1 + x) = x \),

\[ \sigma = \hat{Y} e^{-\beta_3 T + \beta_2 T \ln \dot{\varepsilon}_p} + B \varepsilon_p^n + Y_a \]  

(2.21)

where

\[ \beta_3 = \beta_1 + \left( 1/T \right) \ln \left( V'/V_o \right) \]  

(2.22)

In fact, the definition of the slope \( \beta \) given in Eq.(2.17) and Eq.(2.21) for the thermal component of the flow stress is similar to the one proved experimentally (see for example Armstrong and Campbell, 1973) as follows:

\[ \beta = \beta' - \beta'' \ln(\dot{\varepsilon}_p) \]  

(2.23)

Generally, the proposed model given by Eq.(2.21) and the derivation procedure presented here are quite similar to the well known model proposed by Zerilli and Armstrong (Z-A model). However, the physical parameter \( \beta_1 \) is interpreted differently here. It is used to investigate or introduce the effect of the material length scale, which is considered to be another important factor in controlling the metal behavior under different loading conditions.

It is important to note that the expansion \( \ln(1 + x) = x \) used in the derivation of Z-A model and shown here is valid only for values \( x \ll 1.0 \) (see Fig.2.1). This
variable $x = (k / G_o)T \ln(\dot{\varepsilon}_p / \dot{m}_b \rho v_o)$, however, is both temperature and strain rate dependent and thus, its value increases and approaches the value of one when the temperature increases and the strain rate decreases (see for example, Nemat-Nasser and Isaacs, 1997; Nemat-Nasser et al., 1999). Accordingly, the physical interpretation of the material parameters $\beta_i$ given by the Z-A model (Zerilli and Armstrong, 1987 &1990) as well as these defined in Eq.(2.21) become ineffective and do not represent the real behavior which makes the model parameters appear to be phenomenologically based rather than physically based. This is in spite of the model’s physical basis. In other words, the model derivation is directed to match the experimental evidence given by Eq.(2.23).

Considering the exact value of the expansion $\ln(1 + x)$, the following constitutive relation that has physically interpreted parameters is derived:

$$\sigma_{\text{th}} = Y \frac{V_o}{V'} (1 - \beta_1 T + \beta_2 T \ln \dot{\varepsilon}_p)$$

(2.24)

where the parameters $\beta_1$ and $\beta_2$ are the same as given by Eq.(2.13) and Eq.(2.14) respectively. It is clear that the general form of this model is quite similar to the one derived earlier in Eq.(2.11), assuming $p$ and $q$ values are unity, and provided that the term $(V_o / V')$ is not constant since $V'$ varies with temperature.

![Figure 2.1 Comparison between the approximated and exact values of the expansion of $\ln(1+x)$.](image)
The activation volume for bcc metal deformation is in the range of 5 to 100\text{b}^3 while it is 10 to 100 times larger in the deformation of fcc metals. Hoge and Mukherjee (1977) calculated the activation volumes from the strain rate dependence of the flow stress at constant temperature as a function of the effective stress. These activation volumes decrease with the increase of thermal stresses and are much smaller than those obtained when the intersection mechanism is operative. To consider the strain rate effect as well as the temperature effect on the activation volume, $V'$ used in the constitutive relation, Eq.(2.24) is replaced by a strain rate and temperature dependent activation volume $V'' = V(T, \dot{\varepsilon}_p)$. Although, Hoge and Mukherjee (1977) concluded the existence of temperature and strain rate dependency on the activation volume, they didn’t present an appropriate relation that one may utilize. Moreover, to our best knowledge, no one presented an explicit definition for the activation volume variation with both temperature and strain rate. The following general relation, however, is suggested here using the additive decomposition concept.

$$V'' = V_o \left(1 + \beta_o T^m\right)^{-1} \quad (2.25)$$

here $m$ is an exponent constant and the parameter $\beta_o = f(\dot{\varepsilon}_p)$ is a function of the accumulated plastic strain rate. Eq.(2.25) considers the coupling behavior between temperature and strain rate. Substituting Eq.(2.10) and Eq.(2.24) into Eq.(2.9) with making use of Eq.(2.25), one obtains the modified constitutive relation as follows:

$$\sigma = \dot{Y} \left(1 + \beta_o T^m - \beta_1 T + \beta_2 T \ln \dot{\varepsilon}_p\right) + B\sigma^p + Y_a \quad (2.26)$$

In investigating Eq.(2.26), two important issues are noticed and need to be further discussed. The first one states that, at a given strain rate, the thermal component of the flow stress decreases as the temperature increases taking the power or the polynomial shape. The other point, which agrees with many physically based constitutive relations (including the ones presented here Eq.(2.15) and Eq.(2.21)) shows that the thermal stress, at zero Kelvin temperature, represents the threshold stress and it approaches zero when the temperature reaches higher values and, therefore, the flow stress is represented by the athermal component only. Furthermore, if we assume the room temperature to be our reference temperature, the behavior of the thermal stress will be almost the same as the phenomenological model given by Johnson-Cook (1983).

Comparisons of the proposed constitutive equations (Eq.(2.15) and Eq.(2.21)) to experimental data are presented in section 2.5. Eq.(2.26), however, is not going to be investigated in this chapter.

2.4 Face Centered Cubic Metals (FCC)

In the case of fcc metals, like copper and aluminum, the emergence and evolution of a heterogeneous microstructure of dislocations as well as the long-range intersections between dislocations dominates and controls the mechanisms of thermal activation analysis behavior.
Thus, the thermal activation is strongly dependent on the plastic strain. That is, the increase in the yield point with a decrease in temperature is highly dependent on the strain-hardened states for fcc metals.

Based on the above description, it is clear that the distance $d$ between dislocation intersections and consequently the activation volume play a crucial role in determining an appropriate formulation introducing the effect of plastic strain on the thermal component of the material flow stress. Thus, the activation volume can be related to the distance between dislocation intersections as follows:

$$V_o = m^* d b^2$$

(2.27)

where the constant $m^*$ is usually approximated to a value of 0.5. Moreover, dislocation densities are also related to the distance $d$ through the relationship

$$\rho_m \sim 1/d^2$$

(2.28)

The thermal component of the constitutive equation for the case of fcc metals will have the coupling of temperature, strain rate, as well as plastic strain. The athermal component, however, will be constant and independent of the plastic strain and it pertains totally to the initial yield stress. Zerilli and Armstrong, (1987) provide a discussion of how the initial athermal yield stress $Y_a$ is affected by solute and grain size.

2.4.1 Model 1

For fcc metals, the thermal stress given by Eq.(2.11) preserves the same form except that $\hat{\sigma}$ is no longer related to the threshold yield stress

$$\sigma_m = \hat{\sigma} \left(1 - \left(\frac{\beta T}{\beta T} \right)^{1/p}\right)$$

(2.29)

Utilizing Eq.(2.27) and Eq.(2.28), the multiple slip-crystal flow stress at any strain value is related both to the dislocation densities and strain by the relation given by several authors (see for more details the paper of Zerilli and Armstrong, 1987)

$$\hat{\sigma} \equiv f(b/d) \equiv \sigma_p \varepsilon_p^a$$

(2.30)

Substituting Eq.(2.30) into Eq.(2.29), the first constitutive equation for fcc metals is given as:

$$\sigma = B \varepsilon_p^a \left(1 - \left(\beta_1 T - \beta_2 T \ln \varepsilon_p \right)^{1/q}\right)^{1/p} + Y_a$$

(2.31)

Where $B$ is considered here to be the hardening constant ($\sigma_o$ in Eq.(2.30)).
It can be seen in Eq.(2.31) that, at a given plastic strain value, the thermal stress preserves the same trend shown in bcc metals including that constants $p$ and $q$ are falling in the same range as those given before. Moreover, there is no strain rate and temperature effect on the initial yield stress and, thus, $Y_o$ is constant. This means that for a value of plastic strain equal to zero, the stress strain curves at different temperature and strain rates will have the same starting point ($\sigma = Y_o$), which is not exactly the behavior in some fcc metals. However, this problem can be overcome by introducing a slight strain and temperature effect on the initial yield stress.

2.4.2 Model 2; (Modification of the Material Parameters of the Z-A Model)

As mentioned earlier, the activation volume in fcc metals is much higher than that of bcc metals. Moreover, the activation volume and consequently the thermal stress depend strongly on the plastic strain. On this basis and assuming that the approximate Eq.(2.27), Eq.(2.28) and Eq.(2.30) may be employed in order to determine $V$ at $T = 0.0$, the activation volume may be given as follows:

$$V_o = c\varepsilon_p^{-1/2}$$

(2.32)

Experimental results (Hoge and Mukherjee, 1977) showed that the activation volume does not reduce to zero when there is no plastic strain and also the square root is not an accurate expression for all fcc metals. Therefore, the following formula is suggested which governs most fcc metal behavior:

$$V_o = (c_o + c_t\varepsilon_p^n)^{-1}$$

(2.33)

Substituting Eq.(2.33) into Eq.(2.17) along with the fact that the athermal component of the flow stress in fcc metals is not affected both by temperature and strain rate, the final form of the constitutive relation may be given as follows:

$$\sigma = (Y_o + B\varepsilon_p^n)e^{-\beta_1 T + \beta_2 T \ln \dot{\varepsilon}_p} + Y_a$$

(2.34)

where $Y_o$ indicates the strain rate and temperature dependent component of the initial yield stress. It is, however, approximated to zero in some fcc metals. It should be noted that the above model is almost the same as the one given by Zerilli and Armstrong, (1987). The material parameters $\beta_i$, however, are defined differently as shown in Eq.(2.13) and Eq.(2.22). Besides, these physical parameters are not interpreted accurately since the same expansion $\ln(1+x) = x$ is used (see section 2.4 for more details). Therefore, to have the physical parameters physically interpreted, the proposed model is presented here using the exact value of the expansion $\ln(1+x)$ instead of the approximation one, $\ln(1+x) = x$ such that:

$$\sigma = (Y_o + B\varepsilon_p^n)(1 + \beta_o T^m - \beta_1 T + \beta_2 T \ln \dot{\varepsilon}_p) + Y_a$$

(2.35)
Improvements of the above constitutive relation, Eq.(2.35), as well as numerical comparisons are going to be addressed extensively in chapter 4 that will investigate a proper physically based definition for the activation volume in order to characterize the physical basis of the material flow stress.

2.5 Results, Applications and Discussions

The evaluation of the material parameters of the proposed models are discussed in this section. These models are given by Eq.(2.15) for bcc metals and Eq.(2.31) for fcc metals. Applications of these models as well as comparisons to the available experimental data for Tantalum (Ta), Niobium (Nb), Molybdenum, (Mo), and Vanadium (V) for bcc metals and OFHC Copper for fcc metals are illustrated. Comparisons are also made of the proposed models with both the Z-A models with minor modifications given in Eqs.(2.21) and (2.34), and the Nemat-Nasser and co-workers models. Finally, verification of the physical based material parameters interpreted earlier in sections 2.3 and 2.4 with respect to those fitted experimentally are discussed.

2.5.1 Determination of the Material Parameters

Although various techniques can be used to determine the constants for this model, the following simple approaches have been used for both bcc and fcc metals.

- **BCC Model:**

  For the case of bcc metals, the procedure to determine the constitutive model parameters of Eq.(2.15) is initiated by studying the stress-temperature relations at different values of the plastic strains for a specific strain rate. The stress keeps decreasing until a point is reached where the stress becomes constant with further increase in temperature. This constant value represents the athermal component of the flow stress and is employed to calculate the values of the hardening constants $B$ and $n$ values using the nonlinear least-squares fit. The $Y_a$ value represents the athermal stress at zero plastic strain or the athermal component of the initial yield stress. Thus, subtraction of the above stress increments (athermal stresses) from the overall stress leads to the thermal component of the flow stress which is accounted for by the first term on the right hand side of Eq.(2.15). According to Kocks (2001), the typical values of the exponent $q$ are 3/2 and 2 that is equivalent to a triangle obstacle profile near the top. On the other hand, the typical values of the exponent $p$ are less than 1 and it is chosen here to be 1/2 which characterizes the tail of the obstacle. Once these exponents are determined for a particular mechanism, they become constants.

  Next, the intercept of the constant slope line plotted between $(\sigma - B\varepsilon^p_a - Y_a)^p$ and $T^{1/q}$ at certain strain rate, is employed here to obtain the value of the threshold stress $Y$. Finally, a
graph of \( \left( 1 - \left( \frac{\sigma - Y_a - B \dot{\varepsilon}_p^n}{\dot{Y}} \right)^p \right)^q \) vs \( \ln \dot{\varepsilon}_p \) at fixed temperature is utilized to determine the parameters \( \beta_1 \) and \( \beta_2 \).

- **FCC Model:**

  A similar procedure is followed to determine the material parameters of the fcc metals model given by Eq.(2.31) except that the hardening parameters are coupled with both temperature and strain rate unlike the case for the bcc model. The athermal component of the flow stress \( Y_a \) is obtained using the same steps followed in the above previous bcc procedure except that the hardening parameters no longer belong to the athermal component of the flow stress. That is the temperature is plotted only against the initial yield stress (the stress at zero plastic strain stress). After selecting the proper values for the exponents’ \( p \) and \( q \), a graph for \( (\sigma - Y_a)^p \) versus \( T^{1/q} \) at several plastic strains and a fixed plastic strain rate is plotted. The intercepts of these constant slope lines are employed to determine the hardening parameters \( B \) and \( n \) using the nonlinear least-squares fit. Finally, the parameters \( \beta_1 \) and \( \beta_2 \) are determined by utilizing the constants of the line drawn at a specific temperature and certain plastic strain between \( \left( 1 - \left( \frac{\sigma - Y_a}{B \dot{\varepsilon}_p^n} \right)^p \right)^q \) and \( \ln \dot{\varepsilon}_p \).

  It should be noted that in both bcc and fcc models, the determination of the work hardening coefficients \( B \) and \( n \) are not that simple and straightforward as determining the thermal activation parameters. Theoretically, the nonlinear least-squares method is applied to the stress versus strain data in obtaining \( B \) and \( n \). However, unique values of these coefficients are difficult to achieve depending on the details of the fitting procedure. This problem may be attributed to the presence of upper and lower yield points which complicates the analysis of small strain materials. The accuracy of the hardening coefficients value is very important in determining the adiabatic stress strain curves from which the heat generated by the plastic work plays a crucial aspect in determining the softening or instability points. Details on the difficulties, importance and procedures in determining the material coefficients may be found in the paper by Zerilli and Armstrong (1990).

**2.5.2 Applications and Comparisons**

- **Tantalum (Ta):**

  Tantalum is a bcc metal that has generated a lot of interest in industry due to its density, strength and ductility over a wide range of deformation rates and temperatures. It is been used here as an application for the proposed model. The above mentioned procedure for determining the material parameters for the proposed model simulations is applied to the experimental data presented by Hoge and Mukherjee (1977) and the parameters values are listed in Table 2.1. The results of the model simulations from the above experimental data are also compared with other sets of experimental data (Bechtold, 1955; Mitchell and Spitzig, 1965; Mordike and Rudolph, 1967; and Nemat-Nasser and Isaacs, 1997) as well as with other
The temperature variation of the stresses obtained experimentally by Nemat-Nasser and Isaacs (1997) at 0.05 strain and 5000s$^{-1}$ strain rate, Hoge & Mukharjee (1977) at 0.014 strain and 0.0001s$^{-1}$ strain rate and Bechtold at 0.014 strain and 0.00028s$^{-1}$ strain rate are compared in Fig.2.2 with the results computed using the present model Eq.(2.15) and Z-A model Eq.(2.21). The proposed model, with the parameters obtained using the Hoge & Mukharjee data, predicts results that agree very well both with the data given by Nemat-Nasser and Isaacs (1997) and with the results computed using the Z-A model. The parameter $Y_a$, however, is changed to 133 MPa in order to get a better agreement with Bechtold (1955) data. This change is used to allow for possible differences in solute and grain size effects (see Zerilli & Armstrong, 1990 for more details).

Furthermore, the stress variation with strain rates computed using the proposed model are compared with the experimental data presented by Hoge and Mukharjee (1977) at room temperature and with single crystal data obtained by Mitchell & Spitzig (1965) at 373° K temperature and Mordike & Rudolph (1967) at 200° K temperature. The comparisons illustrated in Fig.2.3 show very good agreement with both the experimental data and the theoretical one presented by the Z-A model. In the case of bcc metals, as discussed earlier in section 2.3, the hardening is independent of both temperature and strain rate effects, and therefore, the predicted stress strain curves using the proposed model or Z-A model will depend completely on the accuracy of determining the hardening parameters which vary from test to test. The hardening parameters, therefore, obtained using certain experimental data will not necessarily matches with the other data set presented by different researchers. In Figure2.4, the adiabatic stress-strain curves predicted using the proposed model are plotted for 0.0001s$^{-1}$ strain rate and at different temperatures and are compared to the Hoge and Mukharjee (1977) data. These results agree well for most temperatures from which the heat generated by the plastic work is calculated using Eq.(2.16).
Figure 2.2 Stress versus temperature proposed model results, for Tantalum (Ta), as compared with experimental data by several authors at different strain rates.

Figure 2.3 Stress versus strain rate proposed model results, for Tantalum (Ta), as compared with experimental data by several authors at different temperatures.
Moreover, Figure 2.5 shows another comparison made with Nemat-Nasser and Isaacs (1997) data at 5000 s\(^{-1}\) strain rate and different initial testing temperatures (\(T_0\)). The adiabatic stress-strain relation agrees very well in the range of 298° K-498° K while they are slightly apart for higher temperatures (598° K-798° K).

Nemat-Nasser and Isaacs (1997) presented a model using the same thermal activation concept proposed in this chapter. However, in their model, they determined the model parameters from a single strain rate test and then generalized their formulation to address different strain rate effects. Furthermore, unlike the proposed model, the evolution of the mobile dislocation density was neglected in their derivation which may overestimate the prediction of the flow stress. This assumption, however, is valid only in the case of low strain rates and becomes inaccurate for the high strain rate problems which is the purpose of the proposed model in this work. The effects of the mobile dislocation density rate on the flow stress will be further discussed in the next section. It should be noted that the thermal component of the flow stress given by Eq.(2.11) is non-negative. Thus, the term between the brackets on the right hand side should be set equal to zero when the temperature exceeds a critical value. This critical value, however, is strain rate dependent and is defined as follows:

![Adiabatic stress-strain curves for proposed model, for Tantalum (Ta), compared to experimental results (Hoge and Mukharjee, 1977) at 0.0001 s\(^{-1}\) strain rate and different initial temperatures.](image-url)
In the temperature variation of the stress curve, the critical temperature defines the starting point of the constant stress which represents the athermal component of the flow stress. Fig. 2.6 shows the calculated critical temperatures for different values of the strain rates using Eq. (2.36) and are compared to those calculated by Nemat-Nasser and Isaacs (1997).

\[ T_{cr} = \beta^{-1} = \left( \beta_1 - \beta_2 \ln \dot{\varepsilon}_p \right)^{-1} \]  \hspace{1cm} (2.36)

Figure 2.5 Adiabatic stress-strain curves for proposed model, for Tantalum (Ta), compared to experimental results (Nemat-Nasser and Isaacs, 1997) at 5000 s\(^{-1}\) strain rate and different initial temperatures.

The adiabatic stress strain curves of the plastically deformed specimens presented here are estimated by assuming the conversion of 90% plastic work into heat, i.e. the temperature increments are calculated using the following relation (Nemat-Nasser and Isaacs, 1997):

\[ T = T_o + 0.433 \int \sigma d\varepsilon_p \]  \hspace{1cm} (2.37)
The instability strains beyond which the material starts softening represent the maximum values in the adiabatic stress strain curves. The following mathematical expression is used in calculating these instability strains:

\[
\frac{d\sigma}{d\varepsilon_p} = Bn\varepsilon_p^{n-1} - \frac{\dot{\gamma} \beta^{1/q}}{pq} T^{(1-q)/q} \frac{dT}{d\varepsilon_p} \left(1 - \left(\frac{\beta T}{\varepsilon}\right)^{1/q}\right)^{(1-p)/p} = 0
\]  

(2.38)

where the parameter \(\beta\) is the same as that given in Eq.(2.12). This equation is solved numerically from which the instability strains increase with temperature and decrease with increasing strain rate.

Figure 2.6 Critical temperatures predicted by the proposed models for several metals compared to Nemat-Nasser & co-workers models, at different strain rates.

- Molybdenum (Mo):

Molybdenum is a refractory bcc metal typically used in high temperature applications. Its key properties include; good thermal and electrical conductivity, good hot strength with high stiffness (Young’s Modulus 317MPa), good strength and ductility at room temperature, high melting point (2885°K) which is exceeded only by those of tungsten and tantalum, and high density (10.2 g/cm³) which is approximately 62% of that of tantalum. Therefore, the ability of
molybdenum to withstand high temperatures and maintain strength under these conditions is responsible for the fact that molybdenum finds most of its application at elevated temperatures. In fact, it can work at temperatures above 1273°K (in non-oxidizing conditions), which is higher than steels and nickel-based superalloys. The study of the deformation behavior of molybdenum leads to better understanding of the deformation mechanisms of bcc metals. Nemat-Nasser et al. (1999) conducted numerous experiments on molybdenum and presented a large set of data at high strain rates and temperatures which will be used here for evaluation of the proposed model.

Table 2.2 Parameters of Molybdenum (Mo) for the proposed model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Proposed Model “Eq.19”</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_1$ (K$^{-1}$)</td>
<td>0.0010922</td>
</tr>
<tr>
<td>$\beta_2$ (K$^{-1}$)</td>
<td>0.00005553</td>
</tr>
<tr>
<td>$\beta_3$ (K$^{-1}$)</td>
<td></td>
</tr>
<tr>
<td>$\hat{Y}$ (Mpa)</td>
<td>2185</td>
</tr>
<tr>
<td>$Y_a$ (Mpa)</td>
<td>65</td>
</tr>
<tr>
<td>$B$ (Mpa)</td>
<td>670</td>
</tr>
<tr>
<td>$n$</td>
<td>0.3</td>
</tr>
<tr>
<td>$p$</td>
<td>0.5</td>
</tr>
<tr>
<td>$q$</td>
<td>1.5</td>
</tr>
</tbody>
</table>

The model parameters for molybdenum (listed in Table 2.2) are determined following the same procedure discussed in section 5.1 and using the experimental data set conducted by Nemat-Nasser and co-workers (Nemat-Nasser et al., 1999). Along with their experimental results, Nemat-Nasser and his co-workers were able to model the material deformation behavior under high strain rates and elevated temperatures based on the same concept used for tantalum. The adiabatic stress strain curves predicted by the present model show very good agreement with both Nemat-Nasser’s and co-worker’s experiments (Nemat-Nasser et al., 1999) and model results for a broad range of temperatures (up to 1000°K) and for two different high strain rates 3100 s$^{-1}$ and 8000 s$^{-1}$ as shown in Fig.2.7 and Fig.2.8 respectively.

In calculating the adiabatic stress strain curves for molybdenum, 100% of the plastic work is assumed to be converted to heat based on the experimental results conducted for different plastic strains (Nemat-Nasser et al., 1999). Thus the temperature evolution during plastic deformation is calculated using the following relation:

$$T = T_0 + 0.39 \int \sigma d\varepsilon_p$$

(2.39)

The strain rate variation of the critical temperature calculated using the proposed model and based on the material parameters listed in Table 2.2 shows higher values than those obtained for other bcc metals until a strain rate of 7500 s$^{-1}$ where they are exceeded by the tantalum’s critical temperature results (see Fig.2.6).
Figure 2.7 Adiabatic stress-strain curves for proposed model, for Molybdenum (Mo), compared to experimental and model results (Nemat-Nasser et al., 1999) at 3100 s\(^{-1}\) strain rate and different initial temperatures.

Figure 2.8 Adiabatic stress-strain curves for proposed model, for Molybdenum (Mo), compared to experimental and model results (Nemat-Nasser et al., 1999) at 8000 s\(^{-1}\) strain rate and different initial temperatures.
• **Niobium (Nb):**

Niobium or columbium as was once known has a melting point of $2741^\circ$K and a density of 8.57 g/cm$^3$. It is a silvery bcc metal that is used as an alloying agent in carbon and alloy steels and in non-ferrous metals, as it improves the strength of the alloy. It is also used in jet engines and rockets. This element has superconductive properties and is used in superconductive magnets which retain their properties in strong magnetic fields. Niobium is used in this work as an application for the present bcc model under a wide range of temperatures and for different strain rates. As is the case in all bcc metals, the model parameters, listed in Table 2.3, are obtained following the determination procedure discussed previously and using the experimental data presented by Nemat-Nasser and Guo (2000).

In Table 2.3, the value of the parameter $\beta_1$ is the same as that found in tantalum which indicates that both metals have the same reference Gibbs free energy, $G_0$ values since the Boltzmann’s constant $K$ is constant for most metals as will be discussed in the following sections. Figs. 2.9 and 2.10 show the adiabatic stress strain results computed using the present model at 3300 s$^{-1}$ and 8000 s$^{-1}$ strain rates respectively. Both the proposed and Nemat Nasser & Guo models show good agreement as compared to the experimental data presented by Nemat-Nasser and Guo (2000) for a wide range of elevated temperatures. However, the proposed model shows better agreement for high temperatures and strain rates.

Similar to molybdenum, a 100% of the plastic work generated during the deformation process under different strain rates is converted to heat as given by Nemat-Nasser and Guo (2000) for the case of niobium. Therefore, the incremental variation of the temperature during the adiabatic process is calculated as follows:

$$T = T_0 + 0.44 \int \sigma d \varepsilon$$ \hspace{1cm} (2.40)

For the Niobium model parameters listed in Table 2.3, the critical temperatures predicted by the present bcc model give results less than those predicted by the tantalum and molybdenum models as varied with strain rates (see Fig.2. 6).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Proposed Model “Eq.19”</th>
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<tbody>
<tr>
<td>$\beta_1$ (K$^{-1}$)</td>
<td>0.00193</td>
</tr>
<tr>
<td>$\beta_2$ (K$^{-1}$)</td>
<td>0.0000937</td>
</tr>
<tr>
<td>$\beta_3$ (K$^{-1}$)</td>
<td></td>
</tr>
<tr>
<td>$\hat{Y}$ (Mpa)</td>
<td>1350</td>
</tr>
<tr>
<td>$Y_a$ (Mpa)</td>
<td>60</td>
</tr>
<tr>
<td>$B$ (Mpa)</td>
<td>440</td>
</tr>
<tr>
<td>$n$</td>
<td>0.25</td>
</tr>
<tr>
<td>$p$</td>
<td>0.5</td>
</tr>
<tr>
<td>$q$</td>
<td>1.5</td>
</tr>
</tbody>
</table>
Figure 2.9 Adiabatic stress-strain curves for proposed model, for Niobium (Nb), compared to experimental and model results (Nemat-Nasser & Guo, 2000) at 3300 s\(^{-1}\) strain rate and different initial temperatures.

Figure 2.10 Adiabatic stress-strain curves for proposed model, for Niobium (Nb), compared to experimental and model results (Nemat-Nasser & Guo, 2000) at 8000 s\(^{-1}\) strain rate and different initial temperatures.
Vanadium (V):

Pure vanadium (V) is a bright white bcc metal, and is soft and ductile with good structural strength. It has found wide range of usage in many fields. About 85% of vanadium is used as ferrovanadium or as a steel additive. Other uses are in producing rust resistant and high-speed tool steels. It is also used in the aerospace industry in titanium alloys, as well as a catalyst in the production of sulphuric acid. Commercially, vanadium is produced by reducing vanadium trichloride with magnesium metal or a mixture of magnesium and sodium or via the calcium reduction of V₂O₅ in a pressure vessel. The purity, which depends on the production method, plays a crucial aspect in characterizing the mechanical properties of vanadium. The material flow stress or the yield stress of vanadium is strongly dependent on temperatures and strain rates. In this regards, we choose this metal to investigate and understand the effect of temperature and strain rate on the mechanical properties of this material and also to extend the applicability of the proposed model to various metals.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Proposed Model “Eq.19”</th>
</tr>
</thead>
<tbody>
<tr>
<td>β₁ (K⁻¹)</td>
<td>0.0021797</td>
</tr>
<tr>
<td>β₂ (K⁻¹)</td>
<td>0.0001392</td>
</tr>
<tr>
<td>β₃ (K⁻¹)</td>
<td></td>
</tr>
<tr>
<td>$\dot{Y}$ (Mpa)</td>
<td>945</td>
</tr>
<tr>
<td>$Y_a$ (Mpa)</td>
<td>60</td>
</tr>
<tr>
<td>$B$ (Mpa)</td>
<td>305</td>
</tr>
<tr>
<td>$n$</td>
<td>0.16</td>
</tr>
<tr>
<td>$p$</td>
<td>0.5</td>
</tr>
<tr>
<td>$q$</td>
<td>1.5</td>
</tr>
</tbody>
</table>

Nemat-Nasser and Guo (2000) modified their bcc model by introducing drag-stress components to the athermal part of the flow stress besides the athermal stress due to hardening. In the proposed model, the athermal part of the yield stress is assumed constant since the strain rate variation of the athermal stress is small. In fact, it is experimentally observed that whenever the initial temperature exceeds the critical temperature ($T>T_{cr}$), the flow stress values predicted by the proposed model noticeably differs from those obtained experimentally. Thus, not only does the strain rate affect the athermal part of the flow stress but also the excess temperature ($T-T_{cr}$) may also contribute to the variation of hardening (athermal) stress. This subject, however, is beyond the scope of this work and will be discussed in more details in the following chapters by investigating the low strain rate effects on some bcc metals that have very low critical temperatures as is the case for Nb and V (see Fig.2.6).

Using the material parameters values listed in Table 2.4, the adiabatic stress strain curves predicted by the present model shows good results as compared to the experimental data at
different initial testing temperatures with 2500 s\(^{-1}\) and 8000 s\(^{-1}\) strain rates as shown in Figs 2.11 and 2.12 respectively. In Fig.2.13, experimental stress strain results at very high strain rates are also used to test the ability of the proposed model to characterize the material flow stress under severe conditions. The comparison shows good agreement in the range of 13500 to 30500 s\(^{-1}\) strain rates.

![Figure 2.11 Adiabatic stress-strain curves for proposed model, for Vanadium (V), compared to experimental and model results (Nemat-Nasser & Guo, 2000) at 2500 s\(^{-1}\) strain rate and different initial temperatures.](image)

The incremental accumulation of the temperature during the adiabatic process is calculated by assuming all the plastic work is converted to heat based on the experimental results presented by Nemat-Nasser and Guo (2000). This evolution is defined by the following relation:

\[
T = T_o + 0.326 \int \sigma d\varepsilon_p \quad (2.41)
\]

It should be mentioned that the proposed model parameters listed in Tables 2.2, 2.3, and 2.4 for Mo, Nb, and V respectively are determined based on two high strain rates results only. Therefore, the flow stress results predicted by the proposed model may differ from those observed experimentally at low strain rates (\(\dot{\varepsilon}_p \leq 10^{-1} \text{s}^{-1}\)).
Figure 2.12 Adiabatic stress-strain curves for proposed model, for Vanadium (V), compared to experimental and model results (Nemat-Nasser & Guo, 2000) at 8000 s\(^{-1}\) strain rate and different initial temperatures.

Figure 2.13 Adiabatic stress-strain curves for proposed model, for Vanadium (V), compared to experimental results (Nemat-Nasser & Guo, 2000) at very high strain rates and room temperature.
Table 2.5 Parameters of OFHC Copper for the proposed and Z-A models.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Proposed Model “Eq.35”</th>
<th>Z-A Model “Eq.38”</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_1$ (K$^{-1}$)</td>
<td>0.0006739</td>
<td>0.000115</td>
</tr>
<tr>
<td>$\beta_2$ (K$^{-1}$)</td>
<td>0.0000355</td>
<td>0.0028</td>
</tr>
<tr>
<td>$\beta_3$ (K$^{-1}$)</td>
<td>0.000115</td>
<td>0.0028</td>
</tr>
<tr>
<td>$Y_o$ (Mpa)</td>
<td>60</td>
<td>65</td>
</tr>
<tr>
<td>$Y_a$ (Mpa)</td>
<td>950</td>
<td>890</td>
</tr>
<tr>
<td>$B$ (Mpa)</td>
<td>0.47</td>
<td>0.52</td>
</tr>
<tr>
<td>$n$</td>
<td>0.5</td>
<td>0.52</td>
</tr>
<tr>
<td>$p$</td>
<td>1.5</td>
<td>1.5</td>
</tr>
</tbody>
</table>

• **OFHC Copper:**

The Oxygen Free High Conductivity (OFHC) Copper is an important fcc metal used in the industry due to its high thermal and electrical conductivity and high ductility combined with low volatility which makes this material indispensable in the electronics industry. It is used here as an application for the proposed model to show the temperature and strain rate variation of the flow stress. The material parameters in Eq.(2.31) are determined using the same procedure explained in the previous section for the experimental data found in the paper by Johnson and Cook (1988). The proposed model parameters along with the Z-A model parameters are listed in Table 2.2. Using the same parameters, the proposed model as well as the Z-A model are further compared with other experimental data provided in the paper by Tanner et al. (1999) and Nemat-Nasser & Li (1998).

A further assessment of the proposed model can be made by comparing the adiabatic stress strain results predicted using the proposed model with both the Z-A model and the experimental data as shown in Fig.2.14. The constants listed in Table 2.5 are obtained from essentially the same data base found in Johnson and Cook (1988). Results obtained using the proposed model compare well with the experimental data for several strain rates and initial testing temperatures. The Z-A model, however, underestimates the stress values in the case of high strain rates and high temperatures. The two models are further compared to the data presented by Tanner et al. (1999) using the same parameter values illustrated in Table 2.5. It appears to be relatively acceptable agreement between the proposed model predictions and the experimental data (see Fig.2.15). In fact, the small difference shown may be attributed to the accuracy in obtaining the hardening parameters which may vary from test to test. In general, the proposed model shows a much stronger reliance on strain rate and temperature at higher strain rates and temperatures.

In the case of copper, the prediction of the adiabatic stress strain curves predicted by the proposed model is obtained based on the assumption of conversion of 90% of the plastic work deformation using the following formula:
This percentage, however, is 10% less than the one used by Nemat-Nasser and Li (1998). Fig. 2.16 shows the adiabatic stress strain results computed for both the proposed model and Nemat-Nasser & Li model and compared to the experimental data at 4000 s\(^{-1}\) strain rate for different initial temperatures. The comparisons show very good agreement between the proposed model predictions and the experimental data at low and high initial testing temperatures.

\[
T = T_o + 0.262 \int \sigma d\varepsilon_p \quad (2.42)
\]

Figure 2.14 Adiabatic stress-strain curves for proposed model, for OFHC Copper, compared to experimental results (Johnson and Cook, 1988) at (451-464) s\(^{-1}\) strain rates and different initial temperatures.

The thermal component of the flow stress given by the proposed fcc model dominates the deformation resistance of the material behavior due to the strain rate and temperature dependence of the hardening stresses. Consequently, the critical temperature \(T_{cr}\), which is calculated similarly to the bcc model in Eq.(2.36) by replacing \(\beta_1\) with \(\beta_3\), predicts values higher than those for the bcc model (see Fig.2.6) due to the fact that the stresses generated by the thermally activated energy in fcc metals are much higher than those found in bcc metals. That is, the athermal component of the flow stress in bcc metals is greater than the one in fcc metals. Similar to the bcc model, the instability strains may be calculated using the following expression:
Figure 2.15 Stress-strain curves, for proposed model, for OFHC Copper, compared to experimental results (Tanner et al., 1999) at room temperature and different strain rates.

Figure 2.16 Adiabatic stress-strain curves, for proposed model, for OFHC Copper, compared to experimental results (Nemat-Nasser & Li, 1998) at 4000s⁻¹ strain rate and different initial temperatures.
\[
\frac{d\sigma}{d\epsilon_p} = \frac{B\epsilon_p^{n-1}}{pq} \left(1 - (\beta T)^{1/q}\right)^{(1-p)/p} \left(pq \left(1 - (\beta T)^{1/q}\right) - \epsilon_p \beta^{1/q} T^{(1-q)/q} \frac{dT}{d\epsilon_p}\right) = 0 \quad (2.43)
\]

This equation shows that the instability strains increase with temperature and decrease with increasing strain rate similar to the bcc model.

### 2.5.3 Verification and Discussion of the Physical Based Parameters

Before checking on the accuracy of the numerical values of the physical parameters, one first needs to investigate the parameter \( \beta_1 \) used in the proposed bcc and fcc models. In fact, this parameter is not constant but rather varies with the accumulation of the mobile and forest dislocation densities which increase with the increase of plastic strains. However, the assumption of assuming \( \beta_1 \) as a constant seems to be acceptable for the case of the bcc model since the hardening parameters (plastic strain) are independent of both temperature and strain rate. Thus, the mobile and the forest dislocation densities used in Eq.(2.13) represent their initial values which are related to the initial yield stress. It should be noted, however, that these initial quantities are generally, strain rate dependent (Hasegawa et al., 2003) which will be disregarded in this work and an average value will be considered instead. On the other hand, the fcc model shows strong coupling between the plastic deformation and the effects of strain rates and temperatures. Consequently, using constant values for the dislocation density in the fcc model is not an accurate assumption unless a proper definition for the dislocation density evolution is made in order to allow for the plastic strains to be factored out and added to the plastic strains which results from the threshold stress dependency as obtained from Eq.(2.29) through Eq.(2.31).

As a matter of fact, it is not appropriate to have a single definition defining the dislocation densities evolution for both bcc and fcc metals. Each type of these two materials, however, has its different behavior with regard to the strain rate and temperature effects. Therefore, bcc and fcc metals need to have two separate evolution relations for the mobile dislocation densities. The bcc evolution relation may be related to the strain rate by a constant whereas the fcc relation should consider the history of dislocation accumulation during the plastic deformation. These facts along with the reality that the dislocation distance \( l \) is not really a constant will be addressed in chapter 5. These modifications may be utilized in determining the grain size effect on the plastic deformation process using the gradient theory developed by Voyiadjis and Dorgan (2001), Dorgan and Voyiadjis (2003), and Voyiadjis et al. (2003).

In general, most metals contain an initial amount of dislocations which naturally exits in the material or generates through the manufacturing process. These dislocation densities, however, help metals deform plastically until a level where no further dislocations generation is allowed which indicates that the saturation limit of dislocation densities is reached and the annihilation process is started. The initial and saturated values of the dislocation densities, however, differ from metal to metal. In this work, numerical values are obtained for the physical parameters used in defining both the bcc and fcc proposed models for tantalum and OFHC copper only.
• **Tantalum (BCC Model):**

In determining the numerical values of the presented physical constants, first one fixes the initial values of the mobile and forest dislocation densities to $5 \times 10^{12} \text{ m}^{-2}$ and $10^{13} \text{ m}^{-2}$ respectively, whereas the saturated values are taken to be $10^{15} \text{ m}^{-2}$ and $5 \times 10^{15} \text{ m}^{-2}$ respectively. To start identifying the numerical values of the physical parameters, the coefficient constants given in Eq.(2.2) are first determined using the same procedure presented by Kubin and Estrin (1990). These constants are obtained at the saturation level where the incremental plastic strain variation of the mobile and forest dislocation densities are zero. As a result, one obtains the following set of constants: $\lambda_1 = 0.3b^2 \times 10^{16}$, $\lambda_2 = 9.45$ and $\lambda_3 = 2.29b \times 10^8$. A value of 0.92 eV/atom is assigned for the Helmholtz free energy, $G_0$. The average value of the Burger vector for tantalum is taken to be around 3.0 Å and the average dislocation distance value $l$ is of the order $10^{-6}$ m.

The reference velocity $v_o = d/t_w$ chosen to be $3.0 \times 10^2 \text{ m/s}$ where $d = b$ and $t_w$ is the time that a dislocation waits at an obstacle. Moreover, the average values of the initial mobile and forest dislocations are assumed to be $10^{13} \text{ m}^{-2}$ for the former and $5 \times 10^{13} \text{ m}^{-2}$ for the latter. Though set arbitrary, these physical quantities are fairly representative.

In neglecting the evolution of the mobile dislocation density ($\dot{\rho}_m = 0.0$), the denominator within the log function given by Eq.(2.13) becomes unity and the parameter $\beta_1$ may be redefined as follows (similar to Nemat-Nasser and Isaacs, 1997):

$$\beta_1 = \frac{K}{G_0} \ln (\bar{mb} \rho_m v_o) \quad (2.44)$$

Fig.2.17 shows the consequence of considering and neglecting the effect of mobile dislocation density evolution on the flow stress as compared to the experimental data at different strain rates (Voyiadjis and Abed, 2003). The results indicate that the assumption of ignoring the evolution effect of the mobile dislocation density is acceptable for low strain rates of loading. This effect, however, increases when the strain rate increases which overestimates the value of the flow stress. On the other hand, the above mentioned effects are less dependent on the temperature variation which one may have the option to neglect (see Fig.2.18). In Figs. 2.17 and 2.18, the value of the parameter $\beta_1$ given in Table 2.1 is replaced by a value of 0.0013254 for the case of no dislocation density evolution effect ($\dot{\rho}_m = 0$).

• **OFHC Copper (FCC Model):**

As was discussed earlier, the dislocation densities ($\rho_m, \rho_f$) given by Eq.(2.13) are not constant and they are generated and accumulated during the plastic deformation process (i.e. they are plastic strain dependent). Since the hardening parameters (plastic strain) of fcc metals show strong dependency on both strain rate and temperature, then the parameter $\beta_i = f(\varepsilon_p)$ may be written as a function of the accumulative plastic strain. For simplicity, however, we assume average values for the forest and mobile dislocation densities which are higher than those of bcc metals. Therefore, the physical quantities taken here might not represent the
accurate values since they are taken based on the aforementioned assumption. In fact, this problem may be solved by substituting from Eq.(2.1) for the mobile dislocation density into Eq.(2.31) after introducing an appropriate definition for the mobile dislocation density evolution as discussed earlier. Hence, the parameter $\beta_1$ will be redefined as follows:

$$
\beta_1 = f(\varepsilon_p) = \frac{k}{G_o} \ln \left( \frac{\varepsilon_p \gamma_o}{l(1 - \hat{m} l \lambda_4 / b + \lambda_4 \varepsilon_p)} \right)
$$

(2.45)

Here $\lambda_4$ represents the combined effect of both immobile and forest dislocation densities on the accumulation of mobile dislocation density during the plastic deformation. The above relation (Eq.(2.45)) is not utilized in this work but will be investigated with a proper definition of the mobile dislocation density evolution in the following chapters.

![Figure 2.17](image)

Figure 2.17 Effect of mobile dislocation density evolution on the strain rate variation of the flow stress using the proposed bcc model (PM) and compared to several experimental data (Ta) at different temperatures.

Generally, the numerical values of the physical parameters for OFHC Copper may be defined similarly to those defined for Tantalum. The initial and saturated values of mobile dislocation densities are taken as $10^{13}$ m$^{-2}$ and $5 \times 10^{15}$ m$^{-2}$ respectively whereas for forest dislocation densities are $5 \times 10^{13}$ m$^{-2}$ and $10^{16}$ m$^{-2}$ respectively. Therefore, the following set of constants is obtained: $\lambda_1 = 0.2 b^2 \times 10^{17}$, $\lambda_2 = 0.37$, $\lambda_3 = 0.181 b^2 \times 10^9$. An average value of 3.3Å for the Burgers vector is selected while the average dislocation distance $l$ is taken to be around a value of $10^{-7}$ m. It is interesting to find that the Helmholtz free energy, ($G_o = 2.43$ eV/atom) is higher than the value assigned for tantalum.
Figure 2.18 Effect of mobile dislocation density evolution on the temperature variation of the flow stress using the proposed bcc model (PM) and compared to several experimental data (Ta) at different strain rates.

Figure 2.19 Effect of mobile dislocation density evolution on the adiabatic stress strain curves of the flow stress using the proposed model (PM) and compared to several experimental data (OFHC Copper) at different strain rates and temperatures.
Also, the reference velocity \( v_0 \approx 131 \text{ s}^{-1} \) is lower since the waiting time \( t_w=O(10^{-11}\text{s}) \] needed by the dislocation to overcome an obstacle is higher than the time required in bcc metals\( t_w=O(10^{-12}\text{s}) \) (Kocks et al., 1975). The dislocation densities increase with the increase of the plastic strains starting from the initial values until they reach their saturated values which represent the maximum value of the flow stress. After that, the dislocation annihilation process starts dominating the behavior of the plastic deformation from which material softening is encountered. In this work, the following average values are selected for the dislocation densities; \( \rho_m = 5 \times 10^{14} \text{ m}^{-2} \) and \( \rho_f = 10^{15} \).

The stress-strain results predicted here using the proposed model is shown in Fig.2.19. In this case, the effect of the mobile dislocation evolution is neglected \( (\dot{\rho}_m = 0.0) \) for different strain rates and temperatures as compared to the experimental data. It is clear that this effect increases as the plastic strain increases which is affected by both the temperature and the strain rate. In calculating these dashed lines in Fig.2.19, a value of 0.0006184 is used for the parameter \( \beta_1 \) instead of the one listed in Table 2.5.
CHAPTER 3

PLASTIC DEFORMATION MODELING OF AL-6XN STAINLESS STEEL AT LOW AND HIGH STRAIN RATES AND TEMPERATURES

3.1 Introduction

Two physically based constitutive models were developed by Voyiadjis and Abed (2004) to simulate the plastic deformation behavior for two different crystal structures of metals; body centered cubic (bcc) and face centered cubic (fcc) that is subjected to high strain rates and temperatures. The two constitutive models were derived based on the concept of thermal activation analysis and the dislocation interaction mechanisms as well as the additive decomposition of the thermal and athermal stresses. Both models were successfully applied to several bcc metals (Tantalum, Molybdenum, Niobium, and Vanadium) and fcc metals (OFHC Copper) over a wide range of temperatures (77K to 1000K) and strain rates (0.001s⁻¹ to 8500s⁻¹). The deformation mechanism of bcc metals is generally attributed to the resistance of the dislocation motion by the Peierls barriers (short-range barriers) provided by the lattice itself. Thus, the behavior of bcc metals shows a strong dependence of the thermal yield stress on the strain rate and temperature whereas, the plastic hardening is hardly influenced by either the strain rate or the temperature and therefore, it contributes to the athermal part of the flow stress. In fcc metals, on the other hand, the emergence and evolution of a heterogeneous microstructure of dislocations as well as the long-range intersections between dislocations dominates and controls the mechanisms of thermal activation analysis behavior. Thus, the thermal activation is strongly dependent on the plastic strain, consequently, the increase in the yield point with a decrease in temperature is highly dependent on the strain-hardened states. Moreover, there is no strain rate and temperature effect on the initial yield stress, which implies that when the plastic strain is zero, the stress-strain curves at different temperatures and strain rates, will have the same starting point.

In this chapter, both bcc and fcc models are utilized in modeling the plastic deformation behavior of AL-6XN stainless steel under low and high strain rates and temperatures. In addition to Iron (bcc), the microstructure of AL-6XN stainless steel is composed mainly of 23.84% of Nickel (Ni) (fcc metal) and 20.56% and 6.21% of Chromium (Cr) and Molybdenum (Mo) (bcc metals) respectively. Table 3.1 shows the major alloy content of the investigated AL-6XN stainless steel as given by Nemat-Naser et al. (2001).

The AL-6XN alloy is a high-strength stainless steel designed to resist chloride pitting, crevice corrosion, stress corrosion cracking, and applications which may come in contact with salts during high temperature processes. Therefore, it is, generally, employed in applications where good strength is required in harsh environments where chloride pitting and stress corrosion cracking is a problem. The study of strain rate and temperature effects on the strength of stainless steel received wide attention that was addressed by many authors (e.g. Ishikawa and Tanimura, 1992; Hecker et al., 1982; Stout and Follansbee, 1986). However, the plastic deformation of AL-6XN at low and high strain rates and temperatures received less attention. Most recently, Nemat-Nasser et al. (2001) investigated the plastic flow of AL-6XN
stainless steel and the corresponding deformation mechanisms first through systematic compression experiments performed over a wide range of temperatures and different strain rates and second through theoretical modeling using the experimental results and based on the mechanisms of thermally activated dislocation motion. In this work, the experimental results provided by Nemat-Nasser et al. (2001) will be utilized in determining the material parameters for the proposed plastic deformation modeling of AL-6XN.

Table 3.1 Major Alloy content of AL-6XN (%) (Nemat-Nasser et al., 2001).

<table>
<thead>
<tr>
<th></th>
<th>C</th>
<th>Cr</th>
<th>Ni</th>
<th>Si</th>
<th>Mn</th>
<th>Mo</th>
<th>N</th>
<th>Cu</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.024</td>
<td>20.56</td>
<td>23.84</td>
<td>0.36</td>
<td>0.41</td>
<td>6.21</td>
<td>0.213</td>
<td>0.2</td>
</tr>
</tbody>
</table>

According to the phase transformation diagram of steel, the percentage of carbon (C) in steel plays a crucial role in determining the phase behavior (ferrite or Austenite) of the material over a wide range of temperatures. It is known that the austenitic steel exhibits a single-phase, face-centered cubic (fcc) structure while the ferrite exhibits a body-centered face (bcc) structure. It should be noted that although the Al-6XN alloy is an austenitic stainless steel material, the plastic deformation or the dislocation interactions in the microstructure scale shows a combination of both bcc and fcc effects under low and high strain rates and temperatures. In other words, both the yield and the hardening stresses are affected by temperature and strain rates as will be shown in the following sections. The objective of this chapter is to characterize the plastic deformation behavior of AL-6XN stainless steel (material contains different compositions that have different crystal structures) using simultaneously both the bcc and fcc models developed recently by Voyiadjis and Abed (2005). Moreover, the classical secant modulus method is utilized here in modeling the true stress strain curves for different temperatures and strain rates.

In section 3.2, a brief discussion about both the bcc and fcc models as related to the nano/micro-quantities are given. Section 3.3 presents the characterizing and modeling of the plastic deformation behavior for the present material at low and high strain rates and temperatures. In section 3.4, the derivation of the classical multiaxial secant modulus as well as the incremental modulus are presented. In addition a uniaxial case of deformation is investigated in order to compare with the available experimental data.

3.2 Microstructural Based Models for BCC and FCC Metals

Dislocations play a main role in determining the inelastic behavior of a metal and its flow stress under different load conditions. Making use of the concept of thermal activation analysis, dislocation movement mechanisms, the concept of the additive decomposition of the flow stress into the thermal and athermal components, and taking into consideration the mobile
dislocation density evolution, Voyiadjis and Abed (2004) proposed the following two physically based constitutive relations for bcc, Eq.(3.1), and fcc, Eq.(3.2), metals:

\[
\sigma = \hat{Y}\left(1 - \left(\beta T - \beta_2 T \ln \dot{\varepsilon}_p\right)^{1/q}\right)^{1/p} + B\varepsilon^n + Y_a \tag{3.1}
\]

\[
\sigma = B\varepsilon^n_p\left(1 - \left(\beta T - \beta_2 T \ln \dot{\varepsilon}_p\right)^{1/q}\right)^{1/p} + Y_a \tag{3.2}
\]

where \(\hat{Y}\) is the threshold yield stress of the Peierls barrier to the initial dislocation motion. \(B\) and \(n\) are the plastic hardening constants, \(Y_a\) represents the temperature-independent yield stress, and the exponents \(q\) and \(p\) are constants defining the shape of the short-range barrier and their range of values is (1.0-2.0) for the former and (0.0-1.0) for the latter. The parameters \(\beta_1\) and \(\beta_2\) are related to the microstructure physical components as follows:

\[
\beta_1 = \frac{k}{G_o} \ln \left(\frac{\bar{m} b^2 \rho_m v_o}{b - \bar{m} l \left(\lambda_1 - b^2 \lambda_2 \rho_m - b \lambda_3 \rho_f^{0.5}\right)}\right) \tag{3.3}
\]

and

\[
\beta_2 = \frac{k}{G_o} \tag{3.4}
\]

where the above nano/micro-physical quantities are defined as follows: \(b\) is the magnitude of the Burgers vector, \(\rho_m\) is the mobile dislocations density, \(\rho_f\) is the forest dislocation density, \(l\) is the dislocation displacement or it can be interpreted as the free path of trapped dislocations, \(\bar{m}\) can be interpreted as the Schmidt orientation factor, \(G_o\) is the reference Gibbs energy at zero absolute temperature \(T=0\), \(v_o = d / t_w\) is the reference dislocation velocity, \(t_w\) is the time that a dislocation waits at an obstacle, and \(d\) is the average distance the dislocation moves between the obstacles. The constant coefficients \(\lambda_i\) are related to the multiplication of the mobile dislocations (\(\lambda_1\)), their mutual annihilation and trapping (\(\lambda_2\)), and their immobilization through interaction with forest dislocations (\(\lambda_3\)).

### 3.3 Plastic Deformation Modeling of AL-6XN Stainless Steel

As explained earlier, the microstructure of AL-6XN stainless steel mainly consists of components that have two types of crystal structures; bcc and fcc. Therefore, a combination of the aforementioned two physically based models is going to be used in order to physically model the plastic deformation of such materials. Moreover, the experimental observations of this material at different strain rates and temperatures are considered. According to Nemat-Nasser et al., (2001), the experimental results of AL-6XN stainless steel reveal some characteristics that need to be addressed in the plastic deformation modeling. The first characteristic is that both the hardening and the yield stress depend on the temperature and the strain rate and their corresponding history, which is not the case if we have either a bcc or fcc
metal structure. Second characteristic is that the microstructure of the material evolves mainly with the temperature history. Third characteristic is that the long-range obstacles are related to the plastic strain as well as the initial yield stress. Finally, the dynamic strain aging takes place when the temperature reaches the critical values (600K to 1000K), becoming weaker when the temperature exceeds 1000K and increasing with strain.

In order to understand quantitatively the deformation behavior of this material, a constitutive description is required. Thus, the above experimental observations should be included and addressed properly in order to have a suitable flow stress model for this material (AL-6XN). The dynamic strain aging effects, however, are not included in the present model since the plastic flow is considered in the range of temperatures and strain rates where diffusion and creep are not dominant. In other words, the plastic deformation is attributed to the motion of dislocations only.

To deform a metal beyond the elastic limit means to activate and move its dislocations through the crystal. Once the dislocations start moving through the crystal, two types of obstacles are encountered that try to prevent dislocation movements through the lattice; long-range and short-range barriers. The long-range obstacles are due to the structure of the material and cannot be overcome by introducing thermal energy through the crystal, while, the short-range barriers can be overcome by thermal energy. Utilizing the two physically based bcc and fcc models, the flow stress of AL-6XN stainless steel consists of thermal and athermal parts: The thermal part is attributed to the short-range barriers which includes the Peierls stress, point defects such as vacancies and self-interstitials, and dislocations intersection with slip planes. On the other hand, the long-range effects such as the stress field of dislocation forests and grain boundaries are independent of strain rate and temperature and thus, contribute to the athermal part of the flow stress. The total flow stress is additively decomposed into the thermal $\sigma_{th}$ and the athermal $\sigma_{ath}$ components as follows:

$$\sigma = \sigma_{th} + \sigma_{ath}$$

(3.5)

As shown from the above two models, the flow stress of a material is a function of some internal microstructural parameters as well as the temperature and strain rate. The internal microstructural components include grain size, Burgers vector, and both the forest and mobile dislocation densities. The assumption used in Eq.(3.5) for the additive decomposition of the flow stress, is a result of experimental observations which show that at certain strain rate, the increase in the temperature beyond such a limit will cause no further degradation on the flow stress. In other words, there is always certain amount of stresses inside the material that is independent of temperature and, therefore, should be added to the total flow stress. This kind of stress is called the athermal stress which is physically interpreted as the resistance of the long-range obstacles to the movement of the thermally activated dislocations.

**3.3.1 Athermal Stress Component of the Flow Stress for AL-6XN**

In most metals, the temperature variation of the flow stress at certain strain and strain rate shows that the flow stress decreases as the temperature increases until a point where no further
decreasing is allowed and the stress becomes constant. This point represents the athermal stress value on the stress axis and the critical temperature value, \( T_{cr} \), on the temperature axis. The critical temperature changes with strain rate while the athermal stress is independent of strain rate. In general, the athermal component of fcc metals consists of one component that is independent of strain (\( Y_a \) in Eq.(3.2)), whereas, an additional strain-dependent component exists in bcc metals (\( B\varepsilon^n \) in Eq.(3.1)). The physical interpretation of the athermal stress component was investigated by many authors. Zerilli and Armstrong (1987) attributed the strain-independent component of the athermal stress to the influence of the solute and the initial dislocation density (originated in the material) on the yield stress. They defined the athermal stress component as the product of the microstructural stress intensity and the inverse square root of the average grain diameter. Nemat-Nasser and Guo (2000) indicated that for bcc metals, the athermal resistance to the motion of dislocations is due to the elastic stress field generated by the dislocations, point defects, grain boundaries, and various other impurities found in the composition of the material. That is, no temperature and strain rate effects are encountered except the temperature dependence on the elastic modulus. Moreover, since the plastic strain increases monotonically and the plastic strain rate is always greater than zero, consequently the plastic strain can be used to define the variation of the mobile dislocation density, the average grain size, and other parameters that affects the athermal component of the flow stress.

For the case of AL-6XN, the above physical interpretations as well as the experimental observations at different strain rates and temperatures lead to the following definition of the athermal component of the flow stress:

\[
\sigma_{ath} = Y_a + B_1\varepsilon_p^n
\]  

where \( B_1 \) and \( n_1 \) represents the athermal hardening parameters and \( Y_a \) is the athermal yield stress. The experimental fitting of these parameters starts by addressing the temperature variation of the flow stress at different strains and strain rates shown in the experimental data presented by Nemat-Nasser et al. (2001). For 0.001s\(^{-1}\) and 0.1s\(^{-1}\) strain rates (see Figs. 3.1 and 3.2), the flow stress becomes independent of the temperature, for the cases above 650K and 775K respectively. However, it needs to exceed temperatures of 1000K for the case of 3500s\(^{-1}\) strain rate (see Fig. 3.3 in Nemat-Nasser et al, 2001). Therefore, the experimental results at 1000K for both 0.001s and 0.1s strain rates will be utilized in determining the athermal components of the flow stress. Examination of the trend of these results, at 1000K temperature, shows that the stress values change with plastic strain which indicates that the athermal flow stress for AL-6XN is strain dependent.

The experimental results of the athermal flow stresses at the two mentioned strain rates (see Fig. 3.4) are almost identical since they are conducted at temperatures beyond the critical ones (\( T>T_{cr} \)). At that stage, the strain rate effect becomes insignificant due to the very high governing temperature from which the flow stress is dominated by the resistance of the long range barriers that could not be overcome by the thermal activation energy.
Figure 3.1 Experimental results of the temperature variation of the flow stress at 0.001 s\(^{-1}\) strain rate and for different plastic strains, for AL-6XN stainless steel (Nemat-Nasser et al., 2001).

Figure 3.2 Experimental results of the temperature variation of the flow stress at 0.1 s\(^{-1}\) strain rate and for different plastic strains, for AL-6XN stainless steel (Nemat-Nasser et al., 2001).
Thus, the athermal part of the flow stress becomes independent of both temperature and
strain rate and is calculated using Eq.(3.6). This approach for estimating $\sigma_{\text{ath}}$ is purely
empirical using the plastic strain as an independent variable. In order to have a physically
based approach, the athermal stress should be directly related to the dislocation density,
average grain size, and other parameters that represent the elastic field of the various
inhomogeneities (Nemat-Nasser and Guo, 2000).

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other parameters that represent the elastic field of the various inhomogeneities (Nemat-Nasser
and Guo, 2000).

![Figure 3.3](image-url)

**Figure 3.3** Experimental results of the temperature variation of the flow stress at 3500s$^{-1}$ strain
rate and for different plastic strains, for AL-6XN stainless steel (Nemat-Nasser et al., 2001).
Figure 3.4 The athermal stress-plastic strain predicted using the proposed model, and compared to the experimental results at 1000K and 0.1s$^{-1}$ and 0.001s$^{-1}$ strain rates.

### 3.3.2 Thermal Stress Component of the Flow Stress for AL-6XN

The thermal activation analysis of AL-6XN under different strain rates shows two different behaviors; of bcc and fcc. The mechanism of bcc metals is defined as the overcoming of the short range barriers (Peierls-Nabarro barriers) through the movement of the initial dislocations (original dislocations), that is, the thermal stress contributes to the yield stress and does not depend on the accumulation of the dislocation densities through the plastic deformation. On the other hand, the cutting of dislocations forests which is attributed to the evolution and the accumulation of the mobile dislocations during the plastic deformation is the principle mechanism in fcc metals, This implies that the thermal stress in fcc is strongly dependent on the plastic strain. Therefore, the thermally activated flow stress of AL-6XN is additively decomposed here into two parts as follows:

$$\sigma_{th} = Y_{th} + H_{th}$$  \hspace{1cm} (3.7)

where both the thermal yield stress $Y_{th}$ and thermal hardening $H_{th}$ are defined as follows:

$$Y_{th} = \hat{Y} \left(1 - \left(\beta_1 T - \beta_2 T \ln \dot{\varepsilon}_p \right)^{1/4}\right)^{1/p}$$  \hspace{1cm} (3.8)
Here, $B_2$ and $n_2$ represent the thermal hardening parameters and their numerical values and are not necessarily the same as those in Eq.(3.6). However, the parameters $\beta_i^1$ and $\beta_i^2$ are the same as those defined in Eqs. (3.3) and (3.4) respectively except that, the parameter $\beta_i^Y$ is related to the initial values of the microstructural quantities (dislocation densities $\rho_m$ and $\rho_f$ and dislocation distance $l$). The parameter $\beta_i^H$ is related to the average values of these quantities. It should be noted that the mobile dislocation density as well as the forest dislocation density is not constant and rather, it evolves with the plastic deformation of the material. Therefore, taking the average value of these dislocation densities in the definition of the parameter $\beta_i^H$ is not an accurate assumption. This problem, however, can be solved by redefining the mobile dislocation density using the Orwan’s relation and assuming that the forest dislocation is related to the plastic strain through the constant $\lambda_4$ which leads to the following expression:

$$
\beta_i^H \approx \frac{k}{G_o} \ln \left( \frac{v_o \varepsilon_p}{1 - \bar{\dot{m}} l \lambda_4 / b + \lambda_5 \varepsilon_p + l \lambda_4 \varepsilon_p^{0.5}} \right)
$$

(3.10)

The above relation given by Eq.(3.10) shows that the parameter $\beta_i^H$ is no longer constant and it varies with the variation of the plastic strain. This makes the thermal flow stress relation more complicated especially in trying to experimentally fit the model parameters. Therefore, one needs to find a consistent physical base to factor out mathematically the plastic strain and incorporate it to the hardening parameters $B_2$ and $n_2$. This problem, however, will be addressed extensively in chapter 5. In this work, however, we choose to use the definition given in Eq.(3.3). Another point that needs to be noted here is that the value of the activation energy $G_o$ differs from one mechanism to another and accordingly, the parameters $\beta_2^Y$ and $\beta_2^H$ will have two different numerical values.

The experimental values of the thermal stress component at each strain rate are calculated by deducting the athermal flow stress component estimated by Eq.(3.6) from the total flow stress. Fig. 3.5 shows the thermal stress for the case of 0.1s$^{-1}$ strain rate for different plastic strains. It is clear that the thermal stress varies with the variation of the plastic strain for temperatures below 1000K while it is strain-independent and vanishes when the temperature passes the critical value (>700K). Hence, the experimental values of the thermal stress at zero plastic strain and for different strain rates are utilized here in determining the thermal yield stress component as shown in Fig. 3.6 as follows:

$$
H_{th} = B_2 \varepsilon_p^{n_2} \left(1 - \left(\beta_1^H T - \beta_2^H T \ln \dot{\varepsilon}_p \right)^{1/q} \right)^{1/p}
$$

(3.9)
Figure 3.5 Experimental results for the temperature variation of the thermal flow stress at 0.1 s\(^{-1}\) strain rate and for various plastic strains.

\[ Y_a = 1100 \left(1 - \left(0.00121T - 0.000061T \ln \dot{\varepsilon}_p \right)^{1/2} \right)^2 \]

Figure 3.6 Temperature variations of the thermal yield stress predicted using the proposed model, and compared to the experimental results at different strain rates.
The final step in modeling the flow stress of AL-6XN is to determine the hardening component of the thermal flow stress. Once the thermal yield stress is estimated, the hardening component of the thermal stress is now obtained by utilizing the net values of the experimental results \( (\sigma - \sigma_{\text{th}} - Y_{th}) \) for different strain rates and specific plastic strain as shown in Fig. 3.7.

Utilizing Eqs. (3.6), (3.7), (3.8) and (3.9), the final expression of the flow stress for AL-6XN stainless steel is given as follows:

\[
\sigma = Y_a + B_1 \varepsilon_p^n + \hat{Y} \left( 1 - \left( \beta_1^Y T - \beta_2^Y T \ln \dot{\varepsilon}_p \right) \right)^{\alpha_1/p}
+ B_2 \varepsilon_p^n \left( 1 - \left( \beta_1^H T - \beta_2^H T \ln \dot{\varepsilon}_p \right) \right)^{\alpha_2/p}
\]

(3.11)

The above relation (Eq.(3.11)) is used to obtain the total flow stress for the cases of isothermal and adiabatic plastic deformation where the temperature is maintained constant for the former and increases with the generation of the plastic work for the latter.

Figure 3.7 Temperature variations of the thermal hardening stress predicted using the proposed model, and compared to the experimental results at 15% plastic strain and for different strain rates.

\[
H_{th} = 2190 \varepsilon_p^{2.31} \left( 1 - \left( 0.00111 T - 0.000051 T \ln \dot{\varepsilon}_p \right) \right)^{2.91/2}
\]
For the adiabatic case of deformation, the heat inside the material increases as the plastic strain increases and therefore, the temperature $T$ is calculated incrementally by assuming that the majority of the plastic work is converted to heat

$$ T = \frac{\chi}{c_p \rho} \int_0^\varepsilon \sigma d\varepsilon_p $$

(3.12)

where $T_o$ is the initial testing temperature, $c_p$ is the specific heat at a constant pressure and $\rho$ is the material density. The Taylor-Quinney empirical constant $\chi$ is often assigned the value of 0.9. However, recent tests reported by Kapoor and Nemat-Nasser (1998) for several metals suggest that, for large strains (e.g., $\varepsilon \geq 20\%$), the value of $\chi$ is essentially equal to one. In this work, the parameter $\chi$ is approximated to a value of 1.0 as verified experimentally by Nemat-Nasser et al. (2001), the mass density $\rho$ for AL-6XN is equal to 7.947 g/cm$^3$ and the temperature-dependent heat capacity $c_p$ is taken as 0.5 J/g K at room temperature (Russell et al., 1980). Eq.(3.12) may be solved numerically or can be integrated without introducing any noticeable errors by either using the mean value theorem or the simple Euler method.

![Graph](image)

Figure 3.8 Critical temperatures predicted by the proposed model for the yield and hardening parts of the thermal flow stress at various strain rates.
The thermal component of the flow stress decreases as the temperature increases until it vanishes when the temperature reaches or exceeds a critical value. In the temperature variation of the stress curve, the critical temperature defines the starting point of the constant stress which, in turn, refers to the athermal component of the flow stress:

\[ T_{cr} = \left( \beta_1^i - \beta_2^i \ln \dot{\varepsilon}_p \right)^{-1} \quad (3.13) \]

It should be noted here, that the thermal component of the flow stress is non-negative. Thus, the thermal yield stress calculated using Eq.(3.7) should be set equal to zero when it becomes negative which indicates that the temperature has exceeded its critical value. The critical temperature, however, is strain rate-dependent and it increases with the increase of the strain rate. Fig. 3.8 shows the strain rate variation of \( T_{cr} \) for both the thermal yield and hardening stresses which are calculated using Eq.(3.13) for the thermal yield and the hardening components. The difference between the \( T_{cr} \) values of the thermal yield and the hardening components may be attributed to two different mechanisms involved in the plastic deformation of each part of the thermal components.

### 3.3.3 Procedure for the Determination of the Material Constants

The numerical values of the material parameters given in Eq.(3.11) are listed in Table 3.2 and calculated after considering separately the effects of strain rate and temperature on the flow stress. The procedure to determine the constitutive model parameters is initiated by studying the stress-temperature relations at different values of plastic strains for a specific strain rate as explained earlier. The constant values of the flow stresses encountered at temperatures above the critical value are used here in order to calculate the values of the athermal hardening constants \( B_1 \) and \( n_1 \) by utilizing the nonlinear least-squares fit. The value of \( Y_a \) represents the athermal stress at zero plastic strain or the athermal component of the initial yield stress. Subtraction of the above stress increments (athermal stresses) from the overall stress leads to the thermal component of the flow stress which is accounted for by the thermal yield stress \( Y_{th} \) and the thermal hardening stress \( H_{th} \) as given by Eqs.(3.8) and (3.9) respectively. According to Kocks (2001), the typical values of the exponents \( p \) and \( q \) are less than 1 for the former and 3/2 and 2 for the latter. In this work, however, values of 3/2 for \( q \), that is equivalent to a triangle obstacle profile near the top, and 1/2 for \( p \), which characterizes the tail of the obstacle, are chosen. Once these exponents are determined for a particular mechanism, they are kept constant.

Next, the thermal stresses at zero plastic strain for different strain rates are used in obtaining the material parameters of the thermal yield stresses. The intercept of the constant slope line plotted between \( \left( \sigma_{\varepsilon_p=0} - Y_a \right)^p \) and \( T^{1/q} \) at certain strain rate, is employed here to obtain the value of the threshold stress \( \hat{Y} \). Furthermore, a graph of \( \left( 1 - \left( \sigma_{\varepsilon_p=0} - Y_a / \hat{Y} \right)^p \right)^q \) versus \( \ln \dot{\varepsilon}_p \) at fixed temperature is utilized to determine the parameters \( \beta_1^y \) and \( \beta_2^y \). A similar procedure is followed to determine the material parameters of the thermal hardening...
parameters as given by the last term of the right hand side of Eq.(3.11). A graph for 
\((\sigma - Y_f - Y_a - B\varepsilon_p^n)^p\) versus \(T^{1/q}\) at several plastic strains and a fixed plastic strain rate is plotted. The intercepts of these constant slope lines are employed to determine the hardening
parameters \(B_2\) and \(n_2\) using the nonlinear least-squares fit. Finally, the parameters \(\beta'\) and \(\beta''\) are determined by utilizing the constants of the line drawn at a specific temperature and certain plastic strain between 
\((1 - ((\sigma - Y_f - Y_a - B\varepsilon_p^n)/B\varepsilon_p^n)^p)\) and ln \(\dot{\varepsilon}_p\).

It should be noted that the determination of the hardening coefficients \(B_i\) and \(n_i\), in both thermal and athermal cases, are not that simple and straightforward from which unique values of these coefficients are difficult to achieve depending on the details of the fitting procedure. This problem may be attributed to the presence of initial upper and lower yield points which complicates the analysis of small strain materials at the initial hardening stage.

Table 3.2 Parameters of AL-6XN stainless steel for the proposed model.

<table>
<thead>
<tr>
<th>Model Parameters Eq.(3.11)</th>
<th>Numerical Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\beta') (K(^{-1}))</td>
<td>0.00121</td>
</tr>
<tr>
<td>(\beta'') (K(^{-1}))</td>
<td>0.00113</td>
</tr>
<tr>
<td>(\beta_2) (K(^{-1}))</td>
<td>0.0000618</td>
</tr>
<tr>
<td>(\beta_2'') (K(^{-1}))</td>
<td>0.000051</td>
</tr>
<tr>
<td>(Y_o) (Mpa)</td>
<td>139</td>
</tr>
<tr>
<td>(\hat{Y}) (Mpa)</td>
<td>1100</td>
</tr>
<tr>
<td>(B_1) (Mpa)</td>
<td>800</td>
</tr>
<tr>
<td>(B_2) (Mpa)</td>
<td>2190</td>
</tr>
<tr>
<td>(n_1)</td>
<td>0.45</td>
</tr>
<tr>
<td>(n_2)</td>
<td>0.71</td>
</tr>
<tr>
<td>(p)</td>
<td>0.5</td>
</tr>
<tr>
<td>(q)</td>
<td>1.5</td>
</tr>
</tbody>
</table>

3.3.4 Justification for the Quantities Used in the Physical Based Parameters

Before checking on the accuracy of the numerical values of the physical parameters, one first needs to recognize the difference of the deformation behavior between thermal yielding (bcc) and thermal hardening (fcc) as related to the physical quantities. For the case of thermal yielding, the dislocation densities as well as the dislocation distances are related to their initial values (i.e., they are independent of the plastic strain). These initial quantities, however, are generally, strain rate dependent (Hasegawa et al., 2003). On the other hand, the thermal
hardening behavior shows strong coupling between the plastic deformation and the effects of strain rates and temperatures. Therefore, the dislocation densities are accumulated up to their saturated values as the plastic hardening evolves such that (Kubin and Estrin, 1990):

\[
\dot{\rho}_m = \left( \lambda_1 / b^2 - \lambda_2 \rho_m - \lambda_3 \rho_f^{0.5} / b \right) \dot{\varepsilon}_p
\]  
(3.14)

This evolution relation, however, is not appropriate for the case of bcc metals (thermal yielding) due to the fact that the thermal stress is independent of the plastic strain and therefore, the history of the dislocation densities during their accumulation or evolution is not involved in the thermal yielding process. As a result, the mobile dislocation density evolution for the thermal yield component of the flow stress is redefined here, after neglecting the parameters \( \lambda_2 = \lambda_3 = 0.0 \), as follows:

\[
\dot{\rho}_m = \left( \lambda_1 / b^2 \right) \dot{\varepsilon}_p
\]  
(3.15)

Consequently, the physical interpretation of the parameter \( \beta_1^y \) takes the following definition:

\[
\beta_1^y = \frac{k}{G_o} \ln \left( \frac{\bar{m} b v_o \rho_{mi}}{1 - \lambda_i \bar{m} b l_i} \right)
\]  
(3.16)

In general, most metals contain an initial amount of dislocations which naturally exits in the material or generates through the manufacturing process. These dislocation densities, however, help metals deform plastically until a level where no further dislocations generation is allowed which indicates that the saturation limit of dislocation densities is reached and the annihilation process is started. The initial and saturated values of the dislocation densities, however, differ from metal to metal. For the present material (AL-6XN stainless steel), the initial density value is taken around \( 5 \sim 15 \times 10^{12} \text{ m}^{-2} \) for the mobile dislocation and \( 10 \times 10^{12} \text{ m}^{-2} \) for the forest dislocation whereas the saturated values of the mobile and forest dislocation densities are set to \( \mathcal{O}(10^{15} \text{ m}^{-2}) \). The constants given in Eq.(3.15) for the case of thermal yield stress and Eq.(3.14) for the case of thermal hardening are determined using the same procedure presented by Kubin and Estrin (1990). The thermal hardening constants given in Eq.(3.9) are obtained at the saturation level where the incremental plastic strain variation of the mobile and forest dislocation densities are zero while the thermal yielding constants are obtained at the initial level of the dislocation densities. As a result, one obtains the following set of constants: \( \lambda_1 = 8.33b^2 \times 10^{15}, \lambda_2 = 7.51 \) and \( \lambda_3 = 2.75b \times 10^7 \) for the case of thermal hardening and \( \lambda_1 = 1.46b^2 \times 10^{14} \) and \( \lambda_2 = \lambda_3 = 0.0 \). A value of 1.4 eV/atom is assigned for the Helmholtz free energy, \( G_o \) for \( \beta_2^y \), whereas \( G_o \) is taken as 1.7 eV/atom for \( \beta_2^H \). The average value of the Burgers vector for AL-6XN is taken to be around 3.0 Å and the dislocation distance \( l \) ranges from an initial value of 10µ decreasing down to a value of 0.1 µ at the saturation level of dislocation densities.
The reference velocity \( v_0 = d/t_w \) is chosen to be \( O(10^4 \text{m/s}) \) for \( \beta_i^\gamma \) and \( O(10^3 \text{m/s}) \) for \( \beta_i^\eta \), where \( d \sim b \) and \( t_w \) is the time that a dislocation waits at an obstacle. It is interesting to find that the reference velocity for thermal hardening is lower than that for thermal yielding which is attributed to the fact that the waiting time needed by the dislocation to overcome Peierls barriers provided by the lattice itself \( [t_w = O(10^{-13} \text{s})] \) is less than the time required to overcome the long-range intersections between dislocations \( [t_w = O(10^{-12} \text{s})] \) (Kocks et al., 1975). In fact, the orders of the numerical values of nano/micro-physical quantities used in this work are fairly representative and chosen from the available experimental work in the literature. Their exact values, however, are selected after determining the numerical values of the model parameters that are related to those quantities.

Once the plastic deformation is defined, the prediction of the uniaxial true-stress true-strain curves for AL-6XN stainless steel is obtained using either the classical secant method or the incremental method which are explained in the following section.

### 3.4 Classical Secant and Incremental Methods

In fact, metals show small elastic strain deformation and therefore, most authors assume that the plastic flow stress is fairly representative in defining the constitutive relation for most metals. In this work, however, we choose to model the true stress-true strain experimental curves by using the classical secant moduli method which is briefly summarized here along with the incremental method (see Suquet, 1997 for a comprehensive presentation).

#### 3.4.1 Classical Secant Method

The classical secant method was initially developed by Berveiller and Zaoui (1979) followed by Tandon and Weng (1988) and applied to metal matrix composites. This method, however, states that the plastic behavior of any phase (e.g. matrix) is approximated by using the secant modulus defined at each step of the deformation path. The resulting local constitutive relation that relates the stress tensor \( \sigma_{ij} \) to the total strain tensor \( \epsilon_{ij} \) can thus be written as follows:

\[
\sigma_{ij} = E_{ijkl}^s \epsilon_{kl}
\]

where \( E_{ijkl}^s \) denotes the secant tensor of the isotropic material (any phase in composites) which is defined by the following relation:

\[
E_{ijkl}^s = k^s \delta_{ij} \delta_{kl} + 2 \mu^s \left( \delta_{ik} \delta_{jl} - \frac{1}{3} \delta_{ij} \delta_{kl} \right)
\]

where \( k^s \) is the secant bulk modulus which is constant when the plastic deformation is assumed incompressible as observed in most metals. Actually, plastic incompressibility produces zero
hydrostatic plastic strain and thus, the total hydrostatic strain pertains totally to the elastic part. Consequently, the secant bulk modulus becomes independent of the plastic strain accumulation and is related only to the initial elastic modulus. This, however, is applicable for the case of multi-dimensional problems which is not involved in the present work. In contrast, the secant shear modulus $\mu^s$ is calculated at each step of the loading path and it can be related to the von Mises equivalent stress $\sigma_{eq}$ and equivalent strain $\varepsilon_{eq}$ as follows (where the indices $e$ and $q$ do not identify tensors but only the equivalent stress and strain scalar quantities):

$$\mu^s = \frac{\sigma_{eq}}{3\varepsilon_{eq}^{eq}}, \quad \varepsilon_{eq} = \sqrt{2\varepsilon_{eq}^{d} \varepsilon_{ij}^{d}} / 3$$

(3.19)

where $\varepsilon_{ij}^{d}$ denotes the deviatoric part of the total strain.

### 3.4.2 Incremental Method

The incremental formulation of the secant modulus, that relates the incremental stress tensor to the incremental strain tensor, can be obtained by differentiating both sides of Eq.(3.17) with respect to the strain as follows:

$$E^T_{ijkl} = \frac{\partial \sigma_{ij}}{\partial \varepsilon_{kl}} = E_{ijkl} + \frac{\partial E^s_{ijmn}}{\partial \varepsilon_{kl}} \varepsilon_{mn}$$

(3.20)

Differentiating Eq.(3.18) with respect to the total strain leads to the following relation:

$$\frac{\partial E^s_{ijmn}}{\partial \varepsilon_{kl}} = 2 \frac{\partial \mu^s}{\partial \varepsilon_{kl}} \left( \delta_{im} \delta_{jn} - \frac{1}{3} \delta_{ij} \delta_{mn} \right)$$

(3.21)

Using the chain rule, the differentiation of the secant shear modulus with respect to the strain tensor is given as follows:

$$\frac{\partial \mu^s}{\partial \varepsilon_{kl}} = \frac{\partial \mu^s}{\partial \varepsilon_{eq}} \frac{\partial \varepsilon_{eq}}{\partial \varepsilon_{kl}}$$

(3.22)

where

$$\frac{\partial \varepsilon_{eq}}{\partial \varepsilon_{kl}} = \frac{2 \varepsilon_{eq}^{d} \left( \frac{\partial \varepsilon_{eq}^{d}}{\partial \varepsilon_{eq}} \right)}{3 \varepsilon_{eq}^{eq}} = \frac{2 \varepsilon_{eq}^{d}}{3 \varepsilon_{eq}^{eq}}$$

(3.23)

The final expression of the incremental secant modulus may by obtained by substituting Eqs. (3.21) and (3.18) into Eq.(3.20) after making use of Eqs.(3.22) and (3.23) as follows:
\[ E_{ijkl}^T = k \delta_{ij} \delta_{kl} + 2 \mu \left( \delta_{ik} \delta_{jl} - \frac{1}{3} \delta_{ij} \delta_{kl} \right) + \frac{4}{3\varepsilon_{eq}} \left( \frac{\partial \mu}{\partial \varepsilon_{eq}} \right) \varepsilon_{ijkl} \varepsilon_{ijkl} \]  

(3.24)

As obvious from the definition of both secant and incremental moduli, the temperature effect on the elastic modulus is not included in this work since we are concerned only about the plastic deformation of AL-6XN. For the same reason, a comparison between the two methods is not considered here and thus, only the secant method is selected to calculate the true-stress true-strain curves for the present material at various strain rates and temperatures.

### 3.4.3 Unidirectional Secant Modulus for AL-6XN

The experimental comparison of the present work is limited to the unidirectional case of deformation because of the limited experimental results in the literature at high strain rates and temperatures for the material under investigation. The basic idea in relating the plastic strain \( \varepsilon^p \) to the total strain \( \varepsilon \) is obtained from the following relation that relates the total stress to the elastic and total strains using the elastic and secant moduli respectively:

\[ \sigma = E_o \varepsilon^e = E^e \varepsilon \]  

(3.25)

thus,

\[ \varepsilon^p = \left( 1 - \frac{E^e}{E_o} \right) \varepsilon = X_1 \varepsilon \]  

(3.26)

where \( E_o \) is the elastic modulus and the scalar variable \( X_1 \), defined above varies with the change of the secant modulus with both stress and strain. Utilizing Eqs.(3.5) and (3.26) together with the use of Eqs. (3.6), (3.7), (3.8) and (3.9), the unidirectional secant modulus for AL-6XN is obtained using the following relation:

\[ E^e = Y_o \varepsilon^{-1} + \hat{Y} X_2 \varepsilon^{-1} + B_1 X_1^n \varepsilon^{n-1} + B_2 X_3 \varepsilon^n \varepsilon^{n-1} \]  

(3.27)

where \( X_2 \) and \( X_3 \) represent the yielding and hardening temperature and strain effects scalar variables respectively which are defined as follows:

\[ X_2 = \left( 1 - \left( \beta_1 T - \beta_2 T \ln \dot{\varepsilon}_p \right)^{1/q} \right)^{1/p} \]  

(3.28)

\[ X_3 = \left( 1 - \left( \beta_1 T - \beta_2 T \ln \dot{\varepsilon}_p \right)^{1/q} \right)^{1/p} \]  

(3.29)

The numerical values of the material parameters shown in Eq.(3.27) are the same as those found in Eq.(3.11) and the adiabatic temperature is calculated similarly as defined in Eq.(3.12). Since the variable \( X_1 \) is a function of the secant modulus, therefore Eq.(3.27), is a nonlinear relation and thus, it should be solved numerically. In addition, the values of the elastic
modulus at different temperatures are measured directly from the experimental stress-strain results for the AL-6XN alloy material investigated by Nemat-Nasser et al., (2001).

The plastic deformation of the AL-6XN stainless steel is calculated using the secant modulus defined in Eq.(3.27). The results are then compared to the experimental results obtained for both low and high strain rates and elevated temperatures. The adiabatic stress-strain curves shown in Figs. 3.9 and 3.10 illustrate the very good correlation between the results predicted by the proposed model and the experimental results presented by Nemat-Nasser et al. (2001) at 3500s\(^{-1}\) strain rate and for different initial temperatures.

Figure 3.9  Adiabatic stress-strain curves predicted by the proposed model, for AL-6XN stainless steel, and compared to the experimental results at 3500 s\(^{-1}\) strain rate and for different initial temperatures.

On the other hand, Figs. 3.11 and 3.12 show the isothermal stress-strain curves calculated by the proposed model which agrees well with the experimental results given by Nemat-Nasser et al. (2001) for the 77K to 1000K range of temperatures and 0.1s\(^{-1}\) and 0.001s\(^{-1}\) strain rates respectively. The proposed model is further verified by comparing the adiabatic stress-strain results predicted by Eq.(3.27) to the other independent tests performed at 8300s\(^{-1}\) strain rate and various initial temperatures. The comparison, generally, shows very good agreement as displayed in Fig.3.13.
Figure 3.10 Adiabatic stress-strain curves predicted by the proposed model, for AL-6XN stainless steel, and compared to the experimental results at 3500 s\(^{-1}\) strain rate and for different initial temperatures.

Figure 3.11 Isothermal stress-strain curves predicted by the proposed model, for AL-6XN stainless steel, and compared to the experimental results at 0.1 s\(^{-1}\) strain rate and for different temperatures.
Figure 3.12 Isothermal stress-strain curves predicted by the proposed model, for AL-6XN stainless steel, and compared to the experimental results at 0.001 s\(^{-1}\) strain rate and for different temperatures.

Figure 3.13 Adiabatic stress-strain curves predicted by the proposed model, for AL-6XN stainless steel, and compared to the experimental results at 8300 s\(^{-1}\) strain rate and for different initial temperatures.
Although the present work is only addressing the unidirectional characterization of the plastic deformation, the multi-dimensional problem can similarly be treated using the secant, Eq.(3.18), or the incremental, Eq.(3.24), tensors along with a proper definition for the loading function. Since the plastic flow stress presented here is a rate dependent, the consistency viscoplastic model developed by Wang (Wang, 1997; Wang et al., 1997) is found more suitable than others in incorporating such a rate dependent yield surface. Moreover, finite deformation analysis should also be considered for the case of large deformation problems (see for example the work of Valanis, 1990; Clayton & McDowell, 2003; Tsakmakis, 2004). This subject is addressed in chapter 7.
CHAPTER 4

A CONSISTENT MODIFIED ZERILLI-ARMSTRONG FLOW STRESS MODEL FOR ELEVATED TEMPERATURES

4.1 Introduction

Large deformation problems, such as high speed machining, impact, and various primarily metal forming operations, require constitutive models that are widely applicable and capable of accounting for complex path of deformation, temperature, and strain rate. The degree of success of any model mainly depends on: (1) the physical basis used in the derivation process producing material parameters that are related directly to the nano-/micro-physical quantities; (2) the flexibility and simplicity of determining material constants from a limited set of experimental data; (3) capturing the important aspects of static and/or dynamic behavior besides being mathematically and computationally accurate. In dynamic problems that introduce high strain rates, the dynamic yield stress is considered the most important expression needed to characterize the material behavior and is also used in finite element codes.

In this regard, the dislocation-mechanics-based constitutive relation for material dynamics calculations developed by Zerilli and Armstrong [1] is considered as one of the most widely used models that have been implemented in many finite element dynamic codes (ABAQUS, DYNA, and others) and used by many authors in different types of low and high strain rates and temperature-related applications (see, for example, [2,3]). Other authors [4-6] reviewed and evaluated the predicted inaccuracies as well as the inconsistencies of the Z-A model when compared to experimental results for different bcc and fcc metals. Yet, no one investigated the impact on the model due to these inconsistencies as well as the model physical basis. The Z-A model incorporates strain, strain rate and temperature dependence in a coupled manner. This model is used in high rates of loading based computer codes. In the Z-A model, the concept of thermal activation analysis for overcoming local obstacles to dislocation motion as well as the dislocations interaction mechanisms are used in deriving two different relations for two different classes of metal crystal structures; body centered cubic (bcc) and face centered cubic (fcc). The differences between the two forms mainly ascribe to the dislocation characteristics for each particular structure. Fcc metals show stronger dependence of the plastic strain hardening on temperature and strain rate. Such effect, however, is mainly captured by the yield stress in most bcc metals. In other words, the thermal flow stress component, which has the coupling effect of both temperature and strain rate, pertains mainly to the yield stress in bcc metals and to the hardening stress in fcc metals. That is to say, the cutting of dislocation forests is the principal mechanism in fcc metals and the overcoming of Peierls-Nabarro barriers is the principal mechanism in bcc metals.

In spite of the Z-A model physical basis, it is found that the definition of the material parameters as related to the microstructure physical quantities is inaccurate. These material parameters lose their physical meaning when used for high temperature and strain rate applications. This is mainly attributed to the use of certain mathematical expansions in the
derivation of the model, as will be discussed later, in simplifying the physical relations of the model parameters. Furthermore, the assumption of using an exponential function in describing the coupling effects of temperature and strain rate on the flow stress produces another inconsistency to the model in spite of the good experimental fitting for some cases of loading. The Z-A model in its current form is not able to capture the athermal temperature, which is a critical value that defines the vanishing stage of the thermal stress. At this critical temperature, the plastic flow stress pertains totally to the athermal component.

The objective of this chapter is to investigate the physical basis of the Z-A constitutive relations and to modify the physical interpretation of the model parameters by introducing validated constitutive relations with material parameters that are related accurately to the nano-/micro-physical quantities. Since the proposed model in this work follows the same physical basis as the Z-A model, a detailed discussion about the physical basis as well as the procedure used in deriving the Z-A relations is given in section 4.2. In section 4.3, the physical interpretation of the Z-A model parameters is investigated and consequently modified relations are proposed. Applications of the proposed modified model for different metals at low and high strain rates and temperatures are performed in section 4.4. Comparisons are also made of the proposed model with both the Z-A model and the experimental results.

4.2 Physical Basis of the Z-A Model

Z-A model is basically derived based on dislocation mechanisms which in fact play a main role in determining the inelastic behavior of a metal and its flow stress under different load conditions. The derivation of the aforementioned dislocation basis model uses Orowan’s equation [7] that defines the dislocation movement mechanisms by relating the equivalent plastic strain rate \( \dot{\varepsilon}_p \) to the density of the mobile dislocations \( \rho_m \), dislocation speed \( v \), and the magnitude of the Burgers vector \( b \) as follows:

\[
\dot{\varepsilon}_p = \tilde{m} b \rho_m v
\]  

(4.1)

where \( \tilde{m} = \left(2 M_{ij} M_{ij} / 3\right)^{1/2} \) can be interpreted as the Schmidt orientation factor and \( M_{ij} \) is the average Schmidt orientation tensor which relates the plastic strain rate tensor \( \dot{\varepsilon}_p \) at the macroscale to the plastic shear strain rate \( \dot{\gamma}^p \) at the microscale as follows:

\[
\dot{\varepsilon}_p = \dot{\gamma}^p M_{ij} = \frac{\dot{\gamma}^p}{2} \left(n_i \otimes v_j + v_i \otimes n_j\right)
\]  

(4.2)

where \( \hat{n} \) and \( \hat{v} \) denote the unit normal on the slip plane and the unit vector in the slip direction respectively. The average dislocation velocity \( v \) can be determined through thermal activation by overcoming local obstacles to dislocation motion. Many authors have introduced velocity expressions for thermally activated dislocation glides (see, for more details, [8-11]). In this regard, the following general expression is utilized:
where \( v_o = 3d \omega \) is the reference dislocation velocity, \( d \) is the average distance the dislocation moves between the obstacles, \( \omega \) is a frequency factor which represents the reciprocal of the waiting time \( t_w \) needed for the dislocation to overcome an obstacle, \( G \) is the shear stress-dependent free energy of activation which may depend not only on stress but also on temperature and the internal structure, \( k \) is the Boltzmann’s constant, and \( T \) is the absolute temperature.

The activation energy \( G \) is expressed in terms of the thermal component of the shear stress \( \tau_{th} \) such that:

\[
G = G_o - \int_0^{\tau_{th}} V \, d\tau'_{th}
\]

where \( G_o \) is the reference Gibbs energy at \( T = 0 \) and \( V^* \) is the activation energy volume which is widely alluded to in the literature as a measure of the Burgers vector \( b \) times the area \( A^* \) swept out by dislocations during the process of thermal activation. At fixed strain rate, the thermal stress diminishes and approaches zero as the temperature increases and reaches critical values. In consequence, the required activation energy \( G \) increases until it approaches its maximum value, \( G_o \), as implied by Eq.(4.4). A mean value of the activation volume \( V \) may be used to characterize the thermal activation process such that [1]:

\[
V = \langle V^* \rangle = \left( \frac{1}{\tau_{th}} \right) \int_0^{\tau_{th}} V \, d\tau'_{th}
\]

Kocks et al. [12] introduced an empirical definition for the activation energy related to the thermal shear stress as follows:

\[
\tau_{th} = \hat{\tau} \left( 1 - \left( G / G_o \right)^{1/q} \right)^{1/p}
\]

where \( \hat{\tau} \) is the threshold shear stress at which the dislocations can overcome the barriers without the assistance of thermal activation. The exponents \( p \) and \( q \) are constants defining the shape of the short-range barrier where their values are within the following ranges \((0.0 < p < 1.0)\) and \((1.0 < q < 2.0)\). According to Kocks [13], the typical value of the constant \( q \) is 2 that is equivalent to a triangle obstacle profile near the top whereas the typical value of the constant \( p \) is 1/2, which characterizes the tail of the obstacle.

The thermal flow stress component, for metals in general, is determined, after making use of Eqs.(4.1)-(4.5), as follows:

\[
\sigma_{th} = \sigma_i \frac{A}{A} \left( 1 - \left( kT / G_o \right) \ln \left( \dot{\varepsilon}_{p} / \dot{\varepsilon}_{p0} \right) \right)
\]
Alternatively, Zerilli and Armstrong expressed the thermal flow stress in Eq.(4.7) using an exponential form in order to capture the experimental observation of some metals:

\[ \sigma_{th} = c_1 e^{-cT} \]  

(4.8)

where the physical material parameter \( c \) and the threshold stress \( c_1 \) (stress at zero Kelvin temperature) are defined as follows:

\[ c_1 = \frac{mG_o}{A_o b} \]  

(4.9)

\[ c = (1/T) \left[ \ln(A/A_o) - \ln(1+(kT/G_o) \ln(\dot{\varepsilon}_p/\dot{\varepsilon}_{po}) \right] \]  

(4.10)

where

\[ \dot{\varepsilon}_{po} = \dot{m} b \rho_{m} v_o \]  

(4.11)

In the above relation, \( A_o \) is the dislocation activation area at \( T = 0 \), \( m \) is the Taylor factor that relates the shear stress to the normal stress (\( \sigma = m \tau \)), and \( \dot{\varepsilon}_{po} \) is the reference equivalent plastic strain rate which represents the highest strain rate value as it is related to the reference dislocation velocity. It should be noticed here that Eq.(4.7) could be recovered simply by substituting Eq.(4.10) into Eq.(4.8) using the following mathematical relations

\[ \ln(a/b) = -\ln(b/a) = \ln a - \ln b \quad \text{and} \quad a = e^{\ln a} \]

Experimental observations show that the parameter \( c \) can be defined as follows [14]:

\[ c = c_3 - c_4 \ln(\dot{\varepsilon}_p/\dot{\varepsilon}_{po}) \]  

(4.12)

Hence, the constant material parameters of the Z-A model, \( c_3 \) and \( c_4 \), are related to the nano/micro-physical quantities by comparing Eq.(4.12) with Eq.(4.10) such that:

\[ c_3 = (1/T) \ln \left( A / A_o \right) \]  

(4.13)

\[ c_4 \ln(\dot{\varepsilon}_p/\dot{\varepsilon}_{po}) = (1/T) \ln \left( 1+(kT/G_o) \ln(\dot{\varepsilon}_p/\dot{\varepsilon}_{po}) \right) \]  

(4.14)

Complying with experimental observations in Eq.(4.12), Zerilli and Armstrong presumed the parameter \( c_3 \) as a constant by considering an implicit temperature dependence of the activation area \( A \). They also simplified Eq.(4.14) using the expansion \( \ln(1 \pm x) \approx \pm x \), where

\[ x = (-kT/G_o) \ln(\dot{\varepsilon}_p/\dot{\varepsilon}_{po}) \]

, in order to obtain a constant form for the parameter \( c_4 \) such that:

\[ c_4 = k / G_o \]  

(4.15)
The Z-A constitutive relations for bcc and fcc metals are then determined utilizing the concept of additive decomposition of the flow stress \((\sigma = (3\sigma_{ij}\sigma_{ij} / 2)^{1/2}\) for the von Mises case), into thermal \(\sigma_{th}\) and athermal \(\sigma_{ath}\) components:

\[
\sigma = \sigma_{th} + \sigma_{ath}
\]

(4.16)

The final form of the thermal and athermal flow stress relations, however, differs from one metal to another depending on their crystal structure. In turn, two different relations for two different types of metals were presented; body centered cubic (bcc) and face centered cubic (fcc).

### 4.2.1 Z-A Relation for BCC Metals

The behavior of most bcc metals such as pure iron, tantalum, molybdenum, and niobium shows a strong dependence of the thermal yield stress on the strain rate and temperature. Moreover, the activation volume \(V\) (and in turn, the activation area \(A\) since \(V = Ab\) where \(b\) is constant) is essentially independent of the plastic strain [14]. In other words, the plastic hardening of most bcc metals is hardly influenced by both strain rate and temperature. The thermal stress is then interpreted physically as the resistance of the dislocation motion by the Peierls barriers (short-range barriers) provided by the lattice itself. Thus, the thermal stress of the Z-A model is written from Eqs.(4.8)-(4.12) as follows:

\[
\sigma_{th} = c_1 \exp\left(-c_5 T + c_4 T \ln\left(\dot{\varepsilon}_p / \dot{\varepsilon}_{p0}\right)\right)
\]

(4.17)

where the material parameters \(c_1, c_3,\) and \(c_4\) are related to the microstructure physical quantities as given by Eq.(4.9), Eq.(4.13), and Eq.(4.15) respectively.

On the other hand, the athermal component of the plastic flow stress for bcc metals is mainly due to the hardening stress that is evaluated from an assumed power law \(c_7\dot{\varepsilon}_p^n\). In addition, an extra stress \(c_6\), which contributes to the athermal component of the flow stress, is attributed to the influence of solutes and the original dislocation density as well as the grain size effect. Thus, \(\sigma_{ath}\) can be defined as follows:

\[
\sigma_{ath} = c_7\dot{\varepsilon}_p^n + c_6
\]

(4.18)

Utilizing Eq.(4.16) together with the definitions given in Eq.(4.17) and Eq.(4.18), the final form of the Z-A constitutive relation for bcc metals is obtained as follows:

\[
\sigma = c_1 \exp\left(-c_5 T + c_4 T \ln\left(\dot{\varepsilon}_p / \dot{\varepsilon}_{p0}\right)\right) + c_7\dot{\varepsilon}_p^n + c_6
\]

(4.19)

Eq.(4.19) clearly shows the uncoupling between the plastic strain hardening and the effect of thermal softening and plastic strain-rate hardening for most bcc metals.
4.2.2 Z-A Relation for FCC Metals

Unlike the case for bcc metals, the thermal activation analysis for most fcc metals like copper and aluminum is strongly dependent on the plastic strain. This, actually, is attributed to the thermal activation energy mechanism which is controlled and dominated by the emergence and evolution of a heterogeneous microstructure of dislocations as well as the long-range intersections between dislocations. In this case, the activation area is related to the plastic strain as follows:

\[ A_o = A_o' \varepsilon_p^{-1/2} \]  \hspace{1cm} (4.20)

In turn, the Z-A thermal flow stress for the case of fcc metals is related to the plastic strain, plastic strain-rate and temperature such that:

\[ \sigma_{th} = c_2 \varepsilon_p^{1/2} \exp \left(-c_1 T + c_4 T \ln \left( \dot{\varepsilon}_p / \dot{\varepsilon}_{po} \right) \right) \]  \hspace{1cm} (4.21)

where the material constant \( c_2 \) is defined as:

\[ c_2 = m G_o / A_o' b \]  \hspace{1cm} (4.22)

The thermal component of the constitutive equation for the case of fcc metals clearly shows the coupling of temperature, strain rate, as well as the plastic strain. The athermal component \( c_6 \), however, is constant and independent of the plastic strain and it pertains totally to the initial yield stress, i.e., to the influence of solutes and the original dislocation density. The Z-A dislocation–mechanics-based constitutive relation for fcc metals is then written as follows:

\[ \sigma = c_2 \varepsilon_p^{1/2} \exp \left(-c_1 T + c_4 T \ln \left( \dot{\varepsilon}_p / \dot{\varepsilon}_{po} \right) \right) + c_6 \]  \hspace{1cm} (4.23)

Although the number of material constants in the fcc relation is less than in the corresponding bcc relation, the procedure steps for determining these constants are almost the same in both relations. The constants \( c_3 \) and \( c_4 \), however, share the same physical interpretation for the bcc and fcc relations.

4.3 Investigation and Modification of the Z-A Plastic Flow Relations

In investigating the physical interpretation of the Z-A constitutive relation parameters, two crucial points are noticed. First, the explicit definition of \( c_3 \) given by Eq.(4.13) clearly indicates that this parameter is not a constant, but rather a temperature dependent parameter. The only way to keep this parameter \((c_3)\) as a constant is when the relation between the activation area \( A \) and the Kelvin temperature \( T \) takes an exponential form which is not necessarily the case in general. Second, the assumption for the expansion given for \( \ln(1 \pm x) \approx \pm x \) in obtaining the parameter \( c_4 \) in Eq.(4.15) is not an accurate one since this expansion is valid only for values \( x \ll 1.0 \). The variable \( x = (G / G_o) = \left(-kT \ln \left( \dot{\varepsilon}_p / \dot{\varepsilon}_{po} \right) / G_o \right) \) is
actually both temperature and strain rate dependent. The percentage change between the exact and approximated $x$-values (initiated at $x \sim 0.1$) affects significantly the prediction of the flow stresses. This because the $x$-values are due to an exponential term that is already multiplied by a large stress number which is the threshold stress, $c_1$, for the bcc model, in Eq.(4.19), and the hardening value, $c_2 \varepsilon_n^i$, for the fcc model, Eq.(4.23).

As widely defined in the literature (see, for example, [15,16]), the numerical values of the reference Gibbs free energy, $G_0$, ranges between 0.6 to 1.0 eV/atom for most bcc metals and 1.5 to 2.5 eV/atom for fcc metals. In addition, the reference plastic strain rate $\dot{\varepsilon}_p$ values are of the order $10^5$ to $10^7$ s$^{-1}$ for most metals whereas, the Boltzmann’s constant $k$ value is taken as $8.62 \times 10^{-5}$ eV/K (1.3807×10^{-23} JK^{-1}). Thus, the numerical investigation of the variable $x$ using average values of the abovementioned quantities elucidates that $x$ increases and approaches the value of 1.0 when the temperature increases and the strain rate decreases as shown in Fig.4.1. It is clear that at strain rates up to $10^3$ s$^{-1}$, the numerical values of the $x$ variable exceeds 0.1 for relatively low temperatures (110-350K). Thus, the Z-A model is physically justified when it is used at temperature and strain rate combinations that fall in the region zone indicated below the horizontal dotted line ($x = 0.1$) shown in Fig.4.1. Conversely, at greater $x$ values (in the region above the aforementioned horizontal dotted line), the physical interpretation of the parameter $c_4$ given by the Z-A model becomes ineffective and does not reflect the real behavior. This, in turn, makes the model parameters appear to be more phenomenologically defined than physically based. Additionally, it is known that the considered mechanism becomes athermal (thermal stresses vanish) when the activation energy $G$ approaches its reference value $G_0$ (i.e., $x = 1.0$) at a critical temperature that is termed the athermal temperature ($T_{cr}$). The Z-A model, in turn, fails to disclose the above behavior since the only way for the thermal stress component to vanish is when $T \to \infty$ (due to the assumed exponential dependence of the temperature). This, in fact, makes the Z-A model physically inconsistent and clearly in contradiction with Eq.(4.4) which is used along with Eqs.(4.1) and (4.3) as the base of the thermal activation analysis.

Zerilli and Armstrong [1,17] applied their model to tantalum and OFHC copper as bcc and fcc metals respectively. they determined the material constants based on experimental results provided by other authors for low and high strain rates and temperatures. For tantalum, the material parameters are obtained from the strain-rate dependence of the lower yield stress at room temperature ($T=300K$) such that $c_4$ is equal to 0.000327 and for the case of OFHC copper is around 0.000115. Comparing the above numerical values of the parameter $c_4$ to its simplified definition given by Eq.(4.15) and using the constant value of $k$, the numerical values of $G_0$ are found to be around 0.26 eV/atom for tantalum and 0.75 eV/atom for OFHC copper. These values, however, are much lower than those obtained in the literature by many authors. For example, Hoge and Mukharjee [18] who provided the experimental results for tantalum used a value of 0.62 eV/atom in their modeling that is necessary to nucleate a pair of kinks. Moreover, Nemat-Nasser and Li [16] employed their experimental results in modeling the plastic flow of OFHC copper at low and high strain rates and temperatures by using a 1.75 eV/atom for the physical quantity $G_0$ (see also [19]). The deviations in $G_0$ between the value given by the Z-A model and that found in the literature is actually attributed to the adoption of the expansion $\ln(1 \pm x) \approx \pm x$ which actually directed the model derivation to match the experimental evidence given by Eq.(4.12).
Furthermore, the Z-A model does not really show an explicit form for the temperature dependence of the activation area. In contrast, the Z-A model introduced an implicit activation area dependence of the temperature through the definition of the material constant $c_3$. This constant value, however, exists only when the exponential relationship mentioned earlier between the temperature and the activation area is defined as

$$A = A_0 e^{c_3 T}$$

which clearly indicates that the effect of the strain rate on the activation area is not considered in the Z-A model. Such effect however, has been investigated by many authors (see, for more details, [20]). The activation area behaves predictably in terms of the effects of parameters such as dislocation density and solid solution concentration. In the classical studies of dislocation plasticity, the activation area is calculated based on the rate sensitivity of the flow stress measured using rate-change or stress relaxation experiments as discussed in [21,22]. The following definition, which depends on both temperature and strain rate effect, is considered one of the ways for measuring the activation area $A$:

$$A = kT / (b \partial \tau / \partial \ln \dot{\varepsilon}_p^*)$$

where $\dot{\varepsilon}_p^* = \dot{\varepsilon}_p / \dot{\varepsilon}_{p0}$. The above relation is used to calculate the activation volumes from the strain rate dependence of the flow stress at constant temperature as a function of the effective stress [17,18]. These activation volumes decrease with the increase of thermal stresses and are
much smaller than those obtained when the interaction mechanism is operative. It is found that the activation area for the fcc metal deformation is 10 to 100 times larger than those found in the deformation of bcc metals which is in the range of 5 to 100b^2.

Eventually, in order to have a solid physically based constitutive relation, an explicit definition is essential for the activation area in terms of temperature and strain rate in order to be used in the definition of the thermal stress given by Eq.(4.7). To the best knowledge, no such definition that is physically derived and explicitly related to both temperature and strain rate currently exists in the literature. At this moment, however, we suggest a new definition for the activation area which is derived utilizing Eq.(4.24) along with Eq.(4.6) after employing the typical values of the exponents p and q mentioned earlier such that:

\[
A = A_o \left(1 - \left((-kT / G_o) \ln \dot{\epsilon}_p^* \right)^{1/2}\right)^{-1} \tag{4.25}
\]

It is obvious from Eq.(4.25) that the activation area increases as the temperature evolves throughout the plastic deformation. Conversely, it decreases as the strain rate increases due to the insufficient time required for dislocations to move inside the lattice. Moreover, A approaches its reference value \(A_o\) at zero Kelvin temperature.

A similar definition for the activation area in Eq.(4.25) may be obtained by directly considering the same variation of the thermal stress with the activation energy given in Eq.(4.6) since the activation area is proportionally related to the threshold stress denoted by \(\hat{\tau}\) or by \(c_1\) as given in Eq.(4.9). This variation may exist at any loading and temperature stages. That is the stress is expected to be proportionally related to the activation area at any temperature, \(\sigma \propto 1/A\), as implied by Eq.(4.24).

In light of the explicit derived definition for the thermal stress along with the suggested temperature and strain dependence of the activation area given in Eq.(4.25), the Z-A constitutive relations are then redefined such that the physical definitions of the model parameters are appropriately justified and related to the nano/micro-structure quantities. These two proposed flow stress relations are defined for both bcc and fcc metals by the following Eqs.(4.26) and (4.27) respectively:

\[
\sigma = c_1 \left(1 - X^{1/2} - X + X^{3/2}\right) + c_5\dot{\epsilon}_p^n + c_6 \tag{4.26}
\]

\[
\sigma = c_5\dot{\epsilon}_p^{0.5} \left(1 - X^{1/2} - X + X^{3/2}\right) + c_6 \tag{4.27}
\]

where the variable \(X = x = (-kT / G_o) \ln \dot{\epsilon}_p^*\) or \(X = c_4T \ln(1/\dot{\epsilon}_p^*)\) and the physical parameters \(c_i\) are the same as previously defined.

Eqs.(4.26) and (4.27) may be used to predict the stress strain curves for both isothermal and adiabatic plastic deformations. For the case of adiabatic deformation, heat inside the material increases as plastic strain increases and therefore, the temperature \(T\) is calculated incrementally by assuming that the majority of the plastic work is converted to heat:
\[ T = \frac{\dot{\varepsilon}}{\varepsilon_p} \int \sigma d\varepsilon_p \quad (4.28) \]

Here \( \rho \) is the material density and \( c_p \) is the specific heat at constant pressure. The Taylor-Quinney empirical constant \( \chi \) is often assigned the values 0.9-1.0 (see, for more details, [23]).

Unlike the Z-A model, the proposed modified flow stress relations, clearly point out that the thermal stress component for both bcc and fcc metals, which is given by the first term on the right hand side of Eqs.(4.26) and (4.27) respectively, vanishes as the variable \( X \) approaches the value of 1 or, in other words, \( G \rightarrow G_0 \). This mechanism, however, coincides well with the thermal activation energy mechanism defined in Eq.(4.4). Based on that, the athermal or critical temperature, \( T_{cr} \) may be calculated by setting \( X = 1 \) such that:

\[ T_{cr} = \left( (-k / G_{0}) \ln(\dot{\varepsilon} / \dot{\varepsilon}_{po}) \right)^{-1} = \left( c_4 \ln(1 / \dot{\varepsilon}^*) \right)^{-1} \quad (4.29) \]

The above definition indicates clearly that \( T_{cr} \) is strain rate dependent and increases as the plastic strain rate increases as will be shown later in the model applications section.

**4.3.1 Further Modifications for the Proposed Model**

The plastic hardening for the proposed model, which is evaluated from an assumed power law dependence mentioned earlier, may alternatively be related to the forest dislocation density through the dislocation model of Taylor [24]. This gives the shear flow stress \( \tau \) in terms of the forest dislocation density \( \bar{\rho}_f \) where \( \bar{\rho}_f = \rho_f - \rho_i \) and \( \rho_i \) denotes the initial dislocation density encountered in the material due to the manufacture process or by nature

\[ \tau = \alpha \mu b \sqrt{\bar{\rho}_f} \quad (4.30) \]

where \( \alpha \) is an empirical coefficient taken to be 0.2 for fcc metals and about 0.4 for bcc metals as given by Nabarro et al. [25]. Nabarro pointed out that Eq.(4.30) can be derived by multiple methods. Ashby [26] splits the difference of the \( \alpha \) values in assuming that \( \alpha = 0.3 \) for most metals. Kubin and Estrin [27] proposed the following set of two coupled differential equations to describe both forest \( \rho_f \) and mobile \( \rho_m \) dislocation density evolutions with plastic strain as follows:

\[ \frac{d\rho_m}{d\varepsilon_p} = \frac{\lambda_1}{b^2} - \lambda_2 \rho_m - \frac{\lambda_3}{b} \rho_f^{1/2} \]

\[ \frac{d\rho_f}{d\varepsilon_p} = \lambda_2 \rho_m + \frac{\lambda_5}{b} \rho_f^{1/2} - \lambda_4 \rho_f \quad (4.31) \]
where the constant coefficients $\lambda_i$ are related to the multiplication of mobile dislocations ($\lambda_1$), their mutual annihilation and trapping ($\lambda_2$), their immobilization through interaction with forest dislocations ($\lambda_3$), and to the dynamic recovery ($\lambda_4$). Klepaczko [28] showed that the growth of dislocation density is nearly linear with regard to the deformation in the first steps of the hardening process, independently of the temperature. This is followed by a recombination of the dislocations that are assumed to be proportional with the probability of dislocation meeting, that is to say of the forest dislocation density. Based on this hypothesis, the following simple relation for the evolution of the forest dislocation density $\rho_f$ was presented:

$$\frac{d\rho_f}{d\varepsilon_p} = M - K_a \rho_f$$

(4.32)

where $M$ is the multiplication factor and $K_a$ is the dislocation annihilation factor which may depend on both temperature and strain rate. Klepaczko and Rezaig [29] showed that for mild steels, both $M$ and $K_a$ could be assumed constant at not so high strain rates and up to the temperature where the annihilation micromechanisms (recovery) start to be more intense. On this basis, the hardening stress for metals may be expressed in terms of the internal physical quantities by substituting the plastic strain evolution of the forest dislocation density Eq.(4.32), after proper integration, into the Taylor definition Eq.(4.30) as follows:

$$B\varepsilon_p^n \approx \overline{B} \left(1 - \exp(-k_a \varepsilon_p) \right)^{1/2}$$

(4.33)

where $\overline{B}$ is the hardening parameter defined as

$$\overline{B} = m \alpha \mu b \left( M / k_a \right)^{1/2}$$

(4.34)

In order to enable one to compare with Z-A model, the above modification for the hardening stress, Eq.(4.33), will not be used in the present application. In addition, the following comparisons will be mainly focusing on the physical justification of the thermal parameters $c_3$ and $c_4$ as well as on the correlation of both the Z-A and the proposed models with the experimental results at different strain rates and temperatures.

4.4 Applications, Comparisons, and Discussion

The modified constitutive relations derived in the previous section for bcc, and fcc metals are evaluated by direct comparison with the experimental results that are provided by several authors for different types of metals and conducted over a wide range of strain rates and temperatures. The evaluation of the material parameters of the proposed model is first initiated by studying the stress-temperature relation at different values of plastic strain and at certain strain rate values. Various numerical techniques can be used to determine the material parameters of the proposed model. However, the Newton-Raphson technique is applied for both bcc and fcc relations utilizing the available experimental results at different strain rates and temperatures. The material constants of the proposed relations (Eq.(4.26) and Eq.(4.27))
and the Z-A relations (Eq.(4.19) and Eq.(4.23)) are listed in Table 4.1 for both OFHC copper and Tantalum. Applications as well as comparisons to the available experimental data for OFHC Copper (fcc) and Tantalum (bcc) using the same material constants are then illustrated. The proposed model is further applied to other bcc metals such as Vanadium and Niobium.

Table 4.1 Parameters of OFHC Cu and Ta for the proposed and Z-A models.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>OFHC Copper</th>
<th>Tantalum</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_1$ (Mpa)</td>
<td>-</td>
<td>1125</td>
</tr>
<tr>
<td>$c_2$ (Mpa)</td>
<td>970</td>
<td>980</td>
</tr>
<tr>
<td>$c_i + k \ln \dot{\varepsilon}_p / G_o$</td>
<td>-</td>
<td>2.8×10^{-3}</td>
</tr>
<tr>
<td>$c_4$ (K^{-1})</td>
<td>3.55×10^{-5}</td>
<td>1.15×10^{-4}</td>
</tr>
<tr>
<td>$\dot{\varepsilon}_p$ (s^{-1})</td>
<td>1.76×10^{8}</td>
<td>-</td>
</tr>
<tr>
<td>$c_5$ (Mpa)</td>
<td>-</td>
<td>300</td>
</tr>
<tr>
<td>$c_6$ (Mpa)</td>
<td>50</td>
<td>65</td>
</tr>
<tr>
<td>$N$</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Figure 4.2 Adiabatic and isothermal stress-strain curves for the proposed model, for OFHC copper, as compared to experimental results [1] and the Z-A model at various strain rates and temperatures.
4.4.1 Application to OFHC Copper (Cu)

The Oxygen Free High Conductivity (OFHC) Copper is used here as an application for the proposed fcc model to show the temperature and strain rate variation of the flow stress. The material parameters of the proposed model, Eq.(4.27), and the Z-A model, Eq.(4.23), are obtained from essentially the same data base found in [30]. The predicted flow stresses, generally, agree well with most experimental data for several strain rates and temperatures. In Fig.4.2, the adiabatic stress-strain calculated using both models predicts good results as compared to the same experimental data. The modified model, however, shows better correlations with the experimental results at higher temperatures (T=730K). On the other hand, both models underestimate the isothermal stress-strain as compared with the experimental results at room temperature.

A further assessment of the proposed model as well as the Z-A model is made, using the same material constant, by comparing the adiabatic and isothermal stress-strain results to other experimental data presented in [16,31] as shown in Fig.4.3 and Fig.4.4 respectively. Results obtained using the proposed model compare well with both experimental data at low and high temperatures (77-1000K\(^\circ\)) and the indicated high strain rates (4000s\(^{-1}\) and 6000s\(^{-1}\)). The adiabatic flow stresses computed by Z-A model, nevertheless, fail to match the experimental results at temperatures greater than 300K\(^\circ\). These predictions, as a point of fact, underestimate the experimental results at high temperatures due to the exponential stress-temperature relationship assumed in the derivation process of the Z-A model.

![Figure 4.3 Adiabatic stress-strain curves for the proposed model, for OFHC copper, as compared to experimental results [16] and the Z-A model at 4000s\(^{-1}\) strain rate and different initial temperatures.](image-url)
Figure 4.4 Adiabatic and isothermal stress-strain curves for the proposed model, for OFHC copper, as compared to experimental results [31] and the Z-A model at different strain rates and room temperature.

For OFHC copper, the adiabatic stress strain curves predicted by the proposed model are obtained based on the assumption of conversion of 90% of the plastic work using the formula defined in Eq.(4.28). Moreover, the specific heat and the material densities are chosen to be 0.383J/g.K° and 8.96g/cm³ respectively.

4.4.2 Application to Tantalum (Ta)

Similar to the Z-A model, the experimental data presented in [18] is utilized here in determining the material constants for the proposed model. The temperature variation of the flow stress obtained experimentally by Hoge & Mukharjee (1977) at 0.014 strain and 0.0001s⁻¹ strain rate is compared with the results computed using both the present model Eq.(4.26) and the Z-A model Eq.(4.19). The proposed model as well as the Z-A model predicts results that agree very well with experimental data as shown in Fig.4.5. The stress variation with strain rates at room temperature computed using both models is compared with the same experimental data. The comparisons illustrated in Fig.4.6 show very good agreement with the experimental results.

The results of both models simulations are also compared with other set of experimental data [15] at 5000s⁻¹ strain rates and elevated temperatures (up to 798K°) as shown in Fig.4.7. The adiabatic stress-strain relations predicted by the proposed model show very good
agreement at all indicated temperatures whereas, the Z-A model fails again to correlate well with other set of experimental results particularly at higher temperatures in spite of the good agreement with the experimental data used in obtaining the model constants. This, in reality, is mainly attributed to the fitted hardening parameters which are affected indirectly by the exponential stress-temperature relationship used in the Z-A model for modeling the thermal yield stresses.

![Stress-temperature results for the proposed and Z-A models, for Tantalum (Ta), as compared with experimental data [18] at 0.0001s\(^{-1}\) strain rates.](image)

Figure 4.5 Stress-temperature results for the proposed and Z-A models, for Tantalum (Ta), as compared with experimental data [18] at 0.0001s\(^{-1}\) strain rates.

In the case of bcc metals, the temperature and strain rate effects emerge clearly at the starting point (initial yielding) of the stress-strain curves whereas, the hardening stress is independent of both temperature and strain rate effects. Therefore, the predicted stress strain curves using the proposed and Z-A models will depend completely on the accuracy of determining the hardening parameters. Moreover, the hardening parameters control the adiabatic stress strain curves by assuming 90% of the plastic work is converted into heat where the temperature evolution is calculated using Eq.(4.28). The specific heat and the material density values for tantalum are chosen to be 0.139J/g.K\(^{\circ}\) and 16.62g/cm\(^3\) respectively.
Figure 4.6 Stress versus strain rates results for the proposed and Z-A models, for Tantalum, as compared to experimental data [18] at room temperature.

Figure 4.7 Adiabatic stress-strain curves for the proposed model, for Tantalum, as compared to experimental data [15] and the Z-A model at 5000s⁻¹ strain rate and different initial temperatures.
4.4.3 Discussion

It is obvious from the proposed model as well as the Z-A model that the thermal component of the flow stress is nearly the same for both bcc and fcc metals. However, the model parameters values and accordingly the physical quantities differ from metal to metal. The physical quantities for OFHC copper and tantalum may be defined after making use of the numerical values of the material constants defined in Table 4.1. For the proposed model, it is found that the Gibbs free energy for Cu ($G_o \approx 2.4$ eV/atom) is higher than the value assigned for tantalum ($G_o \approx 0.9$ eV/atom). This, in fact, is due to the two different thermal activation mechanisms for each metal structure which indicates that the dislocation interaction mechanism necessitates higher activation energy than the Peierls mechanism in overcoming the short-range barriers. The numerical values of $G_o$, however, fall in the same range used in the literature that is mentioned in the previous section.

In general, most metals contain an initial amount of dislocations which are naturally exited or generated through the manufacturing process. These dislocation densities, however, help metals deform plastically until a level where no further dislocation generation is allowed which indicates that the saturation limit of dislocation densities is reached. The initial and saturated values of the dislocation densities, however, differ from metal to metal (see, for more details, [19]). In this work, the mobile dislocation density evolution with the plastic accumulations is not considered and rather an average value of the mobile dislocation density is assumed for both models.

The reference plastic strain rate values obtained for both OFHC copper and tantalum, listed in Table 4.1, are justified by adopting reasonable quantities for the nano/micro-physical parameters. On this basis, the average mobile dislocation densities are found to be in the order of $10^{14}$ m$^{-2}$ for OFHC Cu and $10^{13}$ for Ta. The rational for the differences of $\rho_m$ values in the two materials mainly depends on the dislocation characteristics and interaction mechanisms for each particular structure. It should be noted also that these values are a portion of the total dislocation densities which in addition, include the forest dislocation densities introduced through the hardening parameters. The numerical quantities of the reference velocity ($\dot{\epsilon} = d / t_w$), on the other hand, show lower values for OFHC Cu $O(10^3 s^{-1})$ than Ta $O(10^2 s^{-1})$ since the waiting time $t_w$ needed by the dislocation to overcome an obstacle for the case of fcc metals is higher than the time required in bcc metals [12]. The average values of the Burgers vector are taken as 2.5Å and 2.9Å for OFHC copper and tantalum respectively.

The material constants of the Z-A model for both OFHC Cu and Ta found in [1,17] show some difficulty in trying to relate their numerical values to the nano/micro-physical quantities particularly for the interpretation of the ($c_3 + k \ln \dot{\epsilon}_{p0} / G_o$) constant values listed in Table 4.1. This, as discussed in section 4.3, is due to the improper definition of $c_3$ that is related to the activation area $A$ which is, in fact, a temperature and strain rate dependent parameter as explained in the previous section. Finally, one should admit here that the procedure followed in determining the material constants is found easier for the case of the Z-A model than the one used for the proposed modified model. This, in fact, is at the cost of the accuracy of the physical interpretation for the material parameters.
4.4.4 Application to Other BCC Metals

The proposed model is further verified by comparing the adiabatic stress strain results predicted by Eq.(4.26) to the experimental data of other bcc metals such as Vanadium (V) and Niobium (Nb) conducted at high strain rates and for a wide range of temperatures [32,33]. The material constants for V and Nb are determined using the same procedure followed in Ta and listed in Table 4.2.

Table 4.2 Parameters of V and Nb for the proposed model.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Vanadium</th>
<th>Niobium</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_1$ (Mpa)</td>
<td>945</td>
<td>945</td>
</tr>
<tr>
<td>$c_4$ (K$^{-1}$)</td>
<td>$1.392 \times 10^{-4}$</td>
<td>$1.49 \times 10^{-4}$</td>
</tr>
<tr>
<td>$\dot{\varepsilon}_{\rho_0}$ (s$^{-1}$)</td>
<td>$6.32 \times 10^6$</td>
<td>$7.07 \times 10^6$</td>
</tr>
<tr>
<td>$c_5$ (Mpa)</td>
<td>305</td>
<td>440</td>
</tr>
<tr>
<td>$c_6$ (Mpa)</td>
<td>60</td>
<td>60</td>
</tr>
<tr>
<td>$N$</td>
<td>0.16</td>
<td>0.25</td>
</tr>
</tbody>
</table>

Figure 4.8 Adiabatic stress-strain curves for the proposed model, for Vanadium, as compared to experimental data [32] and the Z-A model at 2500s$^{-1}$ strain rate and different initial temperatures.
The comparisons between the proposed model and the experimental results for the three indicated metals show very good agreement for most loading conditions as displayed in Figs. 4.8 and 4.9. For all of these three metals, a conversion of 100% of the plastic work is considered in computing the adiabatic stress strain curves. The incremental evolution of the absolute Kelvin temperature is obtained, after making use of Eq.(4.28), by employing the specific heat values of 0.498 J/g.K° and 0.265 J/g.K° and the material density values of 6.16 g/cm³ and 8.57 g/cm³ for both Vanadium and Niobium respectively. It should be mentioned here that the damage mechanism is not considered in this work and therefore, the softening behavior captured by the proposed modified models are due to the adiabatic deformation from which the temperature evolves inside the material with the accumulation of the plastic work.

![Figure 4.9 Adiabatic stress-strain curves for the proposed model, for Niobium, as compared to experimental data [33] and the Z-A model at 3300s⁻¹ strain rate and different initial temperatures.](image)

**4.4.5 Evaluation of the Critical Temperature $T_{cr}$.**

Ignoring of the athermal behavior of the thermal activation mechanism for certain temperatures is considered one of the major inconsistencies that the Z-A model suffers due to the assumptions mentioned earlier. The proposed model, on the other hand, is able to introduce this behavior through a strain rate dependent relation of the critical temperature $T_{cr}$ as defined in Eq.(4.34). In fact, $T_{cr}$ is defined as the highest temperature value that corresponds to the
minimum thermal stresses (zero thermal stress) observed during the degradation process of the flow stress as the material temperature increases. Fig. 4.10 shows the strain rate variation of $T_{cr}$ calculated using Eq. (4.34) for the four metals used in this study. It is found that $T_{cr}$ values increase with strain rates increase. Also, the critical temperature value for OFHC Cu is higher than those obtained for the three bcc metals. This disparity may be attributed to the variation of the reference plastic strain rate $\dot{\varepsilon}_{po}$ values and also to the different $c_4$ values that is mainly related to the Gibbs free energy $G_o$.

The variation of $T_{cr}$ results within the three bcc metals is mainly ascribed to the variation of $G_o$ values since the $\dot{\varepsilon}_{po}$ values are approximately of the same order. The higher the reference activation energy values (0.90, 0.62, 0.58 eV/atom for Ta, V, and Nb respectively) needed to overcome the barriers the higher the critical temperature values achieved. Actually, the thermal stress is interpreted as the resistance of the barriers to the dislocation movement, thus, the barriers that need higher activation energy to be overcome require also higher temperature to produce this thermal energy until the resistance of these barriers is completely vanished which indicates zero thermal stresses.

![Figure 4.10 Strain rate variation of the critical temperatures predicted using the proposed model for different types of metals.](image.png)
CHAPTER 5

EFFECT OF DISLOCATION DENSITY EVOLUTION ON THE THERMOMECHANICAL RESPONSE OF METALS WITH DIFFERENT CRYSTAL STRUCTURES

5.1 Introduction

The plastic flow stress for relatively pure metals is determined through the interaction of dislocations, which are moving inside the crystal lattice, with the lattice itself and with the available barriers encountered inside the lattice. Ashby and Frost (1975) pointed out that dislocation motion through the lattice or past an obstacle require the surmounting of an energy barrier by a combination of applied stress and thermal activation. Thus, at the microscale level, the mechanisms associated with dislocation motion and dislocation multiplication, the statistics of mobile dislocation populations, the nature and the statistics of obstacle distributions and the relationship between the externally imposed plastic strain rate and the dislocation kinetics determine the form of the macroscopic plastic response. Moreover, the crystal lattice configuration plays a crucial role in determining the effect of thermal activation on the mechanical response of relatively pure metals which are mainly classified into three common crystal types; body centered cubic (bcc), face-centered cubic (fcc) and hexagonal-close-packed (hcp). Each of these three crystal structures exhibits a characteristic thermomechanical behavior which is associated with the available slip systems and symmetries as well as the nature of dislocation cores. Good reviews of plastic deformation in different crystal structure types of metals are provided by Kubin (1982), Christian (1983), Taylor (1992), Vitek and Duesbury (1998), Chichili et al. (1998), Nemat-Nasser et al. (1999) and Lennon and Ramesh (2004).

A great deal of effort has been investigated in understanding the influence of temperature and strain rate on the flow stress of different structure types of metals. This understanding, however, is essential for the modeling and analysis of numerous processes including high-speed machining, impact, penetration and shear localization. Recently, considerable progress has been made in understanding the role of rate controlling dislocation mechanisms on the temperature and strain rate dependence of the flow stress for metals and alloys. Hoge and Murkherjee (1977) studied the effect of both temperature and strain rates on the lower yield stress of Tantalum as a bcc metal and proposed a model incorporating the combined operation of the Peierls’ mechanism and dislocation drag process. Zerilli and Armstrong (1987) used dislocation mechanics concept to develop a constitutive model that accounts for strain, strain rate and temperature in a coupled manner, which can be incorporated in computer codes for applications related to dynamic loading conditions. Their model considers two different forms for the two different classes of metals (bcc and fcc). The rational for the differences in the two forms mainly depends on the dislocation characteristics for each particular structure. Bcc metals show stronger dependence of the yield stress on temperature and strain rate while in the case of fcc metals the yield stress is mainly affected by strain hardening. In other words, the cutting of dislocation forests is the principal mechanism in fcc metals, while in bcc metals; the overcoming of Peierls-Nabarro barriers is the principal mechanism. Zerilli-Armstrong (Z-A)
model has been derived based on the concept of thermal activation analysis for overcoming local obstacles to dislocation motion. This model has been widely used in many computer codes from which its material parameters, as first believed, are physically interpreted. Very recently, Voyiadjis and Abed (2004) explained that the physical definitions of the Z-A model parameters are, in fact, not accurate because of the assumption made by using the expansion \( \ln(1 + x) = x \) in the model derivation. This expansion, however, is valid only for values \( x \ll 1.0 \) whereas, the definition of the variable \( x \) given by Z-A model indicates that its numerical value increases and approaches the value of one with strain rate and temperature increase. This, in turn, makes the Z-A parameters lose their physical meaning when they are used in high temperature and strain rate applications. In other words, by using the above mentioned expansion, the Z-A model derivation was directed to match the experimental evidence which shows that the temperature degradation of the flow stress can be fitted using an exponential form (see the paper of Voyiadjis and Abed, 2005 for more details).

Klepaczko (1987 & 1988) derived a constitutive model that is based on a consistent approach to the kinetics of macroscopic plastic flow of metals with bcc and fcc structures. His constitutive formalism was applied utilizing one state variable which is the total dislocation density and assuming that plastic deformation in shear is the fundamental mode in metal plasticity. Furthermore, he assumed that at constant microstructure, the flow stress consists of two components; the internal stress and the effective stress. The internal stress is developed by the long-range strong obstacles to dislocation motion whereas; the effective stress is due to thermally activated short-range obstacles. Unlike most experimental observations and theoretical interpretations, Klepaczko pointed out that for certain bcc or fcc metals, athermal and thermal flow stress components that are pertained to the resistance of long and short range barriers respectively are strain rate and temperature dependent. Klepaczko and his co-workers (Klepaczko & Rezaig, 1996 and Rusinek & Klepaczko, 2001) have successfully evaluated the material parameters of the derived constitutive model for different bcc and fcc metals and they were able to study the adiabatic shear banding in mild steel numerically.

Nemat-Nasser and his co-workers (e.g., Nemat-Nasser and Isaacs, 1997, Nemat-Nasser & Li, 1998, Nemat-Nasser et al., 1999, and Nemat-Nasser & Guo, 2000) developed an experimental technique measuring the flow stress of different bcc, fcc and hcp metals and alloys over a broad range of strains, strain rate, and temperatures in uniaxial compression. Some of their experimental results are, actually, used in this work for models evaluation and comparisons. They also presented a constitutive model that characterizes the plastic deformation of different metals and alloys using the thermal activation concept and assuming constant dislocation density throughout the deformation process. That is neither the plastic strain evolution of dislocation density nor the rate multiplication of the dislocation density evolution is considered.

Voyiadjis and Abed (2004) incorporated the production rate of dislocation density in modeling the plastic flow stress for both bcc and fcc metals using the concept of thermal activation analysis as well as the dislocation interaction mechanisms. Some of their models parameters are physically derived and related to the micro-structural quantities. Others, on the other hand, are defined empirically based on the experimental results. It was concluded that the contribution of mobile dislocation density rate to the plastic deformation modeling shows
considerable effect on the prediction of the flow stress particularly in the case of high strain rates and temperatures. Furthermore, Abed and Voyiadjis (2004) used a combination of their bcc and fcc models in characterizing the thermomechanical behavior of AL-6XN stainless steel over a wide range of temperatures and strain rates.

In this chapter, the effect of plastic strain evolution of dislocation density is utilized in determining the plastic flow stress of three major categories of metal structures; body centered cubic (bcc), face centered cubic (fcc), and hexagonal close packed (hcp) over a wide range of temperatures and strain rates. The proposed constitutive models are derived based on the concept of thermal activation analysis, dislocation interaction mechanisms, experimental observations, and the additive decomposition of flow stress to thermal and athermal components.

In section 5.2, the role of dislocation dynamics inside the crystal lattice in determining the general form of the thermal plastic stress is investigated using the well-known Orowans’ (1957) relation that considers the plastic deformation as a dynamic process obtained by the motion of dislocations with an average velocity. In turn, the plastic shear strain rate at the microscale is related to the plastic strain rate tensor at the macroscale using the expression postulated by Bamman and Aifantis (1982). Moreover, the evolution of dislocation density with plastic strain given by Klepaczko (1987) is also utilized in the derivation process of the proposed modeling.

In section 5.3, a constitutive description is presented in order to understand the plastic deformation behavior of bcc, fcc and hcp metals considering the experimental observations as well as the physical basis of the microstructures inside the material. Both the thermal and athermal components of the flow stress are physically derived and all the models parameters are related to the nano and micro-structure quantities. The hardening stresses are characterized using two different definitions of hardening parameters for each metal structure. Finally, the dynamic strain aging and the twinning phenomena encountered in some polycrystalline metals at certain range of strain rates and temperatures are briefly discussed.

In section 5.4, the determination procedure of the proposed bcc, fcc and hcp models parameters is presented. Applications of the proposed models to Niobium, Vanadium, and Tantalum for bcc metals, OFHC Copper for fcc metals and Titanium for hcp are then performed and compared to available experimental results at low and high strain rates and temperatures. Furthermore, Discussions of the model prediction results along with quantification of the nano and micro-quantities are presented. Conclusions are then given in section 5.5.

5.2 Dislocation Dynamics in Crystals Under Plastic Deformation

The plastic behavior of metals can be determined by investigating the dislocation dynamics of their crystals, which are generated, moved and stored during the inelastic deformation. In turn, the most important features that should serve as constituent elements of an appropriate theory of crystal plasticity are the motion, multiplication and interaction of these dislocations.
Orowan (1957) recognized the plastic deformation as a dynamic process by suggesting that the plastic shear strain rate is obtained by the motion of dislocations with an average velocity $v$ such that:

$$\dot{\gamma}^p = b \rho_m v$$  \hspace{1cm} (5.1)

where $\rho_m$ is the dislocation density and $b$ is the Burgers vector.

A theoretical description of plasticity should aim at relating the macroscopic deformation behavior at both the intrinsic properties of the deforming material and the externally imposed deformation conditions. On the microscopic scale, the plastic flow of crystalline materials is controlled by the generation, motion and interactions between dislocations. Thus, the constitutive description must, in principle, bridge the entire hierarchy of length scales, starting from the determination of the single dislocation properties on an atomistic scale and proceeding up to the characterization of the macroscopic material properties. In many cases, conclusions about the macroscopic deformation behavior can be obtained by investigating the temperature and strain rate dependence of the flow stress of pure bcc and fcc metals considering the properties of single dislocations (Zaiser et al., 1999). In relating the plastic shear strain rate at the microscale to the plastic strain rate tensor at the macroscale, the following expression is postulated (Bamman and Aifantis, 1982):

$$\dot{\varepsilon}_{ij}^p = \dot{\gamma}^p M_{ij}$$  \hspace{1cm} (5.2)

where $M_{ij}$ is the symmetric Schmidt orientation tensor which is defined as follows:

$$M_{ij} = \frac{1}{2} \left( n_i \otimes v_j + v_i \otimes n_j \right)$$  \hspace{1cm} (5.3)

where $\hat{n}$ denotes the unit normal on the slip plane and $\hat{v}$ denotes the unit vector in the slip direction. Eq.(5.2) indicates that the climb processes were neglected and plastic incompressibility was assumed since the orientation tensor is traceless. Moreover, the variation of the Schmidt tensor $M_{ij}$ is ignored either by considering that plasticity at the macroscale incorporates a number of differently oriented grains into each continuum point and therefore an average value is assumed or by being the product of two “first order” terms (Aifantis, 1987; Bammann and Aifantis, 1987).

Substituting Eq.(5.1) into Eq.(5.2), the equivalent plastic strain rate $\dot{\varepsilon}_p$ at the macroscale is defined in terms of the mobile dislocation density and dislocation velocity as follows:

$$\dot{\varepsilon}_p = \sqrt{\frac{2}{3} \dot{\varepsilon}_{ij}^p \dot{\varepsilon}_{ij}^p} = \bar{m}b \rho_m v$$  \hspace{1cm} (5.4)
where \( \bar{m} = \left(2M_b M_i / 3 \right)^{1/2} \) can be interpreted as the Schmidt orientation factor. It should be noted that both the mobility \( v \) and the concentration \( \rho_m \) of dislocations increase with increasing external forces (stresses). Nadgorny (1988) showed that one can (and often should) use the dislocation rate as well as the dislocation velocity interchangeably if one considers plastic deformation quantitatively. Consequently, the meaning of the quantities defined in Eq.(5.1) should be subject to refinement. Voyiadjis and Abed (2004) utilized this concept in the derivation of their constitutive models for both bcc and fcc metals. For the present work, however, only the dislocation rate is considered and rather than incorporating the dislocation rate \( (d \rho / dt) \) we consider the variation of the mobile dislocation density with the plastic strain \( (d \rho / d \epsilon_p) \). Therefore, the accumulation of dislocation density from its initial values until reaching its saturated level is considered.

The accumulation process of material dislocation density during the plastic deformation was investigated extensively by many authors (see for example, Klepaczko, 1987; Kubin and Estrin, 1990; Bammann, 2001; and Barlat et al., 2002). Klepaczko (1987) showed that the growth of dislocation density is nearly linear with regard to the deformation in the first steps of the hardening process, independently of the temperature. This is followed by a recombination of the dislocations that are assumed to be proportional with the probability of dislocation meeting, that is to say of the dislocation density. Based on this hypothesis, the following simple relation for the evolution of the total dislocation density \( \rho \) was presented (Klepaczko, 1987):

\[
\frac{d\rho}{d\epsilon_p} = M - K_a (\rho - \rho_i)
\]

(5.5)

where \( M = 1 / bl \) is the multiplication factor, \( l \) is the dislocation mean free path, \( \rho_i \) is the initial dislocation density encountered in the material due to the manufacture process or by nature, and \( k_a \) is the dislocation annihilation factor which may depend on both temperature and strain rate. Klepaczko and Rezaig (1996) showed that for mild steels, both \( M \) and \( k_a \) could be assumed constant at not so high strain rates and up to the temperature where the annihilation micromechanisms (recovery) start to be more intense. It should be kept in mind however, that at saturation, the slope \( d\rho / d\epsilon_p \) approaches a value of zero, which leads to the following definition of the saturated dislocation density \( \rho_s \)

\[
\rho_s = \rho_i + \frac{M}{k_a}
\]

(5.6)

The mobile dislocation density is related to the total dislocation density \( \rho \) by the linear relation \( (\rho_m = f \rho) \), where the fraction \( f \leq 1.0 \) may change with \( \rho \) and temperature (Kelly and Gillis, 1974; Sackett et al., 1977). In fact, it can be shown that the constant value of the fraction \( f \) gives satisfactory quantitative results for most metals (Klepaczko and Rezaig, 1996). In this study, the fraction \( f \) represents only the part of the mobile dislocation density that is thermally affected through Orowan’s equation as will be discussed later.
Kubin and Estrin (1990) proposed the following set of two coupled differential equations to describe both forest $\rho_f$ and mobile $\rho_m$ dislocation density evolutions with plastic strain using the same above mentioned concepts

$$\frac{d\rho_m}{d\epsilon_p} = \frac{\lambda_1}{b^2} - \frac{\lambda_2}{b} \rho_m + \frac{\lambda_3}{b} \rho_f^{1/2}$$

$$\frac{d\rho_f}{d\epsilon_p} = \lambda_2 \rho_m - \frac{\lambda_3}{b} \rho_f^{1/2} - \lambda_4 \rho_f$$

(5.7)

where the constant coefficients $\lambda_i$ are related to the multiplication of mobile dislocations ($\lambda_1$), their mutual annihilation and trapping ($\lambda_2$), their immobilization through interaction with forest dislocations ($\lambda_3$), and to the dynamic recovery ($\lambda_4$).

The dislocations are assumed to move in a periodic potential and the average dislocation velocity $v$ is determined by the thermodynamic probability for achieving sufficient energy temperature $T$ to move past a peak in the potential. In other words, it is determined through thermal activation by overcoming local obstacles to dislocation motion. Many expressions defining the dislocation speed for thermally activated dislocation glides may be found in the literature (Stein and Low, 1960; Gillis and Gilman, 1965; Li, 1968; and Hirth and Nix, 1969). The following general expression, however, is postulated (Bammann and Aifantis, 1982):

$$v = v_o \exp \left( -\frac{G}{kT} \right)$$

(5.8)

where $k$ is the Boltzmann’s constant, and $T$ is the absolute temperature. The reference dislocation velocity $v_o$ represents the peak value where the temperature reaches or exceeds the melting point. It is defined by $v_o = d / t_w$, where $t_w$ represents the time that a dislocation waits at an obstacle and $d$ is the average distance the dislocation moves between the obstacles. The shear stress-dependent free energy of activation $G$ may depend not only on stress but also on the internal structure. Kocks et al. (1975) suggested the following definition to relate the activation energy $G$ to the thermal flow stress $\sigma_{th}$

$$G = G_o \left( 1 - \left( \frac{\sigma_{th}}{\hat{\sigma}} \right)^p \right)^q$$

(5.9)

where $G_o$ is the reference Gibbs energy, $\hat{\sigma}$ is the threshold stress at which the dislocations can overcome the barriers without the assistance of thermal activation ($\sigma_{th} = \hat{\sigma}$ where $G = 0.0$), and $p$ and $q$ are constants defining the shape of the short-range barriers. According to Kocks, (2001), the typical values of the constant $q$ are $3/2$ and $2$ that is equivalent to a triangle obstacle profile near the top. On the other hand, the typical values of the constant $p$ are $1/2$ and $2/3$ which characterizes the tail of the obstacle.
Substituting Eq. (5.5) for the dislocation density evolution (after performing proper integration) and Eq. (5.8) for the dislocation velocity into Eq. (5.4) and making use of Eq. (5.9), the general relation of the thermal flow stress for polycrystalline materials (metals) is defined as follows:

$$\sigma_{th} = \bar{\sigma} \left[ 1 - \left( \beta_1 (\varepsilon_p) T - \beta_2 T \ln \frac{\dot{\varepsilon}_p}{\varepsilon_{ro}} \right)^{1/q} \right]^{1/p}$$  \hspace{1cm} (5.10)

where $\dot{\varepsilon}_p^i$ represents the reference equivalent plastic strain rate in its initial stage while related to the initial mobile dislocation. Its order of magnitude can, however, be anywhere between $10^6$ and $10^9 \text{s}^{-1}$ which characterizes the highest rate value a material may reach as related to the reference (highest) dislocation velocity $v_o$,

$$\dot{\varepsilon}_p^i = \bar{m} b v_o \rho_{mi}$$  \hspace{1cm} (5.11)

The parameters $\beta_1$ and $\beta_2$ are defined as follows:

$$\beta_1 = \frac{k}{G_o} \ln \left( 1 + C_1 \left( 1 - \exp(-k_a \varepsilon_p) \right) \right)$$  \hspace{1cm} (5.12)

and

$$\beta_2 = \frac{k}{G_o}$$  \hspace{1cm} (5.13)

where,

$$C_1 = f \frac{M}{k_a \rho_{mi}}$$  \hspace{1cm} (5.14)

Its worthwhile to mention here that $\beta_1$ is not constant, and rather increases with plastic strain increase. Its value, however, attains the maximum when the mobile part of the total dislocation density reaches its saturated level ($\rho_m = \rho_{ms}$), which is the case at high strains. On the other hand, $\beta_1$ vanishes as the plastic strain approaches zero and, in consequence, the thermal plastic flow pertains totally to the yield stress. In this work, the fraction $f$, which represents the mobile portion amount of the total dislocation density, is assumed constant in order to simplify the determination procedure of the model parameters. Moreover, average values of the quantities $M$ and $k_a$ are considered (Kubin and Estrin, 1990).

In understanding quantitatively the deformation behavior of metals, a constitutive description is required. In fact, any constitutive modeling of crystalline materials like metals should consider the physical basis of the microstructure inside the material as well as the experimental observation during the plastic deformation. However, deforming a metal beyond its elastic limit activates and moves its dislocations through the crystal. In turn, two types of obstacles are encountered that try to prevent dislocation movements through the lattice; short-range and long-range barriers. The short-range are due to dislocations trapping (forest) which
can be overcome by introducing thermal energy through the crystal. On the other hand, the long-range barriers are due to the structure of the material, which cannot be overcome by introducing thermal energy through the crystal. Therefore, the flow stress of any type of metals (\( \sigma = \left(3\sigma_{ij}\sigma_{ij}/2\right)^{1/2} \) of the Von Mises type) will be additively decomposed into two major components; the athermal stress \( \sigma_a \) and the thermal stress \( \sigma_{th} \)

\[
\sigma = \sigma_{th} + \sigma_a \tag{5.15}
\]

The above assumption of additive decomposition for the formulation of the flow stress has been proven experimentally and is used by several authors (see for example, Zerilli and Armstrong, 1987; Nemat-Nasser and Isaacs, 1997; and Nemat-Nasser et al., 1999).

Although Eq.(5.10) represents the general relation of the thermal stress, the final definition of thermal stress as well as athermal stress differs from metal to metal depending on both the microstructure crystal shape (bcc, fcc, and hcp) and on the experimental observations. In the following section, constitutive relations will be proposed for different types of metals applicable to high strain rates and temperatures.

### 5.3 Constitutive Modeling of Polycrystalline Metals

Based on their crystal structure, metals can generally be classified into three major types; body-centered cubic (bcc), face-centered cubic (fcc), and hexagonal close-packed (hcp). The crystal structure and the atom distribution inside the lattice play a crucial role in controlling the dislocation generation and movement during plastic deformation. Each type of metal, however, has its own behavior as coupled to strain rate and temperature. In this section, modeling of the plastic flow is presented for the aforementioned types of metals using the thermal activation energy principle paralleled with systematic experimental observations investigated by many authors. On the other hand, the role of solute/dislocation interaction in metals is not included in this study and therefore, the temperatures and strain rates are considered in the range where dynamic strain aging (DSA) is not effective.

#### 5.3.1 Body Centered Cubic (BCC) Metals

Experimental observations of most bcc metals, such as pure iron, tantalum, niobium, and vanadium show strong dependence of the yield stress on the strain rate and temperature whereas the plastic hardening is hardly influenced by temperature. That is, at a given strain rate and different temperatures or at a given temperature and several strain rates, the variation of the stress strain curves appear only on the yielding point whereas the hardening curves are almost identical (e.g. see Fig.5.1 for the case of Vanadium). This indicates that the thermal component of the flow stress is mainly controlled by the yield stress and nearly independent of the plastic strain.
The thermal stress of bcc metals may be interpreted physically as the resistance of the dislocation motion by the Peierls barriers (short-range barriers) provided by the lattice itself. Moreover, the thermal component of the flow stress for such metals can be determined using the same expression defined in Eq.(5.10). In fact, it is found for most bcc metals that the effect of the variation of $\beta_i$ (or variation of mobile dislocation density) on the thermal flow stress is practically negligible as will be shown in the application section. This behavior, actually, comes out from the fact that the plastic hardening is essentially allotted to the athermal part of the flow stress which is primarily accomplished through the relatively temperature-insensitive long-range barriers.

![Figure 5.1 Adiabatic flow stress of Vanadium for indicated initial temperatures, at 2500s$^{-1}$ strain rate given by Nemat-Nasser and Guo (2000).](image)

It should be mentioned here that the flow stress at a given temperature, $T$, is proportional to an appropriate shear modulus, $\mu$, at this temperature. It is also necessary to have $G$ proportional to $\mu$ ($G \propto \mu b'$) in order for the activation work done by the applied forces during the activation event to be independent of material properties (Kocks, 2001). Zerilli and Armstrong (1987) related, at zero Kelvin temperature, the thermal stress ($\sigma_0$) to the reference Gibbs energy ($G_o$) and dislocation activation area ($A_o$) as follows:

$$\sigma_0 = \frac{mG_o}{A_o b}$$

(5.16)
where $b$ is the magnitude of the Burgers vector and $m$ is the orientation factor that relates the shear stress to the normal stress, $\sigma = m\tau$ where $m = \sqrt{3}$ for the case of the von Mises flow rule. Utilizing Eq.(5.16) with a proper proportional relation of the reference Gibbs energy to the shear modulus, the parameter $\hat{\sigma}$ can be related to the strain-independent internal structure as follows:

$$\hat{\sigma} = m\alpha_o \mu_o b^2 / A_o$$  \hspace{1cm} (5.17)$$

where $\alpha_o$ is a constant which represents the portion of the shear modulus $\mu_o$ contributed to the activation energy both at zero temperature. For bcc metals, the activation area $A_o$ may be considered constant in accordance with the intrinsic Peierls stress.

For most metals, an additional component of stress $Y_a$ is used that is independent of plastic strain and temperature (athermal yield stress component) and related to the internal microstructure quantities that are independent of plastic strain (e.g. grain diameter $D_g$). This component is defined as the product of microstructural stress intensity and the inverse square root of the average grain diameter. Klepaczko (1988) proposed a definition for the stress intensity as related to the shear modulus and the magnitude of the Burgers vector from which the athermal yield stress is finally defined as follows:

$$Y_a = \alpha_i \mu \left( \frac{b}{D_g} \right)^{1/2}$$ \hspace{1cm} (5.18)$$

where $\alpha_i$ is the interaction constant showing the contribution of the above mechanism to the athermal stress.

The final component of the bcc flow stress is attributed to the hardening stress, which is independent of temperature, and consequently contributes to the athermal flow stress part. In fact, both mobile dislocation density and immobile (forest) dislocation density should be considered in the evolution (accumulation) relations for the case of large strain problems (up to 50%). Therefore, the hardening component of the flow stress is related to the effective total dislocation density ($\bar{\rho} = \rho - \rho_i$) where $\rho_i$ is the initial dislocation density encountered originally inside the material. The dislocation model of Taylor (1938) gives the shear flow stress $\tau$ in terms of the total dislocation density $\rho$ as

$$\tau = \alpha \mu b \sqrt{\rho}$$ \hspace{1cm} (5.19)$$

where $\alpha$ is an empirical coefficient taken to be 0.2 for fcc metals and about 0.4 for bcc metals as given by Nabarro et al. (1964) who pointed out that Eq.(5.19) can be derived by multiple methods. Ashby (1970) split the difference of $\alpha$ values in assuming that $\alpha = 0.3$ for most metals. The plastic strain evolution of the effective total dislocation density can be defined, after solving for the differential equation Eq.(5.5), in terms of the internal physical quantities as follows:
\[ \bar{\rho} = \frac{M}{k_a} \left( 1 - \exp(-k_a \varepsilon_p) \right) \] (5.20)

Relating the shear stress to the normal stress by \( \sigma = m \tau \), and substituting \( \bar{\rho} \) defined by Eq.(5.20) instead of \( \rho \) in Eq.(5.19), one has the athermal flow stress in the following form

\[ \sigma_a = Y_a + \bar{B} \left( 1 - \exp(-k_a \varepsilon_p) \right)^{1/2} \] (5.21)

where \( \bar{B} \) is the hardening parameter defined as

\[ \bar{B} = m \alpha \mu b \left( \frac{M}{k_a} \right)^{1/2} \] (5.22)

Alternatively, the plastic hardening for pure bcc metals may be evaluated from an assumed power law dependent on strain. This assumption is observed experimentally and used by many authors (see for example Zerilli & Armstrong, 1987 and Nemat-Nasser et al., 1999). Thus, the athermal flow stress of bcc metals may be given as

\[ \sigma_a = Y_a + B \varepsilon_p^n \] (5.23)

where \( B \) and \( n \) are the hardening parameters. This experimental observation can be physically justified by using alternative explanation for the total dislocation density. In other words, the total dislocation density may also be defined as the interaction between the density \( \rho_s \) for statistically stored dislocations, which are stored by trapping each other in a random way, and density \( \rho_g \) for geometrically necessary dislocations, which are stored in order to maintain the continuity (compatibility) of various components of the material, i.e.

\[ \rho' = \rho_s^\gamma + \rho_g^\gamma \] (5.24)

where the exponent \( \gamma \) is a material parameter. Ashby (1970) pointed out that, in general, the presence of geometrically necessary dislocations will accelerate the rate of statistical storage and that the value of \( \gamma = 1 \) should provide a lower limit on the effective total dislocation density. Based on that, Zhao et al. (2003) argued that the value of \( \gamma \) should be less than or equal to 1 in order to properly estimate the effective total dislocation density.

It is obvious from the above definitions of both dislocation densities that the geometrically necessary dislocation density \( \rho_g \) is related to the strain gradient whereas the statistically stored dislocation density \( \rho_s \) is related to the strain hardening as follows (Zhao et al., 2003):

\[ \rho_g = \hat{f} \frac{\chi}{b} , \quad \rho_s = \left( \frac{\sigma_{ref} \varepsilon_n}{m \alpha \mu b} \right) \] (5.25)
where \( \chi \) is a suitable form of the third-order strain gradient tensor and \( \hat{f} \) is a function of higher order gradients of strain. The function \( \hat{f} \), however, becomes constant when the strain-gradient field is uniform. The coefficients \( \sigma_{\text{ref}} \) and \( N \) represents the material parameters for the assumed power-law hardening rule. Eq.(5.25) may be used for the definition of both effective statistically stored dislocation density \( \bar{\rho}_s \) and effective geometrically necessary dislocation density \( \bar{\rho}_g \) except that they are related to the plastic strain and the plastic strain gradient respectively.

By substituting Eq.(5.25) into Eq.(5.24), the power-law hardening parameters can be related to the effective statistically stored dislocation density \( \bar{\rho}_s \) for the case of uniform plastic straining \( (\bar{\rho}_g = 0) \) as follows:

\[
\sigma_{\text{ref}} \varepsilon_p^N = m\alpha ub\sqrt{\bar{\rho}_s} \tag{5.26}
\]

Although the above equation (Eq.(5.26)) rationalizes the power-low hardening rule by relating it to the internal physical quantities, the hardening parameters \( B \) and \( n \), however, are not explicitly defined as in the case for those given by Eq.(5.21). In turn, the athermal hardening stress may be estimated either by using the physically derived relation given by Eq.(5.21) or by using the empirical relation, Eq.(5.23), obtained through experimental observations.

Accordingly, the total flow stress for bcc metals may be calculated, after making use of the concept of additive decomposition in Eq.(5.15), through one of the following relations:

\[
\sigma = Y_a + B (1 - \exp(-k_\varepsilon \varepsilon_p))^{1/2} + \hat{\sigma} \left( 1 - \left( \beta_1(\varepsilon_p)T - \beta_2 T \ln \frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_p^0} \right)^{1/q} \right)^{1/p} \tag{5.27}
\]

and

\[
\sigma = Y_a + B \varepsilon_p^n + \hat{\sigma} \left( 1 - \left( \beta_1(\varepsilon_p)T - \beta_2 T \ln \frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_p^0} \right)^{1/q} \right)^{1/p} \tag{5.28}
\]

The above relations may be used to predict the stress strain curves for both isothermal and adiabatic plastic deformations. For the case of isothermal deformation, the temperature \( T \) remains constant during the plastic (representing the initial testing temperature, \( T_0 \)) deformation. In the adiabatic case of deformation, heat inside the material increases as plastic strain increases and therefore, the temperature \( T \) is calculated incrementally by assuming that the majority of the plastic work is converted to heat:

\[
T = T_0 + \frac{\dot{\varepsilon}_p}{c_v \rho} \int_0^{\varepsilon_p} \sigma \, d\varepsilon_p \tag{5.29}
\]
here \( \rho \) is the material density and \( c_s \) is the specific heat at constant pressure. The Taylor-Quinney empirical constant \( \zeta \) is often assigned the value of 0.9. However, recent tests have indicated that this parameter may vary with plastic strain (for more details see the work of Kapoor and Nemat-Nasser, 1998). Eq.(5.29) may be solved numerically or can be integrated without introducing any noticeable errors by either using the mean value theorem or the simple Euler method. In this work, Eq.(5.29) is used for all types of metals to determine the evolution of temperature with plastic strain throughout the adiabatic deformation.

It should be noted that the thermal component of the flow stress given by the last term in the right hand side of Eq.(5.27) or Eq.(5.28) is non-negative. Thus, the term between the brackets on the right hand side should be set equal to zero when the temperature exceeds a critical value. The critical temperature, in the \( T \) vs \( \sigma \) curve, defines the starting point of the constant stress which represents the athermal component of the flow stress. This critical value, however, is strain rate dependent and is defined as follows:

\[
T_{cr} = \left( \beta_1 - \beta_2 \ln \frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_p^0} \right)^{-1}
\]  

(5.30)

### 5.3.2 Face Centered Cubic (FCC) Metals

In the case of fcc metals, like copper and aluminum, the mechanisms of thermal activation analysis are dominated and controlled by the emergence and evolution of a heterogeneous microstructure of dislocations (mobile) as well as the long-range intersections between dislocations (forest). On this basis, the thermal activation is strongly dependent on the plastic strain. That is, the increase in the yield point with a decrease in temperature is highly dependent on the strain-hardened states for fcc metals. Experimental observations validate the plastic strain dependence of strain rate and temperature for most fcc metals (Nemat-Nasser and Li, 1998; Tanner et al., 1999; Lennon and Ramesh, 2004). That is, for a certain strain rate and various temperatures, the adiabatic stress vs strain plots clearly show that all curves start approximately from the same point (initial yielding) and each curve hardens differently from each other depending on the corresponding temperature (see Fig.5.2 for the case of OFHC Copper).

The effect of mobile dislocation density is introduced to the flow stress by utilizing Orowan’s equation as derived in the previous section. That is to say, the parameter \( \beta_1 \) plays a significant role in characterizing the effect of dislocations movement on the thermal flow stress during the thermal plastic deformation. Additionally, for the thermal activation analysis behavior, the effect of dislocation intersection mechanisms (mobile and forest) on the flow stress can be described as follows. When dislocation patterns (i.e. cell) are formed, the sources of mobile dislocations become numerous in the cell walls. After deformation, dislocations tend to be trapped on the next cell wall forming a forest of dislocations, which become the major obstacle for a mobile dislocation. Therefore, Introducing thermal energy will facilitate
dislocations in overcoming these types of obstacles and, in consequence, provide hardening to the thermal flow stress.

On this basis, the distance $d$ between dislocation intersections and consequently the activation volume play an additional crucial role in determining an appropriate formulation introducing the effect of plastic strain on the thermal component of the material flow stress. Thus, the activation volume $V$ can be related to the distance between dislocation intersections as follows (Zerilli and Armstrong, 1987; Voyiadjis and Abed, 2004):

$$ V = Ab = db^2 / 2 $$ (5.31)

where $A$ is the activation area. In fact, Gracio (1989) has speculated that in copper, when the plastic strain increases, the mean free path decreases and consequently, the distance between dislocation intersections decreases. Therefore, the forest dislocation densities as well as the plastic strain are related to the distance $d$ through the relationship (Kubin and Estrin, 1990)

$$ d \sim 1/\varepsilon_p^{1/2} \quad \text{and} \quad \rho_f \sim 1/d^2 $$ (5.32)

The multiple slip-crystal flow stress for fcc metals at $T = 0.0$ Kelvin temperature and any strain value is related to both the dislocation densities and strain by the relation given by several authors (see for example Bell, 1965)

$$ \sigma_o = \sigma'_o (b / d) = \sigma_o'^r \varepsilon_p^r $$ (5.33)

Comparing Eq.(5.33) with Eq.(5.10) for the case of zero Kelvin temperature, and employing the argument given by Eqs.(5.31) and (5.32), the activation area $A_o$ for fcc metals, determined by dislocation intersections, is proportional to the inverse square root of plastic strain (and vice versa) as follows (Zerilli and Armstrong, 1987):

$$ A_o = A'_o \varepsilon_p^{1/2} $$

or

$$ A_o^{-1} = A'_o^{-1} \varepsilon_p^{1/2} $$ (5.34)

Eq.(5.34) clearly shows that the activation area decreases as the plastic strain evolves which indicates that the value of the activation area is highest at the initial stage of plastic deformation ($\varepsilon_p = 0$). The initial activation area, however, is a finite quantity, which is not the case as defined in Eq.(5.34) since it will tend to infinity when the plastic strain is zero. In this work, therefore, the definition of the initial activation area is modified incorporating a finite initial activation area $A'_o$, and defined for the case of fcc metals as follows:

$$ A_o^{-1} = A'_o^{-1} + A'^{-1} \varepsilon_p^{1/2} $$ (5.35)
Figure 5.2 Adiabatic flow stress of OFHC Copper for indicated initial temperatures, at 4000s-1 strain rate given by Nemat-Nasser and Li (1998)

Substituting Eq.(5.35) into Eq.(5.16) and since $\sigma_o = \dot{\sigma}$ at $T=0$, the thermal component of the present constitutive equation for the case of fcc metals will incorporate the coupling of temperature, strain rate, as well as plastic strain. On the other hand, the athermal component of fcc flow stress is independent of the plastic strain and it pertains totally to the initial yield stress and is related to the internal structure (grain diameter) as in the case of bcc metals Eq.(5.18). Using the additive decomposition given in Eq.(5.15), the total flow stress may then be defined for the case of fcc metals as:

$$
\sigma = Y_a + (\tilde{B} \dot{\varepsilon}_p^{1/2} + Y_d) \left[ 1 - \left( \beta_1 (\varepsilon_p) T - \beta_2 T \ln \frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_{po}} \right)^{1/q} \right]^{1/p} \quad (5.36)
$$

where the parameters $Y_a$ and $\beta_i$ are the same as defined previously whereas, the hardening parameter $\tilde{B}$ is given as:

$$
\tilde{B} = m\alpha_o \mu_o b^2 / A_o^* \quad (5.37)
$$

It can be seen in Eq.(5.36) that, at a given plastic strain value, the thermal stress preserves the same trend shown in bcc metals including that constants $p$ and $q$ are falling in the same range
as those given before. Moreover, there is no strain rate and temperature effect on the initial yield stress and, thus, $Y_d$ is constant.

In fact, the modification of the activation energy definition given in Eq. (5.35) guided us in introducing an additional component to the thermal flow stress incorporating the election- and phonon- drag effects on the movement of material dislocations. This phenomenon is encountered mainly in fcc and hcp metals at the regions where the plastic strains approach zero with relatively high strain rates (Jassby and Vreeland, 1970 and Zerilli and Armstrong, 1992). An examination of Eq.(5.36) shows that when the plastic strain approaches the limit zero ($\varepsilon_p \rightarrow 0.0$), the solution for the thermal stress approaches the limiting value

$$\sigma_{th} \rightarrow Y_d \left(1 - \left(\frac{k}{G_o} T \ln \frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_o}\right)\right)^{1/\gamma'}$$

(5.38)

where the parameter $Y_d$ may be considered as the resultant drag-stress at the reference velocity $\dot{\varepsilon} = \dot{\varepsilon}_o$ and/or zero Kelvin temperature $T = 0$ defined as

$$Y_d = m\alpha_o \mu_o b^2 / A_o'$$

(5.39)

It’s obvious that the drag-stress component given by Eq.(5.38) is a decreasing function of temperature whereas it increases with the increase of the strain rate. Such a behavior, however, coincides with the experimental results and observations found in the literature (see Vreeland and Jassby, 1971; and Follansbee et al., 1984; Nemat-Nasser and Li, 1998; and Nemat-Nasser et al., 2001). In this regard, Armstrong et al (1993) have noted that the strong upturn in flow stress at high strain rates signifies a strong decrease in the activation area $A$, approaching atomic dimensions, indicative of strongly reduced intersection spacing leading to the dislocation density increase.

Actually, the hardening parameter $\tilde{B}\varepsilon_p^n$ given in Eq.(5.36) can alternatively be derived by a more accurate method by relating the activation area to the forest dislocation density after utilizing both Eqs.(5.31) and (5.32) as follows:

$$A_o = bd / 2 = \tilde{m} b \rho_f^{-1/2}$$

(5.40)

where $\tilde{m}$ is a constant and the evolution of forest dislocation density with plastic hardening may be defined after making use of Eq.(5.5) as follows:

$$\rho_f = \rho_{f0} + \frac{M}{k_a} \left(1 - \exp(-k_a \varepsilon_p)\right)$$

(5.41)
where \( f \) denotes the forest dislocation density fraction of the total dislocation density. Substituting Eq.(5.40) into Eq.(5.17) and utilizing Eq.(5.41), the plastic flow stress of fcc metals can alternatively be determined using the following relation:

\[
\sigma = Y_a + \left( \hat{Y}_d + \hat{B} \left( 1 - \exp(-k_a \varepsilon_p) \right)^{1/2} \right) \left( 1 - \left( \frac{\beta_1 (\varepsilon_p) T - \beta_2 T \ln \left( \frac{\varepsilon_p}{\varepsilon_{po}} \right) \right)^{1/q} \right)^{1/p} \quad (5.42)
\]

where the hardening parameter \( \hat{B} \) and the drag-stress component \( \hat{Y}_d \) are defined by the following two relations:

\[
\hat{B} = \hat{m} \alpha_a \mu_o \sqrt{f} M \quad (5.43)
\]

\[
\hat{Y}_d = \hat{m} \alpha_a \mu_o b \sqrt{\rho_e} \quad (5.44)
\]

where \( \hat{m} = m / \tilde{m} \) is a constant. The plastic flow stress for bcc metals is then determined using either Eq.(5.36) with a power low hardening stress component or Eq.(5.42) with a more accurate physical interpretation hardening stress. Both relations, however, correlate properly with the experimental results.

As a final point, the evolution of the adiabatic temperature for fcc metals is simulated using the same evolution relation given in Eq.(5.29). Moreover, the critical temperature of fcc metals is both strain and strain rate dependent and is defined in the same way as that given in Eq.(5.30).

**5.3.3 Hexagonal Close-Packed (HCP) Metals**

The mechanical behavior of hcp metals, like titanium and zirconium, can be determined by addressing the structure and energies of dislocation cores and planar defects, including twin boundaries and stacking faults. However, different hcp materials have dramatically different mechanical properties which make the modeling of the plastic flow of hcp metals very complicated and not unique over broad temperature and strain rate ranges. In fact, hcp materials often show strong temperature dependent behavior, often associated with changes in deformation modes which, in turn, affect both the polycrystalline ductility and dynamic recrystallization. Although the crystal structure of hcp metals is close-packed like fcc metals, it shows plastic anisotropy and lacks the symmetry needed to be sufficient in satisfying, for instance, the von Mises criterion (Yoo et al., 2002). Since each hcp metal has its own mechanical behavior depending on the internal structure (a/c ratio) and slip plane and direction, we concentrate in this study only on the thermal plastic deformation behavior of titanium. Its alloys are considered to be the most increasingly used hcp metals in structural applications at low and high strain rate of loading.
Observations of the experimental stress-strain results of titanium under high strain rates and elevated temperatures indicated that not only is the yield stress a strong dependent on temperature and strain rates but the strain hardening also changes with temperatures as shown in Fig.5.3.

The above figure (5.3) implies that the thermal activation has the effect of both lowering the yield stress and decreasing the effect of strain hardening. Thus, the macroscopic thermomechanical behavior of hcp metals in general and titanium in particular tends to fall somewhere between that of the fcc and bcc metals. In this regard, the plastic flow stress of hcp metals is related to temperature and strain rates assuming that the plastic flow is mainly accounted for by dislocation motion and intersections, as follows:

\[
\sigma = Y_a + B \varepsilon_p^n + \left( B \dot{\varepsilon}_p^{1/2} + Y_d \right) \left( 1 - \beta_1 (\varepsilon_p) T - \beta_2 T \ln \left( \frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_p^0} \right)^{1/\gamma} \right)^{1/p} \]

Or

\[
\sigma = Y_a + B \left( 1 - \exp(-k_a \varepsilon_p) \right)^{1/2} + B \left( \exp(-k_a \varepsilon_p) \right)^{1/2} + Y_d \left( 1 - \beta_1 (\varepsilon_p) T - \beta_2 T \ln \left( \frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_p^0} \right)^{1/\gamma} \right)^{1/p} \]

The first two terms in Eq.(5.45) and Eq.(5.46) represent the athermal part of the flow stress whereas the third term represents the thermal coupling of plastic hardening and yield stress to the flow stress.

Recent research by Chichili et al. (1998) on \(\alpha\)-Ti indicated that twin-dislocation intersections play an important role on strain hardening at room temperature and for strain rates ranging from \(10^{-5}\) to \(10^2\) s\(^{-1}\). In contrast, the experimental study of Nemat-Nasser et al., (1999) for the plastic flow of commercially pure titanium at strain rates from \(10^{-3}\) to \(10^3\) s\(^{-1}\) and temperatures from 77 to 1000K, with strains exceeding 40% showed that the high density of twins does not necessarily correlate with a higher flow stress. On the other hand, they illustrated that the dynamic strain aging takes place at both low and high strain rates and for a wide range of temperatures. Accordingly, any constitutive relation that deals with the thermomechanical response of titanium should consider not only the role of dislocation activities (dislocation motion and intersections) but also the role of dynamic strain aging as a major event with the role of deformation twinning being uncertain.

In this study, nevertheless, the plastic flow relation defined in Eq.(5.45) is limited to temperature and strain ranges where both twinning and dynamic strain aging is not activated. A brief description of twinning and DSA behaviors is presented in the following sections. The effect of dynamic strain aging on the flow stress of metals, however, is of considerable current interest and an extensive study of this phenomenon is going to be presented in future work.
Dynamic Strain Aging (DSA)

The dynamic strain aging can be interpreted physically as the diffusion of solutes atoms to the mobile dislocations that are temporarily trapped at an obstacle for a certain amount of time before they jump to another obstacle. The activation of DSA takes place when the aging time is equal to the waiting time of these dislocations and therefore, the obstacle strength is increased by certain amount. Dynamic strain aging may be observed at different strain rate levels and certain range of temperatures. It may occur either through a directional diffusion of the dislocation core atmosphere, at high strain rates, or through a bulk diffusion, at low strain rates (Nemat-Nasser et al., 1999).

The dynamic strain aging behavior can be described macroscopically as the sudden increase of the flow stress at certain temperature that normally causes a decrease in the flow stress curve. In other words, at fixed strain and strain rate, and with temperature increase, the decreasing flow stress may suddenly begin to increase at a certain temperature and, after attaining a peak value, may begin to decrease. This sudden increase and decrease of stress forms a noticeable hump in the flow stress-temperature curve. The peak value of the flow stress, however, changes with strain and strain rates. Moreover, the temperature value which indicates the start of the sudden increase in the flow stress is also strain rate dependent.
The range of temperature and strain rate where the DSA is displayed differs from metal structure to another and even from metal to metal within the same crystal structure. Experimental results of Nemat-Nasser and co-workers on bcc and fcc metals (Nemat-Nasser and Issacs, 1997; Nemat-Nasser and Li, 1998; Nemat-Nasser and Guo, 2000; and Cheng and Nemat-Nasser, 2001) show that Niobium exhibits dynamic strain aging at low strain rates only (around $10^{-3} \text{s}^{-1}$) for a temperature range of 450-700K. On the other hand, the DSA behavior is not encountered in Tantalum, Vanadium and OFHC Copper at ranges of $10^{-3}$-$10^{5} \text{s}^{-1}$ strain rates and 77-1000K temperatures. For the case of Titanium, the dynamic strain aging is widely encountered at both low and high strain rates and suitable temperature ranges. It is concluded that the DSA behavior is strain rate dependent for all types of metals and it takes place when the deformation temperature approaches its critical value defined in Eq.(5.30).

As addressed by many authors, the thermomechanical modeling of the extra flow stress produced by the effect of dynamic strain aging is not a straightforward procedure. However, as cited by Barlat et al. (2002), Louat (1981) has given a mathematical expression for the extra flow stress $\sigma_D$ as follows:

$$\sigma_D = \hat{\sigma}_D \left(1 - \exp\left[-\left(\frac{t_w}{t_x}\right)^{2/3}\right]\right)$$  \hspace{1cm} (5.47)

where $\hat{\sigma}_D$ is the maximum stress increase produced by the DSA and $t_x$ is the relaxation time associated with diffusion. Eq.(5.47) indicates that the extra flow stress vanishes as the waiting time $t_w$ approaches zero. This waiting time can simply be related to the plastic strain by utilizing Orowan’s equation, after neglecting the running time of the dislocation between obstacles, as follows

$$t_w = \frac{\bar{m}bd\rho_m}{\dot{\varepsilon}_p}$$  \hspace{1cm} (5.48)

The relaxation time $t_x$ associated with diffusion, on the other hand, is related to the temperature and the microstructure physical parameters as follows (Friedel, 1964; Kubin and Shihab, 1988):

$$t_x = \frac{kTb^2}{3WD\left(c_1/\pi c_o\right)^{3/2}}$$  \hspace{1cm} (5.49)

where $c_o$ and $c_1$ are the bulk solute volume fraction and the saturation solute concentration on dislocations respectively, $D$ is the diffusion coefficient of solute atoms, and $W$ is the absolute value of binding energy between solute and dislocations. Hence, employing Eqs.(5.47), (5.48) and (5.49) with the DSA being effective at $T\rightarrow T_{cr}$, the additional flow stress could suitably be added in calculating the total flow stress for certain metals.
Deformation Twinning Behavior

The unusual difficulty associated with identification of deformation mechanisms within hcp metals may be attributed to the fact that these closed-packed crystal structures often exhibit both slip and twinning during plastic deformation. The presence of twin systems, in certain cases, becomes necessary in order to maintain the compatibility of polycrystalline deformation, and it is expected that twinning shear will contribute to the overall strain. This contribution, however, is still inconsistent and uncertain.

Experiments conducted by Nemat-Nasser et al. (1999) investigated commercially pure titanium over a temperature range of 77-1000K and strain rates of $10^{-3}$-$10^{4}\text{s}^{-1}$ and showed that deformation twins were observed in most temperatures. Moreover, they illustrated that the density of twins increases with increasing strain rate to $2200\text{s}^{-1}$, and when the temperature is decreased to 77K. Besides, they demonstrated that at 10% true strain and low strain rate, the twins start disappearing as soon as the temperature exceeds a limiting value of 600K. However, it is shown that the amount of gross deformation produced by twins is relatively small since the relative atomic movement is limited in deformation twinning and hence, most of the plastic flow occurs by the motion of the twins and their intersections. It is concluded, therefore, that though the deformation of the material undergoes high density of twins at high strain and strain rates, it does not correlate with a higher flow stress.

Chichili et al. (1998), on the other hand, summarized the microstructure characterization of the room temperature deformation of $\alpha$-titanium as follows: (1) the material deformation at low strain rates and low strains is mainly due to dislocation motion with very few twins; (2) at large strains with the same low strain rate level, it is noted that the increase of the numbers of twins as well as a substantial dislocation motion is observed during the deformation; (3) at high strain rates and small strains, densities of both dislocation motion and twins are obviously increased; (4) by increasing both strains and strain rates, the twin density increases even further, with substantial twin-dislocation interactions. It is concluded, however, that even when the material is heavily twinned, the amount of plastic deformation contributed by twinning is measured to be much less that due to dislocations. Consequently, incorporating such effect in the constitutive modeling of pure titanium is still problematic and inconclusive.

5.4 Applications, Comparisons, and Discussions

The proposed constitutive models derived in the previous section for bcc, fcc and hcp metals are further evaluated by direct comparison to the experimental results that are mainly provided by Nemat-Nasser and his co-workers for different types of polycrystalline metals conducted at a wide range of strain rates and temperatures. In this section, the evaluation of the material parameters of the proposed models is first discussed. Applications of these models for predicting the plastic deformation as well as comparisons to experimental results are then illustrated for three bcc metals (Niobium, Tantalum and Vanadium), one fcc metal (OFHC Copper) and one hcp metal (Titanium) over a wide range of temperatures and strain rates. Finally, numerical identification is also presented for the nano/micro-structural physical quantities used in the definition of the proposed models parameters.
5.4.1 Models Parameters Evaluation

Various techniques can be used to determine the material parameters of the proposed models. However, a simple approach is used and similarly applied for all the proposed models with little variation between the three structural types of metals as given by Eq.(5.27) & Eq.(5.28) for bcc metals, Eq.(5.36) & Eq.(5.42) for fcc metals, and Eq.(5.45) & Eq.(5.46) for hcp metals. The evaluation procedure is initiated by studying the stress-temperature relation at different values of plastic strain and at certain strain rate value. Generally, the flow stress decreases as the temperature increases until a point where the stress is constant with further increase in temperature. These constant values represent the athermal part of the flow stress which varies with plastic strain for the case of bcc and hcp metals whereas it is strain independent for the case of fcc metals. Employing the variation of the athermal flow stress with plastic strain, the parameters \( B \) and \( n \) or \( \bar{B} \) and \( k_0 \) for bcc and hcp metals models is calculated using the nonlinear least-squares fit. The \( Y_d \) value, on the other hand, represents the athermal stress at zero plastic strain or the athermal component of the initial yield stress. Subtracting the above stress increments (athermal stress) values from the total flow stress, the thermal component of the flow stress is then determined.

The thermal component of the flow stress is mainly pertained to the yield stress for bcc metals and to the plastic hardening for both fcc and hcp metals. Moreover, the thermal degradation mechanism is captured by selecting proper values of the exponents \( p \) and \( q \) that are chosen here to be 1/2 for the former and 3/2 for the latter for all kinds of metals used in this study. Once these exponents are determined for a particular mechanism, they become constants. Next, the intercepts of the constant slope line plotted between \( \sigma_{th}^p \) and \( T^{1/q} \) at different plastic strains and certain strain rate are employed here to obtain at zero plastic strain, the threshold stress \( \tilde{\sigma} \) for bcc models and the parameter \( Y_d \) for fcc and hcp models. On the other hand, the hardening parameter \( \tilde{B} \) or \( \bar{B} \) for fcc and hcp models are determined using the nonlinear least-square fit technique for the different plastic strain intercept values. Then, for the case of bcc models, a graph of \( \left( 1 - \left( \frac{\sigma_{th}}{\tilde{\sigma}} \right)^p \right)^q \) vs \( \ln \dot{\varepsilon}_p \) is utilized to determine the parameter \( \beta_2 \) and the reference plastic strain rate \( \dot{\varepsilon}_{po}^i \). A similar procedure is followed for the case of fcc and hcp models except that \( \tilde{\sigma} \) is replaced by \( Y_d \). Finally, the parameter \( \beta_1 \) or the constant \( C_1 \) is then determined after detecting all other stress components from the total flow stress at different plastic strain values using the nonlinear least-square fit.

5.4.2 Applications and Comparisons

- **BCC Metals**

Three bcc metals are used in this study as applications for the proposed bcc models: (1) Niobium (Nb) is a silvery bcc metal that is used as an alloying agent in carbon and alloy steels, as it improves the strength of the alloy; (2) Vanadium (V) is a bright white bcc metal, and is soft and ductile with good structural strength. It is used in the aerospace industry in titanium alloys; (3) Tantalum (Ta) has generated a lot of interest in industry due to its density, strength
and ductility over a wide range of deformation rates and temperatures. The material parameters of these bcc metals are determined following the procedure discussed previously. The experimental data presented by Nemat-Nasser and Guo (2000) is utilized for the case of Nb and V metals, whereas the parameters of Ta are obtained using the experimental results presented by Nemat-Nasser and Isaacs (1997) and compared also to different results offered by different authors. The numerical values of the material parameters defined by the proposed bcc models are listed in Table 5.1 for the above-mentioned three metals obtained using the aforementioned procedure.

It is obvious that the only difference between the two proposed bcc models Eq.(5.27) and Eq.(5.28) is with regard to the two different definitions of the plastic hardening component which is mostly associated to the athermal component of the flow stress, i.e., independent of temperature and strain rate. Therefore, the differences of the plastic flow stress predicted by the proposed two bcc definitions emerge only in the athermal component. These differences may be attributed to both the errors accumulated using the nonlinear least-square fit and to the different integration results used in calculating the adiabatic heat accumulated inside the material through the plastic work. Therefore, the predicted stress strain curves using the proposed bcc models will depend totally on the accuracy of determining the hardening parameters which vary from test to test. Moreover, the hardening parameters obtained using certain experimental data will not necessarily match with the other data set presented by different researchers.

<table>
<thead>
<tr>
<th>Model Parameters</th>
<th>Nb</th>
<th>V</th>
<th>Ta</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Y_a$ (MPa)</td>
<td>60</td>
<td>60</td>
<td>50</td>
</tr>
<tr>
<td>$\bar{B}$ (MPa)</td>
<td>415</td>
<td>275</td>
<td>290</td>
</tr>
<tr>
<td>$B$ (MPa)</td>
<td>450</td>
<td>305</td>
<td>330</td>
</tr>
<tr>
<td>$n$</td>
<td>0.25</td>
<td>0.16</td>
<td>0.41</td>
</tr>
<tr>
<td>$k_a$</td>
<td>3.7</td>
<td>9.9</td>
<td>2.5</td>
</tr>
<tr>
<td>$\sigma^*$ (Mpa)</td>
<td>1350</td>
<td>945</td>
<td>1125</td>
</tr>
<tr>
<td>$C_1$</td>
<td>0.25</td>
<td>0.1</td>
<td>0.5</td>
</tr>
<tr>
<td>$\beta_2$ (K$^{-1}$)</td>
<td>0.000149</td>
<td>0.0001392</td>
<td>0.0000937</td>
</tr>
<tr>
<td>$\dot{\epsilon}_{ps}$ ($s^{-1}$)</td>
<td>$7.07 \times 10^6$</td>
<td>$6.32 \times 10^6$</td>
<td>$4.45 \times 10^6$</td>
</tr>
<tr>
<td>$q$</td>
<td>3/2</td>
<td>3/2</td>
<td>3/2</td>
</tr>
<tr>
<td>$p$</td>
<td>1/2</td>
<td>1/2</td>
<td>1/2</td>
</tr>
</tbody>
</table>

Fig.5.4 and Fig.5.5 show the adiabatic stress strain results for niobium computed using the present two bcc models at 3300s$^{-1}$ and 8000s$^{-1}$ strain rates respectively. Generally, both the proposed bcc definitions show very good agreement as compared to the experimental data presented by Nemat-Nasser and Guo (2000) for a wide range of elevated temperatures. In fact,
the difference in the predictions between the two proposed bcc relations for the plastic flow stress is noticeable at low strains (up to 0.1) and it diminishes with strain increase (up to 0.6).

The experimental comparison of the adiabatic flow stress for the case of vanadium agrees well at the strain rate of 2500s\(^{-1}\) and for different temperatures (up to 800K) as shown in Fig.5.6. The agreement, however, is less for the case of higher strain rate (8000s\(^{-1}\)) with a temperature range of 296K to 700K (see Fig.5.7). This may indicate that assuming a constant value of the parameter \(k_a\) (i.e., neglecting the effect of temperature and strain rate) produces inaccurate results in some cases. Furthermore, the prediction of the adiabatic flow stress at different initial temperatures shows more variation between the two proposed bcc relations for the case of a strain rate of 8000s\(^{-1}\) than those obtained at 2500s\(^{-1}\) strain rate.

![Figure 5.4 Adiabatic flow stress of Niobium predicted using the proposed models and compared to experimental results (Nemat-Nasser and Guo, 2000) at 3300s\(^{-1}\) strain rate and indicated initial temperatures.](image)

For the case of tantalum, Eq.(5.27) and Eq.(5.28) show almost identical results when computed at 5000s\(^{-1}\) and temperature range of 298K to 796K. In addition, the adiabatic stress strain curves calculated by those two relations show good correlations with the experimental results provided by Nemat-Nasser and Isaacs (1997) as shown in Fig.5.8.
Figure 5.5 Adiabatic flow stress of Niobium predicted using the proposed models and compared to experimental results (Nemat-Nasser and Guo, 2000) at 8000s\(^{-1}\) strain rate and indicated initial temperatures.

Figure 5.6 Adiabatic flow stress of Vanadium predicted using the proposed models and compared to experimental results (Nemat-Nasser and Guo, 2000) at 2500s\(^{-1}\) strain rate and indicated initial temperatures.
Figure 5.7 Adiabatic flow stress of Vanadium predicted using the proposed models and compared to experimental results (Nemat-Nasser and Guo, 2000) at 8000s$^{-1}$ strain rate and indicated initial temperatures.

Figure 5.8 Adiabatic flow stress of Tantalum predicted using the proposed models and compared to experimental results (Nemat-Nasser and Isaacs, 1997) at 5000s$^{-1}$ strain rate and indicated initial temperatures.
The results of the model simulations from the above experimental data are also compared with other sets of experimental data. Fig.5.9 shows the temperature variation of the flow stresses obtained experimentally by Nemat-Nasser and Isaacs (1997) at 0.05 strain and 5000s\(^{-1}\) strain rate, Hoge & Mukharjee (1977) at 0.014 strain and 0.0001s\(^{-1}\) strain rate and Bechtold (1955) at 0.014 strain and 0.00028s\(^{-1}\) strain rate as compared with those calculated using the proposed model (Eq.(5.28)). The proposed model, with the parameters obtained using the Nemat-Nasser and Isaacs data, predicts results that agree very well with the data given by Hoge & Mukharjee. The parameter \(Y_a\), however, is changed to 133 MPa in order to get a better agreement with Bechtold (1955) data. This change is used to allow for possible differences in solute and grain size effects.

![Figure 5.9 Proposed model results of the temperature variation of the flow stress, for Tantalum Ta, as compared to experimental data obtained by several authors at different strain rates.](image)

Furthermore, the stress variation with strain rates computed using the proposed model Eq.(5.28), are compared with the experimental data presented by Hoge and Mukharjee (1977) at room temperature and with the single crystal data obtained by Mitchell & Spitizig (1965) at 373\(^{\circ}\)K temperature and Mordike & Rudolph (1967) at 200\(^{\circ}\)K temperature. The comparisons illustrated in Fig.5.10 show very good agreement with the experimental results.
The adiabatic stress strain curves of the plastically deformed specimens presented here are estimated using Eq.(5.29) where the thermo-mechanical parameters are listed in Table 5.2 for all metals used in this study. The incremental accumulation of the temperature during the adiabatic process is calculated by assuming a conversion of 100% plastic work into heat is used for Nb, V and Ta based on experimental results presented by Nemat-Nasser and Guo (2000) and Nemat-Nasser and Isaacs (1997).

![Graph of adiabatic stress strain curves](image)

Figure 5.10 Proposed model results of the strain rate variation of the flow stress, for Tantalum Ta, as compared to experimental data obtained by several authors at different temperatures.

<table>
<thead>
<tr>
<th>Physical parameters</th>
<th>Nb</th>
<th>V</th>
<th>Ta</th>
<th>OFHC Cu</th>
<th>Ti</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho$ (g/cm$^3$)</td>
<td>8.57</td>
<td>6.16</td>
<td>16.62</td>
<td>8.96</td>
<td>4.54</td>
</tr>
<tr>
<td>$c_p$ (J/g.K$^\circ$)</td>
<td>0.265</td>
<td>0.498</td>
<td>0.139</td>
<td>0.383</td>
<td>0.523</td>
</tr>
<tr>
<td>$\zeta$</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>0.9</td>
<td>1.0</td>
</tr>
<tr>
<td>$\mu$ (GPa)</td>
<td>37.0</td>
<td>45.0</td>
<td>60.0</td>
<td>45.0</td>
<td>43.0</td>
</tr>
<tr>
<td>$\mu_o$ (GPa)</td>
<td>70.0</td>
<td>75.0</td>
<td>90.0</td>
<td>77.0</td>
<td>75.0</td>
</tr>
</tbody>
</table>
• **FCC Metals**

The Oxygen Free High Conductivity (OFHC) Copper is used here as an application for the proposed fcc models to show the temperature and strain rate variation of the flow stress. OFHC Cu is an important fcc metal used in the industry due to its high thermal and electrical conductivity and high ductility combined with low volatility which makes this material indispensable in the electronics industry. The material parameters of the proposed two fcc relations (Eq.(5.36) and Eq.(5.42)) are listed in Table 5.3 which are determined by following the same procedure explained in the previous section using the experimental data presented by Nemat-Nasser & Li (1998). Using the same parameters, the proposed fcc models are further compared to other experimental data found in the paper by Johnson and Cook (1988).

<table>
<thead>
<tr>
<th>Model Parameters</th>
<th>OFHC Cu</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Y_d$ (MPa)</td>
<td>25</td>
</tr>
<tr>
<td>$\hat{B}$ (MPa)</td>
<td>1175</td>
</tr>
<tr>
<td>$\tilde{B}$ (MPa)</td>
<td>990</td>
</tr>
<tr>
<td>$Y_d$ or $\hat{Y}_d$ (Mpa)</td>
<td>50</td>
</tr>
<tr>
<td>$k_d$</td>
<td>0.9</td>
</tr>
<tr>
<td>$C_1$</td>
<td>40</td>
</tr>
<tr>
<td>$\beta_2$ (K$^{-1}$)</td>
<td>0.0000351</td>
</tr>
<tr>
<td>$\dot{\varepsilon}_{pe}$ (s$^{-1}$)</td>
<td>$6.97 \times 10^6$</td>
</tr>
<tr>
<td>$q$</td>
<td>3/2</td>
</tr>
<tr>
<td>$p$</td>
<td>1/2</td>
</tr>
</tbody>
</table>

Generally, the adiabatic flow stresses calculated using the proposed fcc relations agree well with most experimental data for several strain rates and initial testing temperature. In Fig.5.11, the adiabatic stress strain calculated using both relations Eq.(5.36) and Eq.(5.42) predict very good results as compared with Nemat-Nasser and Li (1998) experimental data at 4000s$^{-1}$ strain rate and different initial temperatures (77K-996K). Eq.(5.42), however, estimates higher stress values than those calculated by Eq.(5.36) at strains up to 0.45. These differences are generally ascribed to the two different definitions used in calculating the hardening stresses. The flow stresses predicted by the proposed fcc relations are further compared to the experimental results conducted by the same authors at lower and higher strain rates (0.1s$^{-1}$ and 8000s$^{-1}$) as shown in Fig.5.12. The comparison shows good agreement as well.
Figure 5.11 Adiabatic flow stress of OFHC Copper predicted using the proposed models and compared to experimental results (Nemat-Nasser and Li, 1998) at 4000s\(^{-1}\) strain rate and indicated initial temperatures.

Figure 5.12 Flow stress of OFHC Copper predicted using the proposed models and compared to experimental results (Nemat-Nasser and Li, 1998) at strain rates of 8000s\(^{-1}\) (adiabatic) and 0.1s\(^{-1}\) (isothermal) and indicated temperatures.
An assessment of the models parameters determined using the experimental data by Nemat-Nasser & Li (1998) can be made by comparing the adiabatic stress strain results with the experimental data found in the paper of Johnson and Cook (1988) as shown in Fig. 5.13. Overall, the predicted results of Eq. (5.36) correlate well with the experimental data at strain rates of 451s⁻¹, 449s⁻¹ and 464s⁻¹ with initial temperatures of 298K, 493K and 730K respectively. However, Eq. (5.42) overestimates the stress values in most cases. This deviation, however, is part of neglecting the temperature and strain rate effects of the parameter $k_a$.

Figure 5.13 Adiabatic flow stress of OFHC Copper predicted using the proposed models and compared to experimental results (Johnson and Cook, 1988) at different strain rates of and temperatures.

In the case of copper, the prediction of the adiabatic stress strain curves predicted by the present model is obtained based on the assumption of conversion 90% of the plastic work deformation to heat calculated using the same relation defined in Eq. (5.29) with the thermo-mechanical parameters listed in Table 5.2.
HCP Metals

The hcp commercially pure titanium (Cp Ti) used in this study has an axial ratio of c/a = 1.587, and is strongly plastically anisotropic as indicated by Nemat-Nasser et al (1999) who conducted both adiabatic and isothermal testing on both annealed and as received samples at low and high strain rates and temperatures. The experimental results clearly show that this material (Ti) is widely affected by the dynamic strain aging phenomenon over most strain rates and temperatures. At strain rates of 0.001s\(^{-1}\) and 0.1s\(^{-1}\), the DSA effect starts clearly at temperature values of 296K up to 500K continuing slightly up to 600K for the case of isothermal process. At higher strain rates with adiabatic deformation (2200s\(^{-1}\) and 8000s\(^{-1}\) strain rates), the appearance of the DSA effects starts at 400K temperature continuing up to 1000K temperature.

As mentioned earlier, the proposed hcp models (Eq.(5.45) & Eq.(5.46)), which did not take into consideration the dynamic strain aging effects, are possibly not accurate in predicting both the adiabatic and the isothermal flow stresses in the strain rate and temperature ranges where the DSA effects are active. This indicates that the flow stresses predicted by the proposed two hcp relations will more likely underestimate the experimental results in theses ranges. The proposed model parameters for titanium are determined using the experimental data presented by Nemat-Nasser et al. (1999) using a combination of the bcc and fcc procedures described earlier. These parameters are listed in Table 5.4. In fact, the proposed hcp model is derived based on the fact that the plastic deformation behavior of most hcp metals shows a combination of both bcc and fcc plastic deformation behaviors.

Table 5.4 The proposed hcp models parameters for Titanium.

<table>
<thead>
<tr>
<th>Model Parameters</th>
<th>Ti</th>
</tr>
</thead>
<tbody>
<tr>
<td>(Y_a) (MPa)</td>
<td>20</td>
</tr>
<tr>
<td>(\hat{B}) (MPa)</td>
<td>2050</td>
</tr>
<tr>
<td>(\hat{B}) (MPa)</td>
<td>2025</td>
</tr>
<tr>
<td>(Y_d) or (\hat{Y}_d) (MPa)</td>
<td>115</td>
</tr>
<tr>
<td>(k_a)</td>
<td>1.31</td>
</tr>
<tr>
<td>(C_1)</td>
<td>0.9</td>
</tr>
<tr>
<td>(\beta_2) (K(^{-1}))</td>
<td>0.0000433</td>
</tr>
<tr>
<td>(\dot{\varepsilon}_p) (s(^{-1}))</td>
<td>(1.95 \times 10^7)</td>
</tr>
<tr>
<td>(q)</td>
<td>3/2</td>
</tr>
<tr>
<td>(p)</td>
<td>1/2</td>
</tr>
<tr>
<td>(\bar{B}) (MPa)</td>
<td>90</td>
</tr>
<tr>
<td>(B) (MPa)</td>
<td>85</td>
</tr>
<tr>
<td>(N)</td>
<td>0.43</td>
</tr>
</tbody>
</table>
Next, assessments of the proposed hcp models are made by comparing the isothermal stresses predicted using both Eq.(5.45) and Eq.(5.46) to the experimental results by Nemat-Nasser et al. (1999) at 0.001s strain rate and different temperatures as shown in Fig. 5.14. The comparison between the predicted results and the experimental data shows good agreement at temperature values of 77K, 673K and 773K whereas they underestimate the experimental results at other temperatures due to the effect of DSA. In Fig.5.15, the adiabatic stress-strain results predicted by the proposed hcp models are compared to the experimental data at a strain rate of 2200s\(^{-1}\) and different initial temperatures. Similarly, the comparison agrees well at temperatures where the DSA is inactive (77K and 296K) whereas, the proposed models predict lower results at temperatures where the DSA effect is dominated.

![Figure 5.14 Isothermal flow stress of Titanium predicted using the proposed models and compared to experimental results (Nemat-Nasser et al., 1999) at 0.001s\(^{-1}\) strain rate and indicated temperatures.](image)

The flow stress prediction of the proposed hcp models are further compared to the experimental results at the strain rate of 0.1s\(^{-1}\) for the case of isothermal deformation process and at the 8000s\(^{-1}\) strain rate for the case of adiabatic deformation as shown in Fig.5.16. Similar comparison results are concluded for both strain rates. In comparing the flow stress results predicted by the proposed two hcp relations, it is found that Eq.(5.46) deviates largely at higher strain rates predicting higher stress values than those calculated using Eq.(5.45). This deviation, however, appears noticeably at strain values up to 30%.
Figure 5.15 Adiabatic flow stress of Titanium predicted using the proposed models and compared to experimental results (Nemat-Nasser et al., 1999) at 2200s$^{-1}$ strain rate and indicated initial temperatures.

Figure 5.16 Flow stress of Titanium predicted using the proposed models and compared to experimental results (Nemat-Nasser et al., 1999) at strain rates of 0.01s$^{-1}$ (isothermal) and 8000s$^{-1}$ (adiabatic) and indicated temperatures.
For the case of titanium, a 100% of the plastic work generated during the deformation process under different strain rates is converted to heat as given by Nemat-Nasser et al. (1999). The temperature accumulation during the plastic deformation is, therefore, calculated using Eq.(5.29) with the thermo-mechanical parameters for Ti given in Table 5.2.

5.4.3 Discussions

In investigating the proposed bcc, fcc and hcp models, the definition of the thermal component of the flow stress is nearly the same for all kinds of metals. However, the model parameters values and accordingly the physical quantities differ from metal to metal. In addition, it is found that the thermal stress for all bcc metals used in this study is independent of strain. That is to say, the effect of the parameter $\beta_1$, which represents the effect of the evolution of the mobile dislocation density that is thermally affected through Orowan’s equation is almost negligible. This, however, supports the experimental observations which indicate that the thermal stresses for most bcc metals are strain independent and mainly controlled by the yield stress. This behavior can be interpreted physically as the resistance of the initial dislocation motion by the Peierls barriers. On the other hand, the thermal component of the flow stress for fcc metals depends mainly on the strain through the evolution of the mobile dislocation density defined by the parameter $\beta_1$ and also through the evolution of the remaining part (mainly forest) of the dislocation density introduced through the hardening parameters definitions given by Eq.(5.37) or Eq.(5.43). For the case of hcp metals, the strain dependence of the thermal stresses is introduced only through the hardening parameters whereas; the effect of $\beta_1$ is very small and can be neglected. Fig.5.17 shows the thermal component of the flow stresses as varying with the plastic strain using the proposed models for V, Nb, Ta, Ti and OFHC Cu at strain rate and temperature values of 8000s$^{-1}$ and 296K respectively.

The consequence of the variation of the parameter $\beta_1$ with plastic strain for fcc metals is observed in determining the values of the critical temperature ($T_{cr}$) that become strain dependent as well. In contrast, the critical temperature for bcc and hcp metals does not depend on plastic strain. In fact, $T_{cr}$ is defined as the highest temperature value that corresponds to the minimum thermal stresses (zero thermal stress) observed during the degradation process of the flow stress as the material temperature increases. Fig.5.18 shows the strain rate variation of $T_{cr}$ calculated using Eq.30 for the five metals used in this study at 0.1 plastic strain. It is found that $T_{cr}$ values increase with strain rates increase. Also, the critical temperature values for OFHC Cu and Ti are higher than those obtained for the three bcc metals. This disparity may be attributed to the variation of the reference plastic strain rate $\dot{\varepsilon}_{po}^i$ values and also to the different $\beta_2$ values that is mainly related to the Gibbs free energy $G_o$. Since $\dot{\varepsilon}_{po}^i$ values for all metals used in this study are approximately of the same order, the value of $G_o$ is considered the major factor that affects the variation of $T_{cr}$ values from one metal to another at a fixed strain rate. The higher the activation energy values (around 2.4, 2.0, 0.92, 0.62, 0.58 eV/atom for Cu, Ti, Ta, V, and Nb respectively) needed to overcome the barriers the higher the critical temperature values achieved. Actually, the thermal stress is interpreted as the resistance of the barriers to the dislocation movement, thus, the barriers that need higher activation energy to be overcome.
require also higher temperature to produce this thermal energy until the resistance of these barriers is vanished which indicates zero thermal stresses.

Figure 5.17 Strain variations of the thermal stresses for several metals using the proposed models at 8000s⁻¹ strain rate and 296K⁰ temperature.

Table 5.5 Numerical values for the physical quantities used in deriving the proposed models parameters for Nb, V, Ta, OFHC Cu and Ti.

<table>
<thead>
<tr>
<th>Physical parameters</th>
<th>Nb</th>
<th>V</th>
<th>Ta</th>
<th>OFHC Cu</th>
<th>Ti</th>
</tr>
</thead>
<tbody>
<tr>
<td>$G_o$ (eV/atom)</td>
<td>0.58</td>
<td>0.62</td>
<td>0.92</td>
<td>2.4</td>
<td>2.0</td>
</tr>
<tr>
<td>$b$ (Å)</td>
<td>3.3</td>
<td>3.1</td>
<td>2.9</td>
<td>2.5</td>
<td>3.0</td>
</tr>
<tr>
<td>$v_o$ (m/sec)</td>
<td>$8.57 \times 10^3$</td>
<td>$8.3 \times 10^3$</td>
<td>$7.71 \times 10^3$</td>
<td>$3.97 \times 10^3$</td>
<td>$5.1 \times 10^3$</td>
</tr>
<tr>
<td>$\rho_{ni}$ (m⁻²)</td>
<td>$5 \times 10^{12}$</td>
<td>$4.9 \times 10^{12}$</td>
<td>$4.1 \times 10^{12}$</td>
<td>$1.4 \times 10^{13}$</td>
<td>$2.55 \times 10^{13}$</td>
</tr>
<tr>
<td>$\rho_{fi}$ (m⁻²)</td>
<td>$2 \times 10^{12}$</td>
<td>$2 \times 10^{12}$</td>
<td>$2 \times 10^{12}$</td>
<td>$1.1 \times 10^{13}$</td>
<td>$2.69 \times 10^{13}$</td>
</tr>
<tr>
<td>$\rho_s$ (m⁻²)</td>
<td>$4.5 \times 10^{15}$</td>
<td>$1.5 \times 10^{15}$</td>
<td>$1.1 \times 10^{15}$</td>
<td>$6.1 \times 10^{15}$</td>
<td>$9.0 \times 10^{15}$</td>
</tr>
<tr>
<td>$A_o$ (m²)</td>
<td>$26b^2$</td>
<td>$27b^2$</td>
<td>$27b^2$</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$D_s$ (mm)</td>
<td>0.013</td>
<td>0.016</td>
<td>0.0375</td>
<td>0.073</td>
<td>0.125</td>
</tr>
<tr>
<td>$A'_o$ (m²)</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>$585b^2$</td>
<td>$321b^2$</td>
</tr>
<tr>
<td>$A''_o$ (m²)</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>$30b^2$</td>
<td>$18b^2$</td>
</tr>
</tbody>
</table>
In general, most metals contain initial amount of dislocations which are naturally exited or generated through the manufacture process. These dislocation densities, however, help metals deform plastically until a level where no further dislocations generation are allowed which indicates that the saturation limit of dislocation densities is reached. The initial and saturated values of the dislocation densities, however, differ from metal to metal. The numerical values of the physical nano- and micro-quantities used in defining the proposed models that are obtained for the indicated metals are listed in Table 5.5. Although these quantities are defined based on the model parameters that are fitted experimentally, their values are found to be reasonable when compared to those available in the literature. The initial dislocation density values are fixed and set around $5 \times 10^{12} \text{m}^{-2}$ for the case of bcc metals and little higher for fcc and hcp metals. Consequently, the saturated values of these dislocation densities are found to be in the order of $10^{15} \text{m}^{-2}$ for all metals. In fact, the effect of initial dislocation density enters the proposed models through the thermal component of the flow stress. This effect, however, is expected to be higher for bcc metals than other metal structures due to the fact that the thermal stress of bcc metals is nearly related to the yield stress (Peierls stress) and not affected by the dislocation density evolution with plastic strain. That is to say, the yielding strength is less when the material contains high initial dislocation density and vice versa. Once the material yields, the evolution of dislocation density along with the initial dislocation density contribution plays a crucial role in determining the flow stress and particularly the thermal stress as in the case for most fcc metals and slightly less for hcp metals. Fig.5.19 shows, for all metals presented here, the variation effect of initial dislocation density generated inside the
material on the flow stress at 298K and 8000s\(^{-1}\) temperature and strain rate respectively. It is obvious that the flow stress decreases with the increase of the originated (initial) dislocation density. The decreasing slopes for bcc metals are higher than those for hcp and fcc metals which supports the abovementioned argument.

Figure 5.19 Initial dislocation density variation of the flow stress, for several metals, computed at 8000s\(^{-1}\) strain rate and 298K\(^{\circ}\) temperature.

It is interesting to note that the Helmholtz free energy values for fcc metals are higher than those found for bcc metals which indicates that the dislocation interaction mechanism necessitates higher activation energy than the Peierls mechanism in overcoming the short-range barriers. Consequently, the waiting time needed by the dislocation to overcome an obstacle is less for bcc \([t_w=O(10^{-12}s)]\) than those required for fcc metals \([t_w=O(10^{-11}s)]\) (Kocks et al., 1975). Therefore, the reference velocity \(v_0 = d / t_w\) values of fcc metals are less than the ones obtained for bcc metals as illustrated in Table 5.5. Moreover, the average values of the Burger vector are chosen to be around 3.3, 3.1, 2.9, 2.5 and 3.0Å for Nb, V, Ta, OFHC Cu and Ti respectively.

In the proposed models, the following typical values; of 1.5 and 0.5 for the exponents \(p\) and \(q\) respectively are used for all metals. Unfortunately, the value of \(\hat{\sigma}\) in the thermal component of the bcc flow stress is sensitive to the choice of \(p\) which characterizes the tail of the obstacle. This sensitivity, however, is less for the case of fcc and hcp metals in obtaining
the parameters $Be_p^\sigma$ and $Y_d$. In fact, $\hat{\sigma}$ represents a parameter which refers to a state of zero Kelvin temperature. It should be noted here that the determination procedure of the proposed bcc, fcc and hcp model parameters is simple and straightforward. However, more caution is required in the numerical techniques used in obtaining the hardening parameters that produce not only the hardening stresses but also the temperature evolving with the plastic work.

Furthermore, two different definitions for the hardening stresses are presented. The first definition is derived based on experimental observations which indicate that the fitting of the hardening stresses can be achieved using the power law definition. On the other hand, the second definition of the hardening parameters is derived using the concept of dislocation density evolution with plastic strain. Both definitions are used in predicting the isothermal and adiabatic flow stresses and compared with the available experimental data. It is found that the power-law definition of the plastic hardening stresses predicts more accurate results than the other definition in most experimental comparisons at different strain rates and temperatures. Actually, the deviation of the predicted results may be attributed to the use of constant values for the parameter $k_a$ assumed in the derivation of the proposed model.

For the bcc metals presented here, it is found that the dynamic strain aging activates when the temperature reaches its critical values. In this stage, dislocations require higher temperatures to overcome the obstacle which consequently increases the waiting time of these dislocations before the obstacle. This, in turn, helps in activating the dynamic strain aging by strengthen the obstacles through the diffusion process of the atoms and accordingly increasing suddenly the flow stress throughout the deformation process. On the other hand, the dynamic strain aging effect is observed in titanium over a wide range of temperatures and at all strain rates. It is found that the DSA phenomenon activates at different temperature depending on the strain rate values. These temperature values increase as the strain rates increase. In the case of OFHC Copper, however, the dynamic strain aging is not observed for most of the strain rates and temperatures used in the presented experimental comparisons. The effect of DSA on the plastic flow simulation along with the strain rate and temperature dependence of the dislocation annihilation factor $k_a$ will be investigated in future work.
CHAPTER 6

THERMODYNAMIC CONSISTENT FORMULATIONS OF VISCOPLASTIC DEFORMATIONS OF BCC AND FCC METALS

6.1 Introduction

Plastic/viscoplastic deformation in metals is a very complex phenomenon originating from highly nonlinear dynamical processes associated with microscopic defects, such as dislocations, voids, and microcracks. While dislocations and their mutual interactions determine the material strength in the absence of other internal defects, they tend to self-organize in the form of patterns. This results into a heterogeneous field of deformation at the microscale although the overall macroscopic field is thought to be homogeneous (Zbib and Rubia, 2002). There has been a significant progress made over the years in the development of theories of plasticity and viscoplasticity for the phenomenological representation of inelastic constitutive properties. In particular, mathematical modeling of metal viscoplasticity developed based on the so-called internal state variable formalism in the thermodynamics of irreversible process. A large number of specialized forms of these modern unified viscoplastic models (e.g., isotropic or anisotropic, fully associative or non-associative, isothermal or non-isothermal, etc.) have been successfully applied to different metals with different crystal structures (Coleman and Gurtin, 1967; Lubliner, 1973; Germain et al., 1983; Lemaitre and Chaboche, 1990; Chaboche, 1989; Arnold and Saleeb, 1994; Robinson and Duffy, 1990; Arnold et al., 1995, 1996; Robinson et al., 1987; Freed and Walker, 1993; Simo and Taylor, 1985, 1986; Voyiadjis and Abed, 2005; Abed and Voyiadjis, 2005).

Experimental observations indicated that the plastic deformation of metals differs from one to another depending on the material crystal structure. This necessitates a proper definition for the material flow stress that can reflect a realistic simulation of the deformation response over a wide range of temperatures and strain rates. As a matter of fact, the material behavior depends to a high degree on the rate of deformation and temperature. At very low, i.e. quasistatic rates of deformation we deal with isothermal processes as the heat produced by dissipation of mechanical energy in the system dissipates immediately outside due to heat flow and radiation. Deformations with higher rates of loading are approximately adiabatic since the energy produced in the system cannot flow off because of the short period of time. Therefore, this leads to an increase in temperature which indicates a strong interaction between the influences of temperature and deformation rate. Unfortunately, most of the recent viscoplastic models have not considered both the role of metal crystal structure and the function of the coupling effect of temperature and strain rates on the adiabatic deformations of metals. In contrast, we found that most of these models use the same yield function for different metals with different crystal structures. Moreover, they tend to decouple the effects of temperature and strain rates as is the case of the Johnson-Cook model. This latter model has been extensively used in the literature to represent the dynamic yield surface for viscoplastic deformation (e.g., Borvik et al., 2001).

Since modern structures exhibit a strong rate dependency especially at elevated temperatures, the constitutive relations which have been developed to describe the behavior of
different types of metals must be able to reproduce these facts. Processes related with high velocities therefore must be described by a rate-dependent viscoplasticity model whereas the same constitutive relations for vanishing velocities must turn over to a rate-independent plasticity. Prior to establishing constitutive relations that can fulfill these conditions; a proper physical interpretation of the phenomena observed during inelastic deformation is needed. This means that the different mechanisms that can explain the dissipation implied by internal changes of the material are to be analyzed (Bruhns, 1987). It is known from appropriate microscopic investigations that in a temperature and strain rate spectrum, in general, different regions can be observed reflecting different mechanisms of inelastic deformation. These are; (1) athermal mechanisms characterized by a yield stress (e.g. fcc metals) or hardening stress (e.g., bcc metals) relatively insensitive to the strain rate; (2) thermally activated dislocation motion characterized by a more noticeably , temperature and rate sensitivity of the yield and hardening stresses.

Classical constitutive models of phenomenological plasticity/viscoplasticity rely heavily on yield functions to distinguish plastic flow from reversible elastic deformation. In this work, two different definitions for the dynamic and static yield functions based on the von Mises yield criterion are introduced for bcc and fcc metals. These are derived based on the concept of thermal activation analysis as well as dislocation interaction mechanisms. It is clear that material rate dependence, no matter how small, leads to well posed boundary value problems with unique solutions. This can be viewed in terms of material rate dependence implicitly introducing a length scale into the boundary value problem formulation. However, the question remains as to whether or not this is the relevant length scale. In this chapter, an explicit definition for a proposed length scale parameter is introduced for both bcc and fcc metals.

Thermodynamics with internal variables offers a solid framework to introduce constitutive equations. It offers both a guideline and some constraints for the choice of thermodynamically consistent evolution equations. A special form uses the notion of a standard generalized material, where the complete thermo-elastic-inelastic behavior is defined from the knowledge of two potentials. These are namely the thermodynamic potential that describes the present state and the dissipative potential for their irreversible evolutions. Introducing mechanical constitutive models into a thermodynamic framework allows the partition of the plastic work into the energy stored by the material and the one dissipated away as heat. In this chapter, a multi-scale constitutive law describing the behavior of polycrystalline bcc and fcc metals will be introduced based on consistent thermodynamic formulations.

6.2 Static and Dynamic Yield Surfaces

In this section, a brief discussion of two different definitions of the yield function based on the von Mises yield criterion is presented for bcc and fcc metals. These definitions were derived (Voyiadis & Abed, 2005 ; Abed & Voyiadis; 2005) based on the concept of thermal activation analysis along with dislocation interaction mechanisms. The proposed definitions are applicable for low (static) and high (dynamic) strain rates over a wide range of
temperatures. A coupled temperature and strain rate effect is considered for dynamic/adiabatic deformation.

### 6.2.1 Yield Function for BCC Metals

Experimental observations for most bcc metals show that at a given strain rate and different temperatures or at a given temperature and several strain rates, the variation of the stress strain curves appear only at the yielding point whereas the hardening curves are almost identical. In this regard, the proposed definition of the yield function for bcc metals is additively decomposed into athermal and thermal components. The former component, which is independent of strain rate, is related to strain hardening as well as to a small portion of the yield stress. The latter component is mainly controlled by the yield stress which shows a coupled effect of temperature and strain rate as introduced through the thermal activation analysis. Thus, the general form of the yield function \( f \) for bcc metals may be given as follows:

\[
f = \sigma_{eq} - Y_a - R(p) - Y_{th}(\dot{p}, T)
\] (6.1)

where \( T \) is the Kelvin temperature, \( p \) is the isotropic hardening and \( \dot{p} \) is the strain rate. Here, the athermal yield stress, \( Y_a \), and the hardening, \( R \), represent the athermal stresses while, the thermal stress is introduced through the yield stress \( Y_{th} \). The equivalent stress, \( \sigma_{eq} \), is defined based on von Mises yield criterion in terms of the deviatoric stress, \( \tau \), and back stress, \( X \), as shown below:

\[
\sigma_{eq} = \left( 3(\tau_{ij} - X_{ij})(\tau_{ij} - X_{ij})/2 \right)^{1/2}
\] (6.2)

Knowing that the deviatoric part of the normal stress is defined as follows:

\[
\tau_{ij} = \sigma_{ij} - \frac{1}{3} \sigma_{mm} \delta_{ij}
\] (6.3)

where \( \sigma_{mm} \) denotes the hydrostatic part of stress and \( \delta_{ij} \) is the Kronecker delta.

In this work, the definition of strain hardening is introduced in two different forms; the first definition is evaluated from an assumed power law dependent on strain. This assumption is observed experimentally and used by many authors (Zerilli & Armstrong, 1987; Nemat-Nasser et al., 1999)

\[
R = B p^m
\] (6.4)

where \( B \) and \( m \) are the hardening parameters. The second definition of strain hardening is derived after considering the plastic strain evolution of the forest dislocation density through the Taylor dislocation relation as shown below (Voyiadjis & Abed, 2005):
\[ R = \bar{B} \left( 1 - e^{-kp} \right)^{1/2} \]  

(6.5)

The parameter \( \bar{B} \) is defined in terms of the microstructure quantities as follows:

\[ \bar{B} = \tilde{m} \alpha \mu b \left( M / k \right)^{1/2} \]  

(6.6)

where \( b \) is the magnitude of the Burgers vector, \( \tilde{m} \) is the orientation factor that relates the shear stress to the normal stress, \( \sigma = \tilde{m} \tau \) where \( \tilde{m} = \sqrt{3} \) for the case of the von Mises flow rule, \( \mu \) is the shear modulus, and \( \alpha \) is an empirical coefficient taken to be 0.3 for most metals. The parameters \( M \) and \( k \) represent the dislocation multiplication and annihilation factors respectively, which are implemented in the evolution equation of the forest dislocation density.

The parameter \( \tilde{m} \) is defined in terms of the microstructure physical quantities as follows:

\[ \tilde{m} = \frac{1}{2} \frac{\mu}{\sigma} \]  

The thermal yield stress given in Eq.(6.1) may be interpreted physically as the resistance of the dislocation motion by the Peierls barriers (short-range barriers) provided by the lattice itself. Its definition introduces the coupling effect of absolute temperature \( T \) and strain rate \( \dot{\rho} \) such that:

\[ Y_{th} = \hat{Y} \left( 1 - \left( \beta_1 T - \beta_2 T \ln \left( \frac{\dot{\rho}}{\dot{\rho}_s} \right) \right)^{1/q_1} \right)^{1/q_2} \]  

(6.7)

where \( \hat{Y} \) denotes the threshold yield stress at which the dislocations can overcome the barriers without the assistance of thermal activation. The constants \( 1.0 < q_1 \leq 2.0 \) and \( 0 < q_2 \leq 1.0 \) define the shape of the short-range barriers. Their typical values, however, are 3/2 and 2 for the former that is equivalent to a triangle obstacle profile near the top and 2/3 and 1/2 for the latter which characterizes the tail of the obstacle (Kocks, 2001).

In equation(6.7), the material parameters \( \beta_1 \) and \( \beta_2 \) are defined in terms of the microstructure physical quantities such that:

\[ \beta_1 = \frac{K}{G_o} \ln \left( \frac{\dot{\rho}_s}{\dot{\rho}_s} \right) \]  

(6.8)

\[ \beta_2 = k / G_o \]  

(6.9)

where \( K \) is the Boltzmann’s constant, \( G_o \) is the Gibbs energy at zero Kelvin temperature, \( \dot{\rho}_s \) is a very low (static) strain rate, and \( \dot{\rho}_s \) is a reference strain rate that is proportional to a frequency factor \( \omega_s = 1 / t_{wo} \), where \( t_{wo} \) is the time that dislocations wait at an obstacle, and \( t_{wo} \) represents its lowest value which is of order equal or less than \( 10^{-13} \) s for most bcc metals. Voyiadjis and Abed (2005) derived the following definition of the reference strain rate in terms of the microstructure physical quantities:

\[ \dot{\rho}_s = \bar{m} \rho_d \omega_o \]  

(6.10)
where $\bar{m}$ can be interpreted as the Schmidt orientation factor, $d$ is the average distance the dislocation moves between the obstacles, $\rho_i = l_i^{-2}$ is the initial dislocation density, and $l_i$ is the initial dislocation distance.

- **Static and Athermal Deformation**

For most bcc metals, the elastic deformations are negligible in comparison with the plastic deformations, and therefore, the total strain rate is assumed to be related mainly to the plastic/viscoplastic strain rate. In static conditions, i.e. at a very low strain rate $\dot{\rho} \leq \dot{\rho}_s$, the thermal part of the yield stress is mainly governed by temperature effect whereas the effect of the strain rate is neglected. Although it may change from a martial to another, this static strain rate is normally taken to be equal to a value less that $10^{-6}$ s$^{-1}$ at which the time of loading is enough for the heat, accumulated due to the plastic work, to dissipate outside the material. In this case the elasto-plastic deformation turns into isothermal conditions and depends mainly on the initial loading temperature. Therefore, substituting Eq.(6.7) into Eq.(6.1), after setting $\dot{\rho} = \dot{\rho}_s$, the static rate-independent yield function for bcc metals is defined as follows:

$$f_s = \sigma_{eq} - Y_o - R - \dot{\gamma} \left( 1 - (\beta_o T)^{1/q_0} \right)^{1/q_2} \quad \text{for } \dot{\rho} \leq \dot{\rho}_s \quad (6.11)$$

In this case, the isothermal elastic-plastic deformation is encountered when the temperature is kept constant throughout the plastic deformation, i.e. $T = T_o$ where $T_o$ is the initial testing temperature. In the classical elasto-plastic flow theory, the static yield function distinguishes between the elastic and inelastic states of deformation. It may also be used to distinguish between the static and dynamic states of rate-dependent deformation. That is

$$f_s < 0 \quad \rightarrow \text{static elastic state},$$

$$f_s = 0 \quad \rightarrow \text{static inelastic state},$$

$$f_s > 0 \quad \rightarrow \text{dynamic inelastic state}. \quad (6.12)$$

The thermal component of the flow stress usually decreases as the temperature increases until it vanishes when the temperature reaches or exceeds a critical value $T_{cr}$ which defines, in the temperature variation of the stress curve, the starting point of the constant stress. In turn, the deformation will be controlled by the athermal component of the flow stress which is non-thermally activated and attributed to the structure of the material, i.e., to the resistance of long-range obstacles that can not be overcome by introducing thermal energy. Since the thermal stress is non-negative, the general form of $T_{cr}$ is determined after setting the term inside the exterior parenthesis in the right hand side of Eq.(6.7) to zero such that:

$$T_{cr} = (\beta_i - \beta_o \ln(\dot{\rho}/\dot{\rho}_s))^{-1} = (\beta_o \ln(\dot{\rho}_o/\dot{\rho}))^{-1} \quad (6.13)$$
It is obvious from the above equation that the athermal temperature required in order for the thermal stresses to vanish increases as the rate of loading increases. In a static deformation, however, the critical temperature becomes constant and corresponds to the static strain rate. Thus, at \( p = \dot{p}_s \), the athermal temperature takes the following constant value:

\[
T_{cr} = (\beta_1)^{-1} = \frac{G_o}{K \ln \left( \dot{p}_a / \dot{p}_s \right)}
\]  

(6.14)

Once the temperature reaches or exceeds the above values defined in Eq.(6.13) or (6.14), the flow stress defined in Eq.(6.1) is reduced, for most bcc metals, to:

\[
f_{ath} = \sigma_{eq} - Y_a - R
\]

(6.15)

where \( f_{ath} \) denotes the athermal rate-independent yield function which is called in this work as the lower limit function. This limit demonstrates the maximum effect of temperature rising on the degradation process of the flow stress. Eq.(6.15) is employed here to distinguish between the thermal and athermal states, that is

\[
f_{ath} \leq 0 \quad \rightarrow \quad \text{athermal state,}
\]

\[
f_{ath} > 0 \quad \rightarrow \quad \text{thermal state}
\]

(6.16)

Before we advance to the rate-dependent formulation, we should recognize the difference between the static and athermal yield functions; the former one corresponds to a specific static strain rate in which the effect of material viscosity is assumed to be negligible. The latter one, on the other hand, represents the lowest inelastic temperature- and rate-independent surface. Though, \( f_a = f_{ath} \) if \( T \geq T_{cr} \), the static yield function should never be less than the athermal yield function (see Figure 6.1).

- **Dynamic Deformation**

  It is well known that the strain localization behavior cannot be characterized using the classical theory of plasticity (rate-independent plasticity) since it does not incorporate material length or time scales and consequently cannot predict mesh insensitivities. A viscoplastic formulation, therefore, helps in characterizing the material rate-dependent deformation and in introducing a physical length scale that plays a crucial role in regularizing some problems encountered in the finite element computations.

  For the case of bcc metals, the coupling effect of the loading rate and deformation temperature is introduced through the thermal component of the yield stress. In this regard, the dynamic yield surface, i.e. at \( \dot{p} > \dot{p}_s \), is defined after substituting Eq.(6.7) into Eq.(6.1), as follows:
In adiabatic conditions for the case of bcc metals, viscoplastic deformation, in its early stages, is controlled by the effect of the strain rate on the yield stress (resistance of the short-range obstacles); the higher the strain rate, the more stiff the metal behaves. This behavior is attributed to the rapid accumulation of dislocation forests which, in turn, work as obstacles preventing the movement of mobile dislocations (surface slipping). Consequently, a large amount of stress is required for the mobile dislocations to overcome these barriers and accordingly a significant expansion of the dynamic yield surface is encountered. In this way, the above yield surface expands until it reaches its maximum, $f_{\text{max}}$, which is termed in this work as the upper limit function such that:

$$f_{\text{max}} = \sigma_{eq} - Y_a - R - \dot{\gamma}$$ (6.18)

where the threshold yield stress $\dot{\gamma}$ represents the highest visco-stress value that a bcc metal may reach that corresponds to a very high strain rate $\dot{\gamma} = \dot{\rho}$ at which the obstacles are destroyed indicating a material fracture. This state of deformation can also be achieved when the temperature reaches the value of zero indicating a very high viscosity of the solid. Therefore, within the framework of continuum mechanics, $f_{\text{max}}$ is utilized to distinguish between the admissible and inadmissible states, that is

$$f_{\text{max}} < 0 \quad \rightarrow \quad \text{admissible state}$$

$$f_{\text{max}} \geq 0 \quad \rightarrow \quad \text{inadmissible state.}$$ (6.19)

In contrast, once dislocations overcome the obstacles, in the admissible state of deformation, plastic strains start accumulating inside the metal causing a significant amount of plastic work which converts to heat. Since there is not enough time for it to dissipate outside, the heat remains inside the material and increases as the plastic strain increases leading to a considerable degradation of the solid viscosity. As a result, the thermo-visco-stress diminishes as the material temperature evolves causing remarkable softening during the material deformation. In this case, the dynamic yield surface gets smaller until it reaches its lower limit, Eq.(6.15), at very high temperatures ($T \rightarrow T_{cr}$) (see Figure 6.1 for further illustration).

Next, a proper definition for the magnitude of the viscoplastic flow is required in order to characterize the dynamic behavior of the material. The viscoplastic multiplier $\dot{\lambda}^{vp}$, as will be derived in the next section, is found to be equivalent to the accumulated plastic strain, $\dot{\lambda}^{vp} = \dot{\rho}$ for the von Mises plasticity. In this section, we will introduce two different definitions for $\dot{\lambda}^{vp}$; the first relation is obtained analogous to the one defined in the well-known viscoplastic model of Perzyna whereas, the second definition is derived after utilizing the same concept used in the Consistency model.
• Perzyna Model

Viscoplasticity is first introduced through the well-known overstress relation of Perzyna (1966) which defines a convex elastic domain in the space of stress and internal variables. The main feature of this model is that the yield function used for describing the viscoplastic strain can become larger than zero; this effect is known as ‘overstress’. Thereby, the magnitude of the viscoplastic flow characterized by the viscoplastic multiplier, $\dot{\lambda}_{vp}$, is proportional to or nonlinear function of the overstress,

\[
\dot{\lambda}_{vp} = \frac{\varphi(f_s)}{\eta_{vp}} \tag{6.20}
\]

where $\eta_{vp}$ is a relaxation time (a viscosity parameter), $\varphi$ are the McCauly brackets with $\langle x \rangle = 0.5 \left( x + |x| \right)$, and $\varphi$ is an arbitrary dimensionless function of the overstress that depends on the static yield function $f_s$ which is considered as the rate-independent yield function. According to Simo (1989), the overstress function $\varphi$ must fulfill the following conditions.

Figure 6.1 Pictorial description of (a) static/dynamic yield functions (b) thermal/athermal yield functions for bcc and fcc metals.
\( \varphi(f_s) \) is continuous in \([0, \infty)\)
\[
\varphi(0) = 0 \rightarrow \dot{\lambda}^{vp} = 0,
\]
so that a rate-independent elastic-plastic model is recovered if \( \eta \rightarrow \) its minimum \( (\eta_0) \), which represents the value at which the viscosity is negligible. In this regard, the following widely-used expression for \( \varphi \) is employed by many authors:
\[
\varphi(f_s) = \left( \frac{f_s}{K} \right)^N
\]
where \( N \) is a calibration parameter. The parameter \( K \), which is used to normalize the overstress function, and is chosen as the initial yield stress (e.g., Desai and Zhang, 1987; Simo, 1989; Sluys, 1992; Wang et al., 1997; Heeres et al., 2002). It may also be used as the hardening stress or the combination of hardening and the yield stresses.

As explained earlier, the viscosity of a solid is mainly affected by the temperature of the viscoplastic deformation. However, this effect is not explicitly included in the above definition of the Perzyna model. The temperature effect is considered very crucial in thermo-viscoplastic deformation particularly in adiabatic conditions. Therefore, in order for the relaxation time to approach its minimum value, an explicit viscosity-temperature relationship is required to impose the effect of the accumulated heat on the adiabatic deformation. This mechanism was avoided by many authors by, inappropriately, introducing an uncoupled temperature-rate effect on the dynamic yield stress. In this kind of modeling, which represents an unrealistic behavior of viscoplastic adiabatic deformation, the viscosity parameter \( \eta \) used in Eq.(6.20) is set to a constant, that is related to a reference value and is normally taken as the minimum, of order \( O(10^{-06}) \), throughout viscoplastic deformation. Having set \( \eta \) to its minimum, the yield stress \( K \) should correspond to a reference temperature and to a very high strain rate. In other words, the normalized overstress function defined in Eq.(6.22), should be chosen such that the overstress reaches its maximum (value of 1) when the strain rate approaches higher values at which \( \eta^{vp} \dot{\rho} \rightarrow 1 \) regardless of the constant value of \( N \). The above argument can mathematically be proven by employing the well-known relationship between the thermo-visco-stress \( \sigma_v^{th} \) and both the temperature and strain rate:
\[
\sigma_v^{th}(T, \tilde{K}, \dot{\rho}) = \bar{\eta} \dot{\rho}
\]
where \( \bar{\eta} \) (MPa.s) denotes the viscosity coefficient that depends on the temperature and the material stiffness \( \tilde{K} \). For models with decoupling effect of temperature and strain rate, the thermo-visco-stress is decomposed additively into visco- and thermal-stress components such that:
\[
\sigma_v^{th} = \sigma_v + \sigma_{th}
\]
where, in this case, the visco-part of the flow stress $\sigma_v$ is defined by substituting Eq.(6.22) into Eq.(6.20) and with simple manipulations one obtains:

$$\sigma_v = \left( \eta^{vp} \dot{p} \right)^{1/N} K$$

(6.25)

Thus, for a certain temperature, the constant $K$ should be set to its maximum value, if, on the other hand, the reference value of the relaxation time is chosen to its minimum value ($< 10^{-6}$ s). The visco-stress approaches its maximum value ($\sigma_v \rightarrow K$) when the rate of loading reaches very high values ($\dot{p} > 10^6$ s$^{-1}$) such that $\eta^{vp} \dot{p} \rightarrow 1$ at which the effect of the exponent $N$ is negligible. Therefore, the constant $K$ should not represent the initial yield condition if, at the same time, a very small value is selected for the relaxation time which is incorrectly used by many authors who used an overstress function similar to the one defined in Eq.(6.22).

An alternative definition for the overstress function is introduced in the literature such that:

$$\varphi(f_s) = \left( \frac{f_s}{K} - 1 \right)^N$$

(6.26)

The above definition should also obey the aforementioned conditions in choosing a proper definition for the parameters $K$ and $\eta$ before implementing them in the thermodynamic based viscoplastic formulation.

It appears that previous constitutive equations of viscoplasticity could be used only if the quantities appearing there are taken as temperature dependent. In general, the temperature-dependent quantities can be $\eta$, $K$, and $\varphi$. The most general case in which these quantities are function of the temperature variable has not been studied in the literature. The main reason for this is that considering the variation of any two of these quantities with temperature is found to give satisfactory correspondence with the experimental data over the entire range of temperature.

In this work, both the viscosity parameter and the overstress function are explicitly considered as temperature-related variables whereas the threshold stress $\hat{Y}$, which represents a reference value at which $T \rightarrow 0$ and/or $\dot{p} \rightarrow \dot{p}_0$ as explained earlier, is chosen in normalizing the overstress function. Consequently, the viscoplastic multiplier in the Perzyna modeling case is obtained, after making use of Eq.(6.7), as follows:

$$\lambda^{vp} = \frac{1}{\eta^{vp}(T)} \varphi(f_s, T, \hat{Y})$$

(6.27)

It is well known that the viscosity parameter, also known as the relaxation time $\eta^{vp}$, is considered the most important parameter in finite element implementation of viscoplasticity. This helps in introducing a physical length scale that is used in regularizing some problems encountered in finite element computations. It allows the spatial difference operator in the
governing equations to retain its ellipticity. In this work, however, at a certain stress value, \( \eta^{vp} \) is exponentially related to the absolute temperature and the microstructure quantities such that:

\[
\eta^{vp} = \eta_o^{vp} \exp \left( \frac{1}{\beta^2 T} \right)
\]  

(6.28)

where \( \eta_o^{vp} \) denotes the reference viscosity parameter which represents the minimum value that is achieved at very high temperatures \( T \to \infty \). This viscosity parameter is explicitly related to the dislocations waiting time, distance between obstacles and the initial dislocation density. As will be discussed later in this section, this helps in introducing a proper definition for a length scale parameter, as follows:

\[
\eta_o^{vp} = (\bar{\mu} \rho \beta d)^{-1} t_w
\]  

(6.29)

The normalized overstress function is defined in terms of the temperature and the static yield function as follows:

\[
\varphi(f_s, T, \hat{Y}) = \exp \left\{ \frac{1 - \left( 1 - \left( \frac{f_s}{\rho} \right) T \right)^{1/q_s}}{\beta^2 T} \right\} \quad \text{for } f_s \geq 0
\]

(6.30)

\[
\varphi(f_s, T, \hat{Y}) = 0 \quad \text{for } f_s < 0
\]

The above overstress definition, actually, provides a smooth transition from the dynamic (viscoplastic) surface to the static (plastic) surface at which the viscoplastic multiplier reduces to its plastic value obtained through \( \dot{f}_s = 0 \). That is to say, \( \dot{\lambda}^{vp} = \dot{\lambda}^p = \dot{p}_s \) when \( f_s = 0 \) or vise versa.

Essentially, some metals show rate dependency even at \( \dot{\rho} < 10^{-5} \text{ s}^{-1} \) which indicates that \( \dot{p}_s \) does not actually exist in real plastic/viscoplastic deformation. Moreover, at high strain rates of adiabatic deformation that is accompanied with high temperatures, \( f_s \) may coincide with \( f_{ath} \) at \( \dot{\rho} > 10^{-5} \text{ s}^{-1} \) designating an actual rate-independent behavior. In these circumstances, the strain rate at which the material becomes athermal and rate-independent could be obtained by rearranging Eq.(6.13), such that:

\[
\dot{p}_{ath} = \dot{p}_o e^{-\frac{1}{\beta^2 T_o}}
\]  

(6.31)
Therefore, we should alternatively use the athermal surface $f_{\text{ath}}$ as the real rate-independent surface in the definition of the normalized overstress function at which the thermo-visco-stress completely vanishes. That is

$$
\varphi(f_{\text{ath}}, T, \hat{Y}) = \exp \left( \frac{1 - \left(1 - \left(\frac{f_{\text{ath}}}{\hat{Y}}\right)^{q_2}\right)}{\beta_1 T} \right) \quad \text{for } f_{\text{ath}} \geq 0
$$

$$
\varphi(f_{\text{ath}}, T, \hat{Y}) = 0 \quad \text{for } f_{\text{ath}} < 0,
$$

so that the athermal rate-independent deformation is recovered when $T \to T_c$, at which the viscosity of the material approaches its minimum ($\eta^{vp} \to \eta_c^{vp}$). It is obvious from Eq.(6.29), that the relaxation time in metals is proportional to the waiting time of dislocations at an obstacle which, in turn, is affected by the temperature. At certain stress value, the rise in heat inside the material helps in diminishing the strength of the obstacles (forests dislocations) such that the mobile dislocations overcome these barriers in a lesser amount of time. That is, an increase of the material temperature during the plastic deformation causes a decrease in the relaxation time and consequently a decrease in the viscosity of the material, which results in a remarkable degradation in the thermo-visco-part of that stress. A further rise in temperature ($T \to T_c$), however, makes the thermo-visco-stress completely vanish at which the yield surface is reduced to its athermal rate-independent state (the lower limit).

### Consistency Model

Alternatively, viscoplasticity may be modeled by incorporating the rate-dependency in a yield function. This concept has been introduced first by Ponthot (1995) who presented a continuous viscoplastic formulation by introducing a zero-valued yield condition which is an extension of traditional elastoplasticity assuming that the ratio of the overstress and the viscosity defines the viscoplastic multiplier. That is

$$
f_d(\sigma, p, X, T, \dot{\lambda}^{vp}) = f_{\text{ath}}(\sigma, p, X) + \varphi^{-1}(T, \dot{\eta}^{vp}, \dot{\lambda}^{vp}) = 0, \quad (6.33)
$$

from which a consistency condition can be derived under a persistent viscoplastic flow when $\dot{f}_d = 0$. Eq.(6.33) corresponds to the usual format in elastoplasticity with the exception of the resistance function being explicitly dependent on $\dot{\lambda}^{vp}$ (see for more details, Carosio et al., 2000).

Wang (1997) formulated the Consistency model, using an argument similar to the above by including the rate of state variables as independent state variables. This model appeared to be an efficient and useful tool in the simulation of Lüders bands and the Portevin-Le Chatelier effects in metal (Heeres et al., 2002). In the Consistency model, the dynamic rate-dependent
yield surface is expressed in a form similar to Eq. (6.17) which is rewritten here, after ignoring $\dot{p}$, as follows:

$$f_d = \sigma_{eq} - Y_a - R - \dot{\nabla} \left( 1 - \beta_2 T \ln(\eta_{\sigma}) \hat{p} \right)^{1/\eta_0} = 0$$ (6.34)

As in the classical elasto-plasticity, viscoplastic loading occurs when $f_d = 0$, while a purely elastic response is generated when $f_d < 0$. The viscoplastic consistency condition then yields:

$$\dot{f}_d = \frac{\partial f_d}{\partial \sigma_{ij}} \dot{\sigma}_{ij} + \frac{\partial f_d}{\partial \dot{X}_{ij}} \dot{X}_{ij} + \frac{\partial f_d}{\partial \dot{p}} \dot{p} + \frac{\partial f_d}{\partial \dot{T}} \dot{T} + \frac{\partial f_d}{\partial \dot{\nabla}} \dot{\nabla} = 0$$ (6.35)

The above consistency condition is utilized to obtain the viscoplastic multiplier after using a more convenient form of Eq. (6.35) such that (Wang et al., 1997):

$$\dot{f}_d = N_q \dot{\sigma}_{ij} - (h_i + h_2 + \theta) \dot{\lambda}^{vp} - y \dot{\lambda}^{vp} = 0$$ (6.36)

where $h_i$, $\theta$, and $y$, which denote the hardening modulus, softening parameter, and the strain-rate sensitivity parameter, respectively, are given as follows:

$$h_i = - \frac{\partial f_d}{\partial X_{ij}} : \dot{X}_{ij} \dot{\lambda}^{vp}$$ (6.37)

$$h_2 = - \frac{\partial f_d}{\partial \dot{p}} \dot{p} \dot{\lambda}^{vp}$$ (6.38)

$$\theta = - \frac{\partial f_d}{\partial \dot{T}} \dot{T} \dot{\lambda}^{vp}$$ (6.39)

$$y = - \frac{\partial f_d}{\partial \dot{\nabla}} \dot{\nabla} \dot{\lambda}^{vp}$$ (6.40)

$$N_q = \frac{\partial f_d}{\partial \sigma_{ij}}$$ (6.41)

According to Eq. (6.36), the viscoplastic multiplier is defined, in the Consistency model, implicitly via a differential equation which was solved by Wang (1997) in a discrete manner. This differential equation, however, may also be solved such that an explicit expression for $\dot{\lambda}^{vp}$ may be obtained and thus the equation may be directly transformed into a numerical scheme (Heeres et al., 2002). The determination of the viscoplastic multiplier along with the parameters defined in Eqs. (6.37)-(6.41) will be demonstrated in the following sections.
The dynamic surface will play a significant role in the viscoplastic finite element formulation described in the next section. This rate-dependent yield surface along with the consistency parameter is subjected to the classical Kuhn-Tucker loading/unloading conditions:

\[ f_d \leq 0, \quad \dot{\lambda}^{\text{vp}} \geq 0, \quad \dot{\lambda}^{\text{vp}} f_d = 0 \] (6.42)

In the Perzyna model, the static yield function, or the athermal yield function in our case, is used, instead of the dynamic yield surface in the Consistency model, to check whether viscoplasticity occurs. Moreover, the two models show different responses during the unloading process. In the Consistency model, the material always unloads elastically regardless of the size and the position of the yield surface, while, in the Perzyna model, viscoplasticity occurs during the first stages of the unloading process. After a sufficient time of unloading, the overstress becomes exhausted, the Perzyna model unloads elastically. This is, however, not the case for bcc metals at which the yield stress controls the viscoplastic deformation. Therefore, it is clear that the assumption for the Consistency model to unload elastically may be accepted for a material with viscoplastic behavior similar to bcc metals.

### 6.2.2 Yield Function for FCC Metals

In the case of fcc metals, the emergence and the evolution of a heterogeneous microstructure of dislocations as well as the long-range intersections between dislocations dominates the mechanism of the thermal activation analysis behavior. Based on that, thermal activation depends strongly on the plastic strain. That is, the increase in the yield point with a decrease in temperature is highly dependent on the strain-hardened states for fcc metals. Using the concept of additive decomposition of the flow stress, the general form of the yield function \( f \) for bcc metals is defined as follows (Voyiadjis and Abed, 2005):

\[ f = \sigma_{eq} - Y_a - R_{th}(p, \dot{p}, T) \] (6.43)

where in this case the thermal part of the flow stress is mainly related to the hardening parameters, \( R_{th} \), while the athermal part is controlled by the initial yield stress, \( Y_a \). The equivalent stress, \( \sigma_{eqs} \), is the same as defined in Eq.(6.2). The back stress, \( X_{ij} \) (kinematic hardening) is assumed in this work as being independent of both temperature and strain rates.

The principle mechanisms for the thermal flow stress of fcc metals is controlled by the cutting of dislocation forests. Hence, the threshold stress that is affected by a coupled temperature and strain rate relation is related to the hardening stresses such that:

\[ R_{th} = \hat{R} \left( 1 - \left( \beta_1 T - \beta_2 T \ln \left( \frac{\dot{p}}{\dot{p}_0} \right) \right)^{1/q_1} \right)^{1/q_2} \] (6.44)

where, similar to those defined for bcc metals, the definition of threshold strain hardening is introduced in two different forms such that:
\[ \hat{R} = \hat{B} p^n \]  
\[ \hat{R} = \hat{B} \left( 1 - e^{-kp} \right)^{1/2} \]  

The parameter \( \hat{B} \) is defined in terms of the microstructure quantities as follows:

\[ \hat{B} = \hat{m} \alpha_o \mu_o b \left( \frac{M}{k} \right)^{1/2} \]

where \( \alpha_o \) is a constant which represents the portion of the shear modulus \( \mu_o \) contributing to the activation energy with both being at zero temperature (Voyiadjis and Abed, 2005). Unlike bcc metals, the parameter \( \beta_i \) given in Eq.(6.44) is not constant but varies with the variation of the accumulated plastic strain such that:

\[ \beta_i = \frac{K}{G_o} \ln \left( \frac{\rho_o \left( 1 + C_i \left( 1 - \exp(-kp) \right) \right)}{\dot{\rho}} \right) \]

where,

\[ C_i = \frac{M}{k \rho_i} \]

It should be mentioned here that the plastic strain dependency of the parameter \( \beta_i \) results from considering the evolution equation of the dislocation density where \( \rho_i \) denotes its initial value. This was not the case for bcc metals since the thermo-viscoplastic behavior is totally attributed to the yield stress in which only the effect of the initial dislocation density is considered. The definition of the other parameters used in Eq.(6.44) is similar to those defined for bcc metals.

• **Static and Athermal Deformation**

Similar to the case of bcc metals, if we consider that the static deformation of fcc metals is encountered at a strain rate equal or less than a specific small value that is chosen to be in the order of \( 10^{-5} \) \( s^{-1} \), then, the static yield function of fcc metals is defined by substituting Eq.(6.44) into Eq.(6.43), after setting \( \dot{p} = \dot{\rho} \), such that:

\[ f_s = \sigma_{eq} - Y_a - \hat{R} \left( 1 - \left( \beta_i T \right)^{1/6} \right)^{1/2} \text{ for } \dot{\rho} \leq \dot{\rho}_s \]

Besides being used to distinguish between the elastic and inelastic states of deformation, the above static yield function is also used to distinguish between the static and dynamic states of rate-dependent deformation as shown in Eq.(6.12).

The critical temperature \( T_{cr} \) at which the thermal component of the flow stress vanishes is related for the case of fcc metals to both the strain and the strain rates such that:
\[ T_{cr} = (\beta_1 - \beta_2 \ln(\dot{\rho}/\dot{\rho}_s))^{-1} \] (6.51)

It's clear from the above definition of the athermal temperature, that \( T_{cr} \) increases as the rate of loading increases and decreases with the accumulation of the plastic strain. In a static deformation, i.e. at \( \dot{\rho} = \dot{\rho}_s \), this critical temperature depends only on the plastic strain as shown below:

\[ T_{cr} = (\beta_1)^{-1} = \frac{G_o}{k \ln\left(\dot{\rho}_o \left(1 + C_1 \left(1 - \exp(-k\rho)\right)\right)/\dot{\rho}_s\right)} \] (6.52)

Once the temperature reaches or exceeds the above critical values, the yield function defined in Eq.(6.43) is reduced, for the case of fcc metals, to a perfect plasticity state of deformation:

\[ f_{ath} = \sigma_{eq} - Y_a \] (6.53)

where \( f_{ath} \) denotes the athermal rate-independent yield function which is also called in this work the lower limit function. This limit demonstrates the maximum effect of temperature rising on the degradation process of the flow stress. It is also used here to distinguish between the thermal and athermal states of deformation as given by Eq.(6.16).

Voyiadjis and Abed (2005) pointed out that the athermal state of deformation for the case of OFHC copper, an example of fcc metals, is achieved only when the temperature reaches a value of \((1000-2500K)\) in the range \((10^{-05}-10^{05}s^{-1})\) of strain rates. Since the range of temperature used in our model applications is \( T \leq 1000K \), the static yield surface will never coincide with the athermal yield surface at this range of temperatures, i.e., at \( T < T_{cr} \), (see Figure 6.1).

**Dynamic Deformation**

In fcc metals, the coupling effect of temperature and strain rates is introduced through the thermal component of the flow stress which is mainly controlled by hardening. The dynamic yield surface, i.e. at \( \dot{\rho} > \dot{\rho}_s \), is then defined by substituting Eq.(6.44) into Eq.(6.43) as follows:

\[ f_d = \sigma_{eq} - Y_a - R\left(1 - (\beta_1T - \beta_2T \ln(\dot{\rho}/\dot{\rho}_s))^{1/q_1}\right)^{1/q_2} \text{ for } \dot{\rho} > \dot{\rho}_s \] (6.54)

In adiabatic conditions for fcc metals, the viscoplastic deformation in its early stages is controlled by the effect of the strain rate on the hardening stress at which dislocations interact with the quick accumulation of dislocation forests resulting in high stresses as the strain rate increases. Consequently, a considerable expansion of the dynamic yield surface is encountered. In this way, the above yield surface expands until it reaches its maximum state, \( f_{max} \), which is called in this work the upper limit function such that:
where the threshold stress \( \hat{R} \) represents the highest visco-stress value that an fcc metal may reach which corresponds to a very high strain rate \( \dot{\rho} = \dot{\rho}_o \) at which the obstacles are destroyed indicating a material fracture. This state of deformation can also be achieved when the temperature reaches the value of zero indicating a very high viscosity of the solid. Therefore, within the framework of continuum mechanics, \( f^{\text{max}} \) is utilized to distinguish between the admissible and inadmissible states similar to those given in bcc metals (see Eq.(6.19)). As the plastic strain accumulates, the plastic work increases and converts into heat inside the material causing significant degradation for the material viscosity as a result of the weakening of most of the dislocations barriers. As a result, the thermo-visco-stress diminishes as the material temperature evolves causing remarkable softening for the material deformation. In this case, the dynamic yield surface gets smaller until it reaches its lower limit, Eq.(6.53), at very high temperatures \( (T \to T_{cr}) \) (see Figure 6.1 for further illustration). Although the critical temperature is so high for most fcc metals, it is still feasible to use the athermal yield surface instead of the static yield surface in the Perzyna model of viscoplastcity as will be shown later in this section.

- **Perzyna Model**

In a similar way to bcc metals, both the viscosity parameter and the overstress function are explicitly considered as temperature-related variables whereas the threshold hardening stress \( \hat{R} \), which represents a reference value at which \( T \to 0 \) and/or \( \dot{\rho} \to \dot{\rho}_o \) as explained earlier, is chosen in normalizing the overstress function. Consequently, the viscoplastic multiplier in the Perzyna modeling case is obtained after making use of Eq.(6.44), as follows:

\[
\lambda^{vp} = \frac{1}{\eta^{vp}(T)} \varphi(f_s,T,\hat{R})
\]  

(6.56)

In addition to the temperature and the microstructure quantities, the viscosity parameter, \( \eta^{vp} \), for the case of fcc metals, is also related to the plastic strain through the reference viscosity parameter \( \eta_o^{vp} \) at which the evolution of dislocation density is considered. That is

\[
\eta^{vp} = \eta_o^{vp} \exp \left( \frac{1}{\beta T} \right)
\]  

(6.57)

In a similar way to the case of bcc metals, \( \eta_o^{vp} \) denotes the minimum value of the viscosity parameter achieved at very high temperatures \( T \to \infty \). In addition to the accumulated plastic strain, this viscosity parameter is explicitly related to dislocations waiting time, distance between obstacles and the dislocation density as follows:
\[ \bar{\pi}_o^{vp} = \left( \bar{m} b d \left( \rho_i + \frac{M \left( 1 - \exp(-kp) \right)}{k} \right) \right)^{-1} t_{wo} \] (6.58)

Since the hardening stress dominates the thermo-visco-plastic deformation, its threshold value is used in normalizing the overstress function that is defined in terms of temperature and the static yield function as follows:

\[
\varphi(f_s, T, \hat{T}) = \begin{cases} 
\exp \left( 1 - \left( 1 - \left( f_s / \hat{R} \right)^{\beta_1} \right)^{\frac{\beta_2}{\beta_1}} \right) & \text{for } f_s \geq 0 \\
0 & \text{for } f_s < 0 
\end{cases}
\] (6.59)

where \( \beta_1 \) is a strain-dependent parameter as defined in Eq(6.48). In the above definition of the overstress, viscoplasticity occurs as soon as \( f_s > 0 \) while classical thermal plasticity is recovered when \( f_s = 0 \) in which \( \dot{\lambda}^{vp} = \dot{\lambda}^p = \dot{\rho}_s \). On the other hand, the material is in the elastic state of deformation when \( f_s < 0 \).

Alternatively, one may use the athermal yield function \( f_{ath} \) which, as defined in Eq.(6.53), represents a perfectly plastic deformation as the indicator for the overstress function instead of the static yield function as follows:

\[
\varphi(f_{ath}, T, \hat{T}) = \begin{cases} 
\exp \left( 1 - \left( 1 - \left( f_{ath} / \hat{R} \right)^{\beta_1} \right)^{\frac{\beta_2}{\beta_1}} \right) & \text{for } f_{ath} \geq 0 \\
0 & \text{for } f_{ath} < 0 
\end{cases}
\] (6.60)

In this case, the thermo-visco-plastic deformation occurs as soon as the athermal yield function exceeds zero \( f_{ath} > 0 \).

As the case in bcc metals, the viscosity of fcc metals is also proportional to the dislocation waiting time at an obstacle. It is affected by both the temperature and the accumulative plastic strain. The rise of the heat inside the material diminishes the strength of the obstacles such that the mobile dislocations overcome these barriers in a smaller amount of time at which the viscosity of the material decreases. Moreover, the large amount of accumulated plastic strain that evolves during the viscoplastic deformation gives an indication of obstacle weakness, i.e., viscosity degradation. A further rise in temperature \( (T \rightarrow T_o) \) makes the thermo-visco-stress completely vanish at which the yield surface is reduced to its athermal rate-independent state.
(the lower limit). This kind of deformation, however, is achieved at extremely high temperatures.

- **Consistency Model**

The dynamic rate-dependent yield surface for the case of fcc metals is expressed similar to Eq.(6.54) which is rewritten here such that it becomes valid for any value of strain rate:

\[
f_d = \sigma_{eq} - Y_a - \tilde{R} \left( 1 - \left( -\beta_2 T \ln(\eta_a T p) \right)^{1/\eta_2} \right)^{1/\eta_2} = 0
\]  
(6.61)

where the viscosity parameter \( \eta_a \) varies with the variation of plastic strain as defined in Eq.(6.58). In the Consistency model, viscoplastic loading occurs when \( f_d = 0 \), while a purely elastic response is generated when \( f_d < 0 \). The viscoplastic consistency condition then yields:

\[
\dot{f}_d = N_q \ddot{\sigma}_{ij} - \left( h_1 + h_2 + \theta \right) \dot{\lambda}^{vp} - y \dot{\lambda}^{vp} = 0
\]  
(6.62)

where the hardening modulus \( h_i \), the softening parameter \( \theta \), and the strain-rate sensitivity parameter \( y \), are defined similar to the ones given in Eqs.(6.37)-(6.41). However, as will be shown in the following section, the definitions of these parameters differ from those obtained for bcc metals since the thermo-visco-plastic stresses are different. Using the differential equation, Eq.(6.62), a closed form expression for the viscoplastic multiplier may be derived and directly transformed into a numerical scheme. This definition is presented in the following section. Moreover, the above rate-dependent yield surface along with the consistency parameter is also subjected to the classical Kuhn-Tucker loading/unloading conditions defined in Eq.(6.42).

Both the Perzyna and the Consistency models show different responses during the unloading process. In the Consistency model, the material always unloads elastically regardless of the size and the position of the yield surface, while, in the Perzyna model, viscoplasticity occurs during the first stages of the unloading process. For the case of fcc metals, the assumption of elastic unloading in the Consistency model is found to be not accurate since the viscoplastic deformation is initiated as soon as the athermal yield function exceeds zero.

**6.2.3 Length Scale Definition**

Sluys (1992) pointed out that viscosity introduces implicitly a length scale parameter, \( \ell \), into the dynamic initial boundary value problem such that:

\[
\ell = a c \eta^{vp}
\]  
(6.63)
where \( c = \sqrt{E/\rho} \) denotes the velocity of the propagation of the elastic waves in the material, \( E \) is Young’s modulus, \( \rho \) is the mass density, and \( a \) is a proportionality factor that depends on the particular initial-boundary value problem under consideration and may also depend on the microscopic properties of the material.

Similarly, the following definition for the length scale parameter \( l_i \), which is taken for the case of bcc metals as the initial value of dislocation distance, is proposed here after making use of Eq.(6.29) such that:

\[
l_i = \left( \bar{a} v \eta \right)^{1/2}
\]  

(6.64)

where \( \bar{a} = \bar{m}b \) and \( v = d / t_w \) is the dislocation velocity that is equivalent to the velocity of the propagation of the elastic waves defined in Eq.(6.63). The proposed length scale for bcc metals is independent of the plastic strain since the hardening parameter is not much included in the viscoplastic deformation. Hence, the viscoplastic behavior of bcc metals is mainly controlled by the presence of the initial dislocation density.

In the case of fcc metals, the accumulated plastic strain plays a significant role in the viscoplastic deformation. This effect is extended to the definition of the proposed length scale which varies with the accumulation of the plastic strain during the viscoplastic deformation. Hence, the following definition for the length scale parameter \( l \), which is taken here as the active value of dislocation distance, is proposed after making use of Eq.(6.58) such that:

\[
l = \frac{l_i}{\left( 1 + C_i \left( 1 - \exp(-kp) \right) \right)}
\]  

(6.65)

where \( l_i \) is the initial value of dislocation spacing defined in Eq.(6.64). The plastic strain dependence of the length scale may be attributed to the dislocations interactions mechanism encountered in fcc metals at which the total mobile dislocation density is involved in determining the thermo-viscoplastic deformation.

Utilizing the material parameters given in the previous chapter, the initial value of dislocation distance for Tantalum (Ta), Vanadium (V), Niobium (Nb), and OFHC Copper (Cu) is given in Table (1). Moreover, the variation of the length scale with the variation of plastic strain for the aforementioned metals is also illustrated in Figure 6.2. It is obvious that the variation of the length scale with the plastic strain for the case of bcc metals is almost negligible, while, there is a significant variation for the case of fcc metals. The dislocation distance decreases as the plastic strain increases which is mainly pertained to the evolution of dislocation density during the plastic strain accumulation. This dislocation density evolution reaches it saturated level for most of the above metals at almost 15% plastic strain as shown in Figure 6.2.
Figure 6.2 Variation of the length scale parameter with the variation of accumulated plastic strain.

Table 5 Numerical values for the physical quantities used in deriving the proposed models parameters for Nb, V, Ta, OFHC Cu and Ti.

<table>
<thead>
<tr>
<th>Length Scale</th>
<th>Nb</th>
<th>V</th>
<th>Ta</th>
<th>OFHC Cu</th>
</tr>
</thead>
<tbody>
<tr>
<td>$l_i$ (µm)</td>
<td>0.45</td>
<td>0.45</td>
<td>0.49</td>
<td>0.27</td>
</tr>
</tbody>
</table>

6.3 Thermodynamic Formulations of the Viscoplastic Model

A thermodynamically consistent mathematical formulation within the context of small deformation is presented in this section as a framework to introduce constitutive equations. Thermodynamics with internal state variables offers both guidelines and some constrains for the choice of evolution equations. Thermo-elastic-viscoplastic deformation behavior in the absence of damage is considered in this work that is defined using two potentials; the
The thermodynamic potential to describe the present state and the dissipative potential for the irreversible evolutions. The formal potential is described through the Helmholtz free energy

$$\psi = e - sT$$

where $s$ is the specific entropy, $e$ is the internal energy and $T$ is the absolute temperature. An inelastic body is one in which the strain is determined by the stress and by some additional internal variables. The form of the Helmholtz potential in terms of observable and internal state variables can be given as follows:

$$\psi = \psi\left(\varepsilon^e, T, p, \alpha_{ij}\right)$$

where $p$ and $\alpha_{ij}$ characterize the isotropic (scalar) and kinematic (second-order tensor) hardening in plasticity/viscoplasticiy respectively. For small strain deformation, the total strain tensor is additively decomposed into elastic, $\varepsilon^e$, and viscoplastic, $\varepsilon^{vp}$, components as follows:

$$\dot{\varepsilon}_{ij} = \dot{\varepsilon}^e_{ij} + \dot{\varepsilon}^{vp}_{ij}$$

The time derivative of Eq.(6.67) with respect to its internal state variables is given by:

$$\dot{\psi} = \frac{\partial \psi}{\partial \varepsilon^e_{ij}} \dot{\varepsilon}^e_{ij} + \frac{\partial \psi}{\partial T} \dot{T} + \frac{\partial \psi}{\partial p} \dot{p} + \frac{\partial \psi}{\partial \alpha_{ij}} \dot{\alpha}_{ij}$$

The choice of evolution equations in a form that does not allow any reversible changes is important. Reversible changes produce instantaneous changes of the internal variables and result in incompatibility with thermodynamics (Chaboche, 1991). The determination of these internal state variables is achieved through the use of the fundamental laws of thermodynamics; the conservation of mass, balancing laws, linear and angular momenta, the conservation of energy, and the second law of thermodynamics which reduces to the Clausius-Duhem inequality. These fundamental laws are expressed as follows (Lubliner, 1990):

(i) Conservation of mass

$$\dot{\rho} + \rho \dot{v}_{i,j} = 0$$

(ii) Balance of linear momentum

$$\sigma_{ij,j} + \rho b_i = \rho \dot{v}_i$$

(iii) Balance of moment of momentum

$$\sigma_{ij} = \sigma_{ji}$$

(iv) Conservation of energy (first law of thermodynamics)

$$\rho \dot{e} = \sigma_{ij} \dot{\varepsilon}_{ij} + \rho r_{ext} - q_{i,j}$$
(v) The Clausius-Duhem inequality

\[ \sigma_{y} \dot{e}_{ij} - \rho (\nabla + s \dot{T}) - q_{i} \frac{T}{T} \geq 0 \]  

(6.74)

where \( \rho, v, b, r_{ext}, \) and \( q \) denote the mass density, the velocity vector, the body force vector, the density of external heat, and the heat flux vector. Substituting the rate of the Helmholtz free energy, Eq. (6.69), along with the decomposition of the total strain tensor, Eq.(6.68), into the above Clausius-Duhem inequality, Eq.(6.74), one obtains the following thermodynamic constraint:

\[
\left( \sigma_{y} - \rho \frac{\partial \psi}{\partial e_{ij}} \right) \dot{\varepsilon}_{ij} - \rho \left( s + \frac{\partial \psi}{\partial T} \right) \dot{T} + \sigma_{y} \dot{e}_{ij}^{vp} - \rho \frac{\partial \psi}{\partial p} \dot{p} - \rho \frac{\partial \psi}{\partial \alpha_{ij}} \dot{\alpha}_{ij} - q_{i} \frac{T}{T} \geq 0 
\]

(6.75)

The above Eq.(6.75) must be valid for arbitrary reversible changes in the observable variables, so that the first two terms must vanish independently which result in the following thermodynamic state laws:

\[
\sigma_{ij} = \rho \frac{\partial \psi}{\partial \varepsilon_{ij}}; \quad s = -\frac{\partial \psi}{\partial T}
\]

(6.76)

The remaining terms in the inequality, Eq.(6.75), correspond to the dissipation energy, \( \Pi \)

\[
\Pi = \sigma_{y} \dot{e}_{ij}^{vp} - R \dot{p} - X_{y} \dot{\alpha}_{ij} - q_{i} \frac{T_{j}}{T} \geq 0
\]

(6.77)

where the isotropic hardening \( R \) and the kinematic hardening \( X \) represent the thermodynamic conjugate forces associated with the fluxes of the viscoplastic internal state variables \( p \) and \( \alpha \) respectively. By analogy, these forces may be expressed as follows:

\[
R = \rho \frac{\partial \psi}{\partial p}; \quad X_{y} = \rho \frac{\partial \psi}{\partial \alpha_{ij}}
\]

(6.78)

The dissipation energy defined in Eq.(6.77) may be considered as separated into viscoplastic (intrinsic) and thermal dissipation inequalities such as(Coleman and Gurtin, 1967):

\[
\Pi = \Pi^{vp} + \Pi^{th} \geq 0,
\]

(6.79)

where

\[
\Pi^{vp} = \sigma_{y} \dot{e}_{ij}^{vp} - R \dot{p} - X_{y} \dot{\alpha}_{ij} \geq 0,
\]

(6.80)

\[
\Pi^{th} = -q_{i} \frac{T_{j}}{T} \geq 0
\]

(6.81)
However, such decomposition does not exist in this work due the fact that both $R$ may depend on temperature. Therefore, the total dissipation energy function given in Eq.(6.77) is considered.

Introducing mechanical constitutive models into a thermodynamic framework allows the partition of the plastic work into the energy stored by the material (due to hardening) and the one dissipated as heat. In the case of dissipative processes, the viscoplastic dissipation potential is expressed as a continuous and convex scalar valued function of the flux variables as shown below:

$$\Theta^{vp} = \Theta^{vp} \left( \dot{\varepsilon}_{ij}^{vp}, \dot{p}, \dot{\alpha}_{ij} \right)$$  \hspace{1cm} (6.82)

Using the Legendre-Frenchel transformation of the above viscoplastic dissipation potential, one can obtain complementary laws in the form of the evolution laws of flux variables in terms of the dual variables.

$$F = F \left( \sigma_{ij}, R, X_{ij} \right)$$  \hspace{1cm} (6.83)

It is obvious that the above intrinsic potential is attributed only to the viscoplastic mechanical process. In this regard, the evolution laws of the internal state variables are obtained using the maximum dissipation principle after utilizing the calculus of function of several variables with the Lagrange multiplier, $\lambda^{vp}$ as follows:

$$\Omega = \Pi - \dot{\lambda}^{vp} F$$  \hspace{1cm} (6.84)

According to the maximum dissipation principle, the viscoplastic dissipation function is maximized over all other possible admissible states by the actual state of the thermodynamic forces. Therefore, the following conditions are used to maximize the objective function $\Omega$ as follows:

$$\frac{\partial \Omega}{\partial \sigma_{ij}} = 0; \quad \frac{\partial \Omega}{\partial X_{ij}} = 0; \quad \frac{\partial \Omega}{\partial R} = 0$$  \hspace{1cm} (6.85)

The generalized normality hypothesis is recovered here after substituting Eq.(6.85) into Eq.(6.84). Thus, the corresponding following thermodynamic flow laws are obtained

$$\dot{\varepsilon}_{ij}^{vp} = \dot{\lambda}^{vp} \frac{\partial F}{\partial \sigma_{ij}}; \quad \dot{\alpha}_{ij} = -\dot{\lambda}^{vp} \frac{\partial F}{\partial X_{ij}}; \quad \dot{p} = -\dot{\lambda}^{vp} \frac{\partial F}{\partial R}$$  \hspace{1cm} (6.86)

In the following, a proper definition for the viscoplastic potential as well as the Helmholtz free energy is required in order to present thermodynamic consistent constitutive relations that are able to describe the thermomechanical behavior (isotropic and adiabatic processes) of the material.
6.3.1 Definition of the Helmholtz Free Energy Function

The choice of the form of the Helmholtz free energy function $\Psi$ is very important since it constitutes the basic for deriving the constitutive equations. It is possible to decouple the Helmholtz free energy into a potential function for each of the internal state variables in such a way that an analytical expression for the thermodynamic potential is given as a quadratic form of its tensorial internal state variables. The scalar (isotropic) internal state variables, on the other hand, are not necessarily to be defined in a quadratic form as indicated by Chaboche (1991) who also pointed out that using a non-quadratic form for the definition of the tensorial internal state variables (e.g. kinematic hardening) always leads to abnormal effects such as dissymmetric and abnormal concavities of the stress strain responses. It should be clearly stated here that the definition of the specific free energy function should take into consideration the deformation condition (rate independent/rate dependent and/or isothermal/adiabatic) as well as the material type (bcc metals, fcc metals, steel alloys, concrete, etc.). For example, at high strain rates of (viscoplastic) adiabatic deformation, a significant temperature rise is produced as the accumulated plastic work converts mostly into heat stored inside the material where there is no enough time for it to be transferred elsewhere. Under rate independent condition (very low strain rates), however, the deformation behavior tends to be isothermal all around the body. Experimental observations show that the viscoplastic hardening for most fcc metals is strongly affected by the temperature and strain rate whereas, this effect seems to be negligible for the case of bcc metals. Thus, introducing a unique form of the free energy definition for all types of materials and loading conditions is not an accurate assumption in thermodynamic consistent formulations for constitutive relations.

The complexity of any model is directly determined by the form of the Helmholtz free energy and by the number of conjugate pair of variables. In this work, however, we postulate the following general definition of the elastic-thermoviscoplastic energy $\psi$ for both bcc and fcc metals:

$$\rho\psi = \frac{1}{2} e_{ij}^e E_{ijkl} e_{kl}^e + \frac{1}{3} C \alpha_i \alpha_j + \rho\psi(p) \quad (6.87)$$

where $E_{ijkl}$ is the fourth order elastic tensor, and both the coefficient $C$ and function $\psi(p)$ may depend on temperature and strain rate. In this work, however, only the isotropic hardening of fcc metals is considered as temperature and strain rate dependent as confirmed by the thermoviscoplastic behavior of each metal structure elucidated in the previous section. Thus, the form chosen for the function $\psi(p)$ differs from one metal structure to another.

In general, the thermodynamic potential $\psi(p)$ is chosen in a form that is able to restitute adequately the relation between $R$ and $p$. Therefore, the following temperature and rate dependent definitions for the case of fcc metals are postulated:

$$\rho\psi(p) = \frac{1}{2} B \hat{R} p \left(1 - \exp(-kp)\right)^{1/2} \quad (6.88)$$
\[ \rho \psi(p) = \frac{\overline{J} \hat{R}}{m+1} p^{m+1} \]  \hspace{1cm} (6.89) 

so that the aforementioned two different definitions for the hardening parameter \( R \) are recovered. The temperature and rate-dependent coefficient, \( \overline{J} \), is defined as follows:

\[ \overline{J} = \left( 1 - \left( -\beta T \ln(\overline{\eta}) \right)^{1/q_1} \right)^{1/q_2} \]  \hspace{1cm} (6.90)

On the other hand, the definitions of the thermodynamic potential \( \psi(p) \) for the case of bcc metals are chosen such that no temperature and strain-rate effect is considered which reflects the real thermo-viscoplastic behavior of such structures of metals: These two definitions are assumed as follows:

\[ \rho \psi(p) = \overline{B} p (1 - \exp(-kp))^{1/2} \]  \hspace{1cm} (6.91)

\[ \rho \psi(p) = \frac{B}{m+1} p^{m+1} \]  \hspace{1cm} (6.92)

where all of the above material parameters are defined in the previous section. The above proposed definition of \( \psi(p) \) allows the derivation of the hardening stresses in which two different relations for the isotropic hardening, using Eq(6.78)\(_1\), may be written. For fcc metals, the general definition of the hardening stress is given as follows:

\[ R = \overline{J} \hat{R} \]  \hspace{1cm} (6.93)

where \( \hat{R} \) may take, using Eqs.(6.88) and (6.89), the following two different relations:

\[ \hat{R} = \hat{B} (1 - \exp(-kp))^{1/2} \]  \hspace{1cm} (6.94)

\[ \hat{R} = \hat{B} p^n \]  \hspace{1cm} (6.95)

Furthermore, Using Eqs.(6.91) and(6.92), the hardening stresses are defined for the case of bcc metals as follows:

\[ R = \overline{B} (1 - \exp(-kp))^{1/2} \]  \hspace{1cm} (6.96)

\[ R = B p^n \]  \hspace{1cm} (6.97)

In the same way, the constitutive equations for stress, Eq.(6.76)\(_1\), and back stress, Eq.(6.78)\(_2\), may be written based on the thermodynamic potential given in Eq.(6.87) as follows:
\[ \sigma_{ij} = E_{ijkl} \varepsilon_{kl} = E_{ijkl} (\varepsilon_{kl} - \varepsilon_{kl}^{vp}) \] (6.98)

\[ X_{ij} = \frac{2}{3} C \alpha_{ij} \] (6.99)

where \( \varepsilon_{ij} \) is the total strain tensor that is additively decomposed into elastic \( \varepsilon_{ij}^{e} \) and viscoplastic \( \varepsilon_{ij}^{vp} \) components.

### 6.3.2 Plastic Dissipation Potential and Yield Criterion

In order to obtain non-linear evolution rules for the viscoplasticity hardening variables, one may assume the existence of a viscoplastic potential \( F \) such that it is not equal to the yield surface \( f \). This postulate is essential to obtain non-linear kinematic hardening rules, which gives a more realistic characterization of the material response in the deformation process. In this work, the following definition for the viscoplastic potential is proposed:

\[ F = f + \frac{3\gamma}{4C} X_{ij} X_{ij} \] (6.100)

where \( \gamma \) and \( C \) are material constants used to adjust the units of the equation. The von Mises type of yield function \( f \) differs from one metal structure to another. For bcc metals, the athermal yield function discussed in the previous section is chosen as the rate-independent yield function

\[ f = \sigma_{eq} - Y_a - R(p) \] (6.101)

whereas, the thermal yield surface is chosen as the dynamic (rate-dependent) yield function such that.

\[ f_d = \sigma_{eq} - Y_a - R(p) - Y(p, \dot{p}, T) \equiv 0 \] (6.102)

where

\[ Y(p, \dot{p}, T) = \hat{Y} \left(1 - (-\beta_z T \ln(\eta_{o}^{vp} \dot{p}))^{1/q_t} \right)^{1/q_t} \] (6.103)

Analogously, the following athermal (rate-independent) and dynamic (rate-dependent) yield functions are chosen for the case of fcc metals.

\[ f = \sigma_{eq} - Y_a \] (6.104)

\[ f_d = \sigma_{eq} - Y_a - R(p, \dot{p}, T) \equiv 0 \] (6.105)
It should be stated here that Eqs.(6.15) and (6.104) are utilized here in the overstress function to determine the viscoplastic multiplier, \( \dot{\lambda}^{vp} \), in the Perzyna viscoplastic model for bcc and fcc metals respectively. The dynamic yield functions, Eqs.(6.102) and (6.105), are, alternatively, employed in the Consistency model in order to obtain \( \dot{\lambda}^{vp} \) for bcc and fcc metals respectively. In this work, however, the evolution of the internal variables and accordingly the constitutive equations will be derived using of the dynamic yield functions for both bcc and fcc metals. Thus, the three relations given in Eq(6.86) yield

\[
\dot{\varepsilon}_{ij}^{vp} = \dot{\lambda}^{vp} \frac{\partial \sigma_{ij}}{\partial \sigma_{ij}} = \dot{\lambda}^{vp} \frac{3(\tau_{ij} - X_{ij})}{2\sigma_{eq}} = \dot{\lambda}^{vp} N_{ij}
\]

(6.107)

\[
\dot{\alpha}_{ij} = \dot{\lambda}^{vp} N_{ij} - \frac{3\gamma}{2C} \dot{\lambda}^{vp} X_{ij}
\]

(6.108)

\[
\dot{p} = \dot{\lambda}^{vp}
\]

(6.109)

where \( N_{ij} = \frac{\partial f_d}{\partial \sigma_{ij}} = -\frac{\partial f_d}{\partial X_{ij}} \) is the normal to the yield surface that defines the direction of the viscoplastic strain. The above evolution equations, Eqs.(6.107)-(6.109) are valid for both bcc and fcc metals. The rate of accumulative viscoplastic strain given in Eq.(6.109), coincides with the definition obtained using the following relation:

\[
\dot{\varepsilon}_{ij}^{vp} = \frac{2}{3} \dot{\lambda}^{vp} \frac{\partial \sigma_{ij}}{\partial \sigma_{ij}} \dot{\varepsilon}_{ij}^{vp} = \dot{\lambda}^{vp}
\]

(6.110)

where

\[
\frac{\partial f_d}{\partial \sigma_{ij}} \frac{\partial f_d}{\partial \sigma_{ij}} = N_{ij} N_{ij} = \frac{3}{2}
\]

(6.111)

By taking the time rate of Eq.(6.99) and making use of Eq.(6.108), the evolution equation for the kinematic hardening parameter \( \dot{X}_{ij} \) is related to \( \dot{\lambda}^{vp} \), \( X_{ij} \), and \( N_{ij} \) for both bcc and fcc metals as follows:

\[
\dot{X}_{ij} = \frac{2}{3} C \dot{\lambda}^{vp} N_{ij} - \gamma \dot{\lambda}^{vp} X_{ij}
\]

(6.112)

In contrast, the definition of the evolution equation for the isotropic hardening parameter is not unique for the case of bcc and fcc metals. Two different relations are proposed here for each
metal structure. That is, for bcc metals, the following two forms of \( \dot{R} \) are derived after taking the time derivative of Eq.(6.96) and Eq.(6.97) such that:

\[
\dot{R} = \frac{\partial R}{\partial p} \dot{p} = \frac{k}{2R} \left( \hat{B}^2 - \hat{R}^2 \right) \hat{\lambda}^{vp} \tag{6.113}
\]

\[
\dot{R} = mR \left( \frac{B}{R} \right)^{1/m} \hat{\lambda}^{vp} \tag{6.114}
\]

Since the isotropic hardening for the case of fcc metals is temperature and strain dependent as shown in Eq.(6.93), the evolution equation for \( \dot{R} \) takes the following complex form:

\[
\dot{R} = \frac{\partial R}{\partial p} \dot{p} + \frac{\partial R}{\partial T} \dot{\hat{T}} \tag{6.115}
\]

where,

\[
\frac{\partial R}{\partial p} = \frac{\partial \dot{\hat{R}}}{\partial p} \frac{\partial \hat{\Omega}}{\partial p} + \dot{R} \frac{\partial \hat{\Omega}}{\partial p} \tag{6.116}
\]

\[
\frac{\partial R}{\partial T} = \dot{R} \frac{\partial \hat{\Omega}}{\partial T} = \dot{R} \zeta \ln(\eta_o^{vp} \dot{p}) \tag{6.117}
\]

and

\[
\zeta = \frac{\beta_2}{q_1 q_2} \left( 1 - \left( -\beta_2 T \ln(\eta_o^{vp} \dot{p}) \right) \right)^{1/\alpha_1} \left( -\beta_2 T \ln(\eta_o^{vp} \dot{p}) \right)^{1/\alpha_2} \tag{6.118}
\]

Since \( \dot{R} \) has two different definitions as shown in Eqs.(6.94) and (6.95), the partial derivative of \( R \) with respect to \( p \), Eq.(6.116), may, accordingly, have two different definitions:

\[
\frac{\partial R}{\partial p} = \frac{k}{2} \left( \hat{B}^2 - \hat{R}^2 \right) + \dot{R} T k C_i \hat{\zeta} \left( \frac{\hat{B}^2 - \hat{R}^2}{\hat{B}^2 - C_i \hat{R}^2} \right) \tag{6.120}
\]

or

\[
\frac{\partial R}{\partial p} = m \left( \frac{B}{R} \right)^{1/m} + \dot{R} T k C_i \zeta \left( \frac{\exp(-k(\hat{B}/\hat{R})^{1/m})}{1 + C_i (1 - \exp(-k(\hat{B}/\hat{R})^{1/m}) \right)} \tag{6.121}
\]

Finally, the evolution equation of the stress tensor in terms of the incremental evolution of the total and viscoplastic strain tensors is determined by taking the time derivative of Eq.(6.98) such that:
\[
\dot{\sigma}_{ij} = E_{ijkl} (\epsilon_{kl} - \epsilon_{kl}^{vp}) = E_{ijkl} (\dot{\epsilon}_{kl} - \dot{\lambda}^{vp} N_{ij})
\]  
(6.122)

Assuming plastic incompressibility, the deviatoric part of the above stress evolution equation is written as follows:

\[
\dot{\epsilon}_{ij} = \dot{\sigma}_{ij} - \frac{1}{3} \dot{\sigma}_{mm} \delta_{ij} = 2 \mu (\dot{\epsilon}_{ij} - \dot{\lambda}^{vp} N_{ij})
\]  
(6.123)

where \( e_{ij} = e_{ij}^{e} + e_{ij}^{vp} \) denotes the deviatoric strain tensor and \( \mu \) is the shear modulus.

Next, the evolution of the temperature during the adiabatic viscoplastic deformation, which is considered very necessary in constitutive modeling of metals, is introduced utilizing the concept of conservation of energy.

### 6.3.3 Evolution Equation of Temperature (\( \dot{T} \))

Viscoplastic adiabatic deformation of metals is not only influenced by the rate of loading but also by the initial testing temperature as well as its evolution as the plastic work accumulates. Substituting for the internal energy density rate \( \dot{\psi} \) after taking the time rate of Eq.(6.66), into the first law of thermodynamics, Eq.(6.73), yields the following energy balance relation:

\[
\rho \left( \dot{\psi} + s \dot{T} + \dot{s} T \right) - \sigma_{ij} \dot{e}_{ij} - \rho r_{ext} + q_{i,i} = 0
\]  
(6.124)

By ignoring the temperature gradient effect, assuming no external heat during the adiabatic deformation, and substituting for \( \dot{\epsilon}_{ij} \) from Eq.(6.68) and \( \dot{\psi} \) from Eq.(6.69), the following thermomechanical heat balance equation is obtained:

For bcc metal

\[
\rho c_p \dot{T} = \sigma_{ij} \dot{e}_{ij}^{vp} - X_{ij} \dot{\alpha}_{ij} - R \dot{p}
\]  
(6.125)

where \( c_p = T \partial s / \partial T \) is the tangent specific heat capacity at constant pressure. Eq.(6.125) can further be simplified, by utilizing Eqs.(6.107)-(6.109) for the definition of \( \dot{e}_{ij}^{vp} \), \( \dot{\alpha}_{ij} \), and \( \dot{p} \) respectively, such that the temperature is evaluated during the thermo-viscoplastic deformation by the following evolution equation:

\[
\dot{T} = z \dot{\lambda}^{vp}
\]  
(6.126)

where

\[
z = \frac{1}{\rho c_p} \left( \sigma_{eq} - \frac{3 \gamma}{2C} X_{ij} X_{ij} - R \right)
\]  
(6.127)
It is obvious from the definitions of the evolution equations, that most of these state variables are driven by the incremental evolution of the viscoplastic multiplier. This, however, necessitates a proper definition for the evolution of $\dot{\lambda}^{vp}$ which was explained earlier in the previous sections and a brief description is given in the following section.

### 6.3.4 Determination of the Viscoplastic Multiplier ($\dot{\lambda}^{vp}$)

As indicated earlier, the definition of the viscoplastic multiplier is determined for both bcc and fcc metals using a similar definition of the Perzyna and the Consistency models.

- **Perzyna Model**

In the Perzyna approach, the viscoplastic multiplier is defined for the case of bcc metals as follows:

$$
\dot{\lambda}^{vp} = \frac{1}{\eta^{vp}(T)} \exp \left( \frac{1 - \left( f / \bar{Y} \right)^{q_z}}{\beta_z T} \right) \text{ for } f \geq 0
$$

$$
\dot{\lambda}^{vp} = 0 \quad \text{for } f < 0
$$

where $f$ denotes the athermal rate-independent yield function defined in Eq.(6.15) and $\eta^{vp}$ represents the temperature dependent viscosity parameter given in Eq.(6.28). On the other hand, the viscoplastic multiplier for fcc metals is given by the following relation.

$$
\dot{\lambda}^{vp} = \frac{1}{\bar{\eta}^{vp}(T)} \exp \left( \frac{1 - \left( f / \hat{R} \right)^{q_z}}{\beta_z T} \right) \text{ for } f \geq 0
$$

$$
\dot{\lambda}^{vp} = 0 \quad \text{for } f < 0
$$

here $f$ is chosen for the case of fcc metals as the athermal rate-independent yield function defined in Eq.(6.104) and $\bar{\eta}^{vp}$ is related, in this case, to both the temperature and the plastic strain as given by Eq.(6.57). The deformation Kelvin temperature starts with its initial value $T_o$ and accumulates according to Eq.(6.126), that is

$$
T = T_o + z \dot{\lambda}^{vp}
$$

(6.130)
• **Consistency Model**

Alternatively, the Consistency model is employed to define \( \dot{\lambda}^{vp} \) using the dynamic yield function given by Eqs (6.102) and (6.105) for bcc and fcc metals respectively. In this way, the dynamic yield function behaves in a similar way to the role of the static yield function in rate-independent plasticity. That is, the consistency coefficient, \( \dot{\lambda}^{vp} \), is obtained by applying the consistency condition on the dynamic yield surface, i.e. \( \dot{f}_d = 0 \). Thus, substituting Eqs.(6.122) for \( \dot{\sigma}_y \), (6.112) for \( \dot{X}_{ij} \), (6.126) for \( \dot{T} \), (6.110) for \( \dot{p} \), and \( \dot{p} = \dot{\lambda}^{vp} \), into the consistency condition, Eq.(6.35), yields, after making use of Eq.(6.111), the following general definition of the differential equation of \( \dot{\lambda}^{vp} \):

\[
\ddot{\lambda}^{vp} + \frac{H}{y} \dot{\lambda}^{vp} = \frac{2\mu}{y} N_{ij} \dot{X}_{ij}
\]

(6.131)

where

\[
H = 3\mu + C - \gamma N_{ij} X_{ij} + h_z + \theta
\]

(6.132)

The definitions of the scalars \( h_2 \), \( \theta \), and \( y \) for bcc metals differ from those obtained for fcc metals. These differences are attributed to the fact that the effect of temperature and strain rate is related to the yield stress for bcc metals and to the hardening stress for fcc metals. Thus, using Eq.(6.38), (6.39), and (6.40), the following definitions are obtained for \( h_2 \), which takes two different forms due to two different hardening definitions, \( \theta \), and \( y \) respectively for the case of bcc metals:

\[
h_2 = \frac{k}{2R} \left( B^2 - R^2 \right) \quad \text{for} \quad R = B \left( 1 - \exp(-kp) \right)^{1/2}
\]

(6.133)

\[
h_2 = mR \left( B / R \right)^{1/m} \quad \text{for} \quad R = Bp^m
\]

(6.134)

\[
\theta = \hat{Y} \zeta \ln(\eta_o^{vp} \dot{p})
\]

(6.135)

\[
y = \hat{Y} T \zeta / \dot{p}
\]

(6.136)

where \( z \) is given in Eq.(6.127) and the scalar \( \zeta \) is defined for the case of bcc metals as follows:

\[
\zeta = \frac{\beta_2}{q_1 q_2} \left( 1 - \left( -\beta_2 T \ln(\eta_o^{vp} \dot{p}) \right)^{1/q_1} \right)^{-1/q_2} \left( -\beta_2 T \ln(\eta_o^{vp} \dot{p}) \right)^{-1/q_1}
\]

(6.137)

For the case of fcc metals, the definitions of \( h_2 \), \( \theta \), and \( y \) take the following forms:
Having defined all the parameters of the above incrementally-linear differential equation, Eq.(6.131), the consistency parameter \( \lambda^{vp} \) can then be derived either by solving the differential equation in a discretized manner (Wang, 1997), solving the linearized differential equation using the Laplace transformation (Heeres et al., 2002) or by using the following algorithmic closed-form expression:

\[
\lambda(t) = \hat{\lambda}(0) + \frac{1}{y'} \left( N_y \varepsilon_y(t) - N_y \varepsilon_y(0) \right) - \frac{H}{y'} \left( \lambda(t) - \lambda(0) \right)
\] (6.142)

Once the value of \( \lambda^{vp} \) is obtained during a specific discrete time step at a given strain, the values of the stresses and other state variables are accordingly updated. In the next chapter, an algorithmic treatment for the proposed multi-scale viscoplastic model will be presented with applications to different boundary value problems.
CHAPTER 7
ALGORITHMIC TREATMENTS AND APPLICATIONS

7.1 Introduction

The high concentration of strains in small areas is a real physical phenomenon which can be observed in engineering structures and in laboratory specimens when, in particular, they are made of materials with a descending portion of physical relation and when they are loaded sufficiently high. Even in cases when the increase of loads is slow, the increase of strains in the areas of strain concentration is fast and associated with higher than average dissipation of energy. Therefore, plastic strain localization may be considered as a symptom of the initiation of structural failure. Usually, strain concentration is observed in ductile materials (e.g. metals) but a similar phenomenon may be observed in composites made of one brittle component and the other ductile (Garstecki, 2003). The strain localization may appear in static and dynamics problems particularly in wave propagation.

In fact, the problem of strain localization still remains a challenging problem for future research. The localization of deformation into narrow bands of intense straining is a characteristic feature of inelastic deformation. It has been proved in the literature (e.g., Needleman, 1988) that using rate independent models in the analysis of structures made of materials that exhibit softening leads to ill posed problems. Theoretically, for rate independent solids, localization is associated with a change in the character of the governing equations. That is, the type of the partial differential equations changes from elliptic into hyperbolic in statics and conversely in dynamics. Consequently, numerical solutions to localization problems for rate-independent solids exhibit inherent mesh dependence. The minimum width of the band of localized deformation is set by the mesh spacing. Furthermore, global quantities such as the overall stiffness characteristics of the body depend on the mesh size used to resolve the band of localized deformations. Therefore, rate independent theories without any type of regularization cannot be used in the analysis where strain localization appears. A possible way to overcome this problem is to introduce rate dependent models into the formulation. In this regard, the introduction of Perzyna’s type viscoplasticity model (e.g., Glema et al., 2001; Lodygowski et al., 1994; Kang, 2004; ) or the Consistency’s type of viscoplasticity model (e.g., Carosio et al., 2000, Wang and Sluys, 2000; Heeres et al.,2002) may be recommended as they naturally regularize initial value problems in which the type of governing equations does not change during the expected strain localization which leads to well posed problem. This may be viewed in terms of material rate dependence implicitly introducing a length scale into the boundary value problem formulation.

Large-scale finite element numerical simulations provide a feasible approach for assessing the performance of inelastic structural components operating under complex thermomechanical and multiaxial loading conditions. The global solutions for any discretized finite element model are typically achieved, from the computational point of view, by an increment iterative procedure (e.g., Newton-Raphson technique). The mathematical forms, accuracy and stability properties of a selected integration procedure will directly affect the accuracy and efficiency of the overall finite element solution. The development of stress
integration algorithms with improved performance has received considerable attention in the recent literature on computational plasticity and viscoplasticity. In this regard, due to their stability and wide range of applicability, a number of well-established implicit schemes of time integration have been attracted the attention of many authors for plasticity and viscoplasticity (Simo and Taylor, 1985, 1986; Simo, 1991; Ju, 1990; Loret et al, 1992; Lush et al., 1987; Caddemi and Martin, 1991; Hornberger and Stamm, 1989; Auricchio and Taylor, 1994; Freed and Walker, 1992; Saleeb, 1993; Kojic and Bathe, 1987; Bathe, 1996).

The very efficient implementations of the implicit integration scheme using the radial return schemes for metals corresponding to the special case of full isotropy (both elastic and inelastic responses). This is enabled by the complete reductions of the rate tensor equations to a final single/scalar nonlinear equation; e.g. in terms of the effective stress, or equivalently the plastic multiplier or the “magnitude” of the inelastic strain vector. In order to achieve a strong algorithmic treatment for any complex viscoplasticity constitutive models used for large-scale deformation, the following three tasks are required (Saleeb et al., 2000); (1) a detailed study of the mathematical structure of the viscoplastic equations, and the corresponding integrated field of stress and internal state variables, (2) development and implementation of the implicit backward-Euler stress-updating algorithm, and the associated nonlinear iteration equation solver (e.g, Newton Raphson technique), (3) testing the convergence, stability, and accuracy properties of the algorithms.

In this chapter, algorithmic issues for the consistent viscoplastic models derived in chapter 6 are first discussed for both bcc and fcc metals within the context of small strain deformation using the Perzyna and the Consistency viscoplastic models. The algorithm is then extended to account for the objectivity of stress integration in finite strain viscoplasticity. On the theoretical side, the general framework is developed in the specific context of the fully implicit (backward Euler) difference scheme which is known to exhibit excellent convergence and accuracy characteristics in large scale computations that involve large time steps, particularly with complex anisotropic inelastic models (Ortiz and Popov, 1985). The radial return algorithm which is a special case of the backward-Euler method is used to introduce a nonlinear scalar equation in terms of the viscoplastic multiplier for the case of the Consistency viscoplastic model and in terms of the equivalent stress for the case of Perzyna viscoplastic model. Consistent algorithmic tangent stiffness matrices are derived for both small and finite strain viscoplastic models.

The extension of a small strain constitutive relation to finite strains requires the consideration of finite rotations. The development of objective rates has been studied extensively in the literature in introducing stress update algorithms (e.g, Simo and Marsden, 1984; Simo and Ortiz, 1985; Cuitino and Ortiz, 1982; Rodriguez-Ferran et al., 1997). In this study, we will adopt a stress integration methodology that is called a “local rotated representation” explained in section 7.4 in which the problem may be reduced to the numerical integration of an initial value problem that generates a one-parameter subgroup of proper orthogonal transformation. Finally, several numerical examples are introduced to test the proposed algorithm and its implementation in the ABAQUS finite element code and also to study the initiation and growth of shear bands using the previous bcc and fcc metals with their material parameters.
7.2 Viscoplastic Constitutive Relations

In the previous chapter, a thermodynamic consistent elastic-viscoplastic model has been proposed to simulate the uniaxial/multiaxial deformations of bcc and fcc metals at low and high strain rates and temperatures. In this chapter, however, the governing equations of rate-dependent viscoplasticity derived in the previous chapter will now be summarized and algorithmically treated using both the Perzyna and the Consistency viscoplastic models. In this work, the standard additive decomposition of the strain rate $\dot{\varepsilon}$ into elastic $\dot{\varepsilon}^e$ and viscoplastic $\dot{\varepsilon}^{vp}$ parts is adopted such that:

$$
\dot{\varepsilon} = \dot{\varepsilon}^e + \dot{\varepsilon}^{vp}
$$

(7.1)

The stress rate and the back stress rate are written for both bcc and fcc metals as follows:

$$
\dot{\sigma} = E : (\dot{\varepsilon} - \dot{\varepsilon}^{vp})
$$

(7.2)

$$
\dot{X} = \frac{2}{3} C \dot{\varepsilon}^{vp} - \gamma \dot{\lambda}^{vp} X
$$

(7.3)

where $\gamma$ and $C$ are material constants and ($:$) denotes tensor contraction ($E : \varepsilon = E_{ijkl} \varepsilon_{kl}$) and the fourth-order elasticity tensor is defined as follows:

$$
E_{ijkl} = K \delta_{ij} \delta_{kl} + 2\mu \left( \delta_{ik} \delta_{jl} - \frac{1}{3} \delta_{ij} \delta_{kl} \right)
$$

(7.4)

where $K$ is the bulk modulus, $\mu$ is the shear modulus, and $\delta_{ij}$ is the Kronecker delta. In a strain-driven process the total strain tensor is regarded as an independent variable, usually known, and the evolution of the viscoplastic strain rate tensor is defined by the viscoplastic flow rule such that:

$$
\dot{\varepsilon}^{vp} = \dot{\lambda}^{vp} \frac{\partial f}{\partial \sigma} = \dot{\lambda}^{vp} N
$$

(7.5)

where $N$ represents the unit normal to the yield surface pointing out the direction of the viscoplastic strain in the stress space. It is written as follows:

$$
N = \frac{3}{2\sigma_{eq}} (\tau - X)
$$

(7.6)

where $\tau$ is the deviatoric component of the Cauchy stress tensor $\sigma$ (i.e. $\tau_{ij} = \sigma_{ij} - \frac{1}{3} \sigma_{eq} \delta_{ij}$), $X$ is the back-stress tensor or the kinematic hardening conjugate force, and $\sigma_{eq}$ is known as the equivalent stress defined in the deviatoric space as follows:
\[ \sigma_{eq} = \sqrt{\frac{3}{2} (\tau - X) : (\tau - X)} \] (7.7)

As shown in the previous chapter, we have two different definitions of isotropic hardening for each type of metal structure. For bcc metals, the hardening rules evolve as follows:

\[ \dot{R} = \dot{\lambda}^{vp} \frac{k}{2R} (\dot{B}^2 - R^2) \quad \text{for} \quad R = B(1 - e^{-kp})^{1/2} \] (7.8)

\[ \dot{R} = \dot{\lambda}^{vp} mR (B / R)^{1/m} \quad \text{for} \quad R = Bp^m \] (7.9)

where \( B, k, \) and \( m \) represent the hardening parameters. The above definitions take the following two different forms for the case of fcc metals after including the effects of temperature and strain rate:

\[ \dot{R} = \dot{\lambda}^{vp} \frac{\overline{k}}{2\overline{R}} (\dot{B}^2 - \dot{R}^2) \quad \text{for} \quad \dot{R} = \dot{B}(1 - e^{-kp})^{1/2} \] (7.10)

\[ \dot{R} = \dot{\lambda}^{vp} m\overline{R} (\dot{B} / \dot{R})^{1/m} \quad \text{for} \quad \dot{R} = \dot{B}p^m \] (7.11)

where the temperature and strain rate effects are introduced through the scalar parameter \( \overline{J} \) as follows:

\[ \overline{J} = \left(1 - \left(-\beta_2 T \ln(\eta_{vp} \dot{\rho})\right)^{1/q_1}\right)^{1/q_2} \] (7.12)

where \( \beta_2 \) is a constant and the viscosity parameter \( \eta_{vp} \) is proportional to the dislocation waiting time as well as other microstructural quantities as explained in chapter 6. The viscosity parameter depends on the viscoplastic strain and helps in introducing a proper definition for the length scale.

The role of temperature is considered very important in the case of adiabatic deformation that is a result of the high strain rate of loading. The evolution of the temperature is given by the following relation.

\[ \dot{T} = \dot{\lambda}^{vp} z \] (7.13)

where

\[ z = \frac{1}{\rho c_p} \left( \sigma_{eq} - \frac{3\gamma}{2C} X : X - R \right) \] (7.14)

where \( \rho \) denotes the material density and \( c_p \) represents the tangent specific heat capacity at constant pressure.
The static yield function used in the Perzyna’s way of viscoplastic modeling is chosen here to be equivalent to the athermal yield function. Its definition along with the dynamic yield surface used in the Consistency model is given as follows:

For bcc metals:

$$f^a = \sigma_{eq} - Y_a - R$$

(7.15)

$$f^d = \sigma_{eq} - Y_a - R - \dot{\dot{Y}}\left(1 - \left(-\beta_2 T \ln(\eta_{eq}^p \dot{\rho})\right)^{1/q_2}\right)^{1/q_2} = 0$$

(7.16)

For fcc metals:

$$f^a = \sigma_{eq} - Y_a$$

(7.17)

$$f^d = \sigma_{eq} - Y_a - \dot{R}\left(1 - \left(-\beta_2 T \ln(\eta_{eq}^p \dot{\rho})\right)^{1/q_2}\right)^{1/q_2} = 0$$

(7.18)

In the following we elaborate on the finite element implementation of the proposed viscoplastic model for both bcc and fcc metals. An implicit stress integration algorithm is introduced based on the radial return algorithm (Krieg and Krieg, 1977) and the backward-Euler integration algorithm using the Perzyna viscoplastic model as well as the Consistency model at which the radial return algorithm of elasto-thermoplasticity is directly extended to the case of elasto-thermoviscoplasticity.

7.3 Algorithmic Treatment and Computational Aspects

In any numerical scheme employed for the analysis of elasto-viscoplastic problems, it eventually becomes necessary to integrate the constitutive equations governing the material behavior. The precision with which the constitutive relations are integrated has a direct impact on the overall accuracy of the analysis. In this section, an implicit stress integration algorithm is proposed based on the radial return and the backward-Euler integration algorithms. The radial return algorithm is a widely successful method due to its good numerical performances and its well established numerical properties. In general, this method consists of;

1. the time-integration of the differential algebraic system, leading to an algebraic system that is solved by adopting backward-Euler time integration formula;
2. the formulation of the solution algorithm for the obtained algebraic system that is solved by the radial return map or what is called the radial map.

In displacement-based finite element formulations, stress updates take place at the Gauss points for a prescribed nodal displacement. In other words and as for most numerical schemes which are built to solve a constitutive equation, we suppose that the strain history path is known. We are then interested in the evolution of the other problem variables, in particular the stresses, the viscoplastic strain, and the total strain. We start by assuming that the load history interval is divided into a certain number of sub-intervals. For the interval from step $n$ to $n+1$, we start from time $t_n$ with the known converged state ($\sigma_n, X_n, R_n, T_n, \varepsilon_{eq}^n, \ldots$), to calculate, after
a certain increment of time, $\Delta t$, the corresponding values at time $t_{n+1} = t_n + \Delta t$ by applying the implicit backward-Euler scheme to the previous equations such that the following discrete equations may be found:

\[
\sigma_{n+1} = \sigma_n + \Delta \sigma = E : (\varepsilon_{n+1} - \varepsilon_{n+1}^v) \tag{7.19}
\]

\[
\varepsilon_{n+1}^v = \varepsilon_n^v + \Delta \varepsilon^v \tag{7.20}
\]

\[
\Delta \varepsilon^v = \Delta \lambda^v N_{n+1} \tag{7.21}
\]

\[
N_{n+1} = \frac{3}{2\sigma_{n+1}^q} (\tau_{n+1} - X_{n+1}) \tag{7.22}
\]

\[
\sigma_{n+1}^q = \sqrt{\frac{3}{2} (\tau_{n+1} - X_{n+1}) : (\tau_{n+1} - X_{n+1})} \tag{7.23}
\]

\[
X_{n+1} = X_n^v + \frac{2}{3} C \Delta \lambda^v N_{n+1} - \gamma \Delta \lambda^v X_{n+1} \tag{7.24}
\]

\[
\tau_{n+1} = \sigma_{n+1} - \frac{1}{3} \text{tr}(\sigma_{n+1}) \mathbf{1} = E : \varepsilon_{n+1} - 2 \mu \Delta \lambda^v N_{n+1} \tag{7.25}
\]

\[
T_{n+1} = T_n + \Delta \lambda^v z_{n+1} \tag{7.26}
\]

\[
z_{n+1} = \frac{1}{\rho c_p} \left( \sigma_{n+1}^q - \frac{3\gamma}{2C} X_{n+1} : X_{n+1} - R_{n+1} \right) \tag{7.27}
\]

For bcc metals,

\[
R_{n+1} = R_n + \Delta \lambda^v \frac{k}{2 R_{n+1}} (B^2 - R_{n+1}^2) \tag{7.28}
\]

or

\[
R_{n+1} = R_n + \Delta \lambda^v m R_{n+1} \left( B / R_{n+1} \right)^{1/m} \tag{7.29}
\]

For fcc metals,

\[
R_{n+1} = R_n + \Delta \lambda^v \frac{k}{2 \hat{R}_{n+1}} (\hat{B}^2 - \hat{R}_{n+1}^2) \bar{\theta}_{n+1} \tag{7.30}
\]

or

\[
R_{n+1} = R_n + \Delta \lambda^v m \hat{R}_{n+1} \left( \hat{B} / \hat{R}_{n+1} \right)^{1/m} \bar{\theta}_{n+1} \tag{7.31}
\]

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\[
\bar{\mathcal{G}}_{n+1} = \left( 1 - \left( -\beta_2 T_{n+1} \ln(\bar{\eta}^p_{n+1}) \frac{\Delta \lambda^p}{\Delta t} \right) \right)^{1/q_2} \tag{7.32}
\]

where \( \beta_2 = K / G_o \) is a material constant.

The assumption of elastic isotropy and plastic incompressibility is employed in determining the deviatoric stress \( \tau \) given in Eq.(7.25) in terms of the shear modulus, the deviatoric strain \( \epsilon \), and the Kronecker delta \( \mathbf{I} \). Moreover, von Mises plasticity is also assumed in the definition of the above yield functions.

In a strain-driven process, the new value of the total strain is known \( \epsilon_{n+1} \) and the unknowns are \( (\sigma_{n+1}, X_{n+1}, R_{n+1}, T_{n+1}, \epsilon^p_{n+1}, \ldots) \) which are driven by the value of \( \Delta \lambda^p \). To perform this update, the aforementioned equations need to be discretized and cast into a residual format (Borja, 1991; Groen, 1997; Suiker, 1998; and Heeres et al., 2002). In this regard, as an example, we obtain for the stress

\[
r_{\sigma} = \sigma_{n+1} - E : (\epsilon_{n+1} - \epsilon^p_{n+1}) \tag{7.33}
\]

In order to solve for the other state variables, the above residual relation is similarly applied and utilized, after requiring the following condition to hold with a prescribed tolerance:

\[
r(\sigma_{n+1}, \phi_{n+1}, \Delta \lambda^p) = 0 \tag{7.34}
\]

where \( \phi_{n+1} \) includes the scalar and tensor internal state variables \( (X_{n+1}, R_{n+1}, T_{n+1}, \ldots) \).

In general, the residuals are interrelated, and therefore, the solution has to be obtained in an iterative manner. Accordingly, the above set of nonlinear equations can be solved by applying a standard Newton-Raphson procedure with respect to the following unknowns:

\[
x = [\sigma_{n+1}, \phi_{n+1}, \Delta \lambda^p]^T \tag{7.35}
\]

The resulting solution scheme is given by:

\[
x^{i+1} = x^i - J(x^i)r(x^i) \tag{7.36}
\]

where the superscript \( i \) and \( i+1 \) refer to the previous iteration and to the current iteration respectively. With regard to the above definitions of the internal state variables, the Jacobian matrix takes a very complex form defining the inverse of the derivative of the residuals with respect to the internal state variables. That is,
\[ J(x') = \left( \frac{\partial r_{n+1}}{\partial x'_{n+1}} \right)^{-1} \]  

(7.37)

The solution given in Eq.(7.36) constitutes a general mean to solve the set of nonlinear equations (7.19)-(7.31) but, from the computational point of view, it does not represent an efficient solution. In fact, the evaluation of the Jacobian matrix Eq.(7.37) requires the derivatives of the state variables which can become a heavy burden for the solution algorithm. For realistic material models, higher order derivatives of the above functions may not be available or be extremely laborious to compute. In such cases, having an algorithm which only makes use of the essential response functions may be most desirable. Therefore, the return mapping algorithm, which is a special form of the backward-Euler procedure, aims to circumvent the aforementioned drawbacks.

### 7.3.1 Radial Return Mapping (for the Consistency Model)

A number of authors have advocated the use of return mapping (or radial return) algorithms for the integration of elastoplastic and elasoviscoplastic constitutive relations (e.g. Krieg and Krieg, 1977; Ortiz and Simo, 1986; Kang, 2004). Such algorithms satisfy the increment viscoplastic consistency requirement and enjoy good accuracy and stability properties. As we mentioned earlier, the internal state variables \( \phi \) at \( t_n \) are assumed to have been determined and known and we are concerned with solving for the stresses \( \phi_{n+1} \) at \( t_{n+1} \) after a certain time increment \( \Delta t \) and a given value of \( \Delta \varepsilon \).

In this section, the elastic predictor-viscoplastic corrector method is used along with the Consistency model for solving the above constitutive equations. In the Consistency approach the methodology used for plasticity is directly extended for the case of viscoplasticity by using, instead of the rate-independent yield function, the dynamic yield function that is defined at the end of the considered discrete time step as follows:

for bcc metals, 
\[
 f_{n+1}^d = \sigma_{n+1}^a - Y_a - R_{n+1} - \hat{Y} \left( 1 - \left( -\beta_2 T_{n+1} \ln (\bar{T}_o^{vp} \frac{\Delta \lambda^{vp}}{\Delta t}) \right)^{1/q_1} \right)^{1/q_2} = 0
\] (7.38)

for fcc metals, 
\[
 f_{n+1}^d = \sigma_{n+1}^{eq} - Y_a - \hat{R}_{n+1} \left( 1 - \left( -\beta_2 T_{n+1} \ln (\bar{T}_o^{vp} \frac{\Delta \lambda^{vp}}{\Delta t}) \right)^{1/q_1} \right)^{1/q_2} = 0
\] (7.39)

at which the converged stress should obey the above yield condition. In addition, the discrete counterpart of the Kuhn-Tucker conditions defined in the previous chapter become:
As in the continuum case, the Kuhn-Tucker conditions, Eq.(7.40), define the appropriate notion of loading/unloading. These conditions are reformulated in a form directly amenable to computational implementation by introducing the so-called the trial elastic state \((\sigma_{n+1}^*, \phi_{n+1}^*, f^*)\) where the superscript * is an indication of a trial state. From a physical standpoint, the trial elastic state is obtained by freezing the plastic/viscoplastic flow during the time step. As a matter of fact, this state arises naturally in the context of an elastic-viscoplastic operator split.

In the first step, the elastic predictor problem is solved with the converged values of the reversible state variables obtained at the previous time step. If a trial elastic stress state \(\sigma^*\) lies outside the yield surface, it will be taken as the initial condition for the solution of the viscoplastic corrector problem. The scope of this second step is to return the stresses to the yield surface or in some other way to ensure that the stresses remain at least very close to the surface.

**Crossing the Yield Surface**

The initial elastic predictor needed as a step to move forward from the elastic state to the inelastic state (forward-Euler procedure) can be cautiously obtained by setting \(\Delta \varepsilon = \Delta \varepsilon^*\), such that:

\[
\sigma_{n+1}^* = \sigma_n + E : \Delta \varepsilon
\]

For this tentative stress state, the dynamic yield criterion is given, for the case of bcc and fcc metals, by:

for bcc metals,

\[
f_{n+1}^{d*} = \sqrt{\frac{3}{2} \left( \tau_{n+1}^* - X_{n+1} \right) \cdot \left( \tau_{n+1}^* - X_{n+1} \right) - Y_n - R_n - \hat{\gamma} \left( 1 - \left( -\beta_i T_n \ln(\eta_{o}^{vp} \frac{\Delta \lambda^{vp}}{\Delta t}) \right)^{1/q} \right)^{1/q} \right)}
\]

for fcc metals,

\[
f_{n+1}^{d*} = \sqrt{\frac{3}{2} \left( \tau_{n+1}^* - X_{n+1} \right) \cdot \left( \tau_{n+1}^* - X_{n+1} \right) - Y_n - \hat{\gamma} \left( 1 - \left( -\beta_i T_n \ln(\eta_{o}^{vp} \frac{\Delta \lambda^{vp}}{\Delta t}) \right)^{1/q} \right)^{1/q} \right)}
\]

With the above definition of the trial state of the yield function, the elastic and viscoplastic states of the material deformation are determined. In other words, the material is still elastic if \(f_{n+1}^{d*} \leq 0\) which also implies that the trial stress \(\sigma_{n+1}^*\) is accepted as the converged stress \(\sigma_{n+1}\). On the other hand, viscoplastic deformation is indicated if \(f_{n+1}^{d*} > 0\) which requires a proper
return to the yield surface as the trial stress cannot be accepted as \( \sigma_{n+1} \). In this case, the strain increment contains both the elastic and viscoplastic components and the converged stress that satisfies the dynamic yield surface Eqs.(7.38) or (7.39) can be written using Eq.(7.41) along with Eq.(7.19) as follows:

\[
\sigma_{n+1} = \sigma_{n+1}^* - E : \Delta \varepsilon^p = \sigma_{n+1}^* - 2\mu N_{n+1} \Delta \lambda^p
\]  

(7.44)

Eq.(7.44) is considered as the base of the backward-Euler return at which the term \( E : \Delta \varepsilon^p \) represents the viscoplastic corrector. If the initial yield surface has been crossed during the initial trial increment, the location of the intersection of the elastic stress vector with the yield surface (point \( b \) in Figure 1) is, then, required.

In such circumstances, we require

\[
f(\sigma_a + \alpha \Delta \sigma) = f_b = 0
\]  

(7.45)

where \( \Delta \sigma \) denotes the increment of stress at which the yield stress is crossed for the first time and \( \alpha \Delta \sigma \) is the portion of the stress increment necessary to bring the trial stress state to the initial yield surface. Where the original stresses, \( \sigma_a \) are such that

\[
f(\sigma_a) = f_a < 0
\]  

(7.46)

while, in the case of \( \alpha = 1 \), the elastic stresses \( \sigma_c = \sigma_a + \Delta \sigma \) give

\[
f(\sigma_a + \Delta \sigma) = f_c > 0
\]  

(7.47)

As indicated by Eq.(7.45), the portion \( \alpha \) can be determined by employing the dynamic yield surface Eq.(7.38) for the case of bcc metals or Eq.(7.39) for the case of fcc metals, leading to a quadratic equation for the determination of \( \alpha \). Alternatively, we can use a truncated Taylor series with \( \alpha \) as the only variable to set up an iterative scheme (Crisfield, 1997). Such a scheme might start with the following linear interpolation as an initial estimate

\[
\alpha_i = \frac{-f_a}{f_c - f_a}
\]  

(7.48)

where, in this case, the yield function of Eqs.(7.42) and (7.43) is utilized for bcc and fcc metals respectively. Due to the nonlinearity in the function \( f \), the above linear interpolation is not enough to evaluate the exact value of \( \alpha \) from the first iteration and therefore, further iterations are required. A truncated Taylor series is, then, used to give a first change in \( \alpha \), \( \Delta \alpha \), such that:

\[
f_a = f_i + \frac{\partial f}{\partial \sigma} \frac{\partial \sigma}{\partial \alpha} \Delta \alpha = f_i + N_{n+1}^* : \Delta \sigma \Delta \alpha = 0
\]  

(7.49)
where \( f_i \) is computed with the stresses at the old iteration, i.e., \( \sigma = \sigma_a + \alpha_i \Delta \sigma \). By making use of Eqs.\( (7.48) \) and \( (7.49) \), the scalar \( \alpha \) would then be updated using the following relation

\[
\alpha = \alpha_i + \Delta \alpha = \frac{-f_a}{f_i - f_a} + \frac{-f_i}{N_{\alpha_i} \cdot \Delta \sigma} \quad (7.50)
\]

Having computed the intersection point, the remaining portion of the trial stress increment (or the strain increment), which is \((1 - \alpha) \Delta \sigma\), can be treated in an elasto-viscoplastic manner.

Following the initial predictor, we may need to obtain the real values of the stresses that coincide with the updated dynamic yield function. It is clear from the above definitions of the state variables that the converged stresses can be readily obtained if the increment of the viscoplastic strain \( \Delta \varepsilon^{vp} \) is found, i.e., if the viscoplastic multiplier \( \Delta \lambda^{vp} \) is determined.

With the Consistency model, two different methodologies may be adopted to calculate \( \Delta \lambda^{vp} \); by discretizing the consistency condition of the dynamic yield surface or by solving a nonlinear scalar relation (return mapping algorithm) of the viscoplastic multiplier.
• Consistency Condition

In the consistency model, with the fact that the viscoplastic flow direction is defined similar to Eq. (7.21), the viscoplastic multiplier is determined by the discretized consistency condition of the dynamic yield surface, Eqs. (7.38) and (7.39) for bcc and fcc metals respectively.

\[ f_{i+1}^d = f_i^d + \Delta f_i^d = 0 \]  
(7.51)

where \( f_i^d \) is the \( i \)th residual of the yield function. For clarity we omit the subscript \( n+1 \) from the increment of a state variable \( \Delta \left( \right)_{n+1} \) in the following equations since all of the increments are provided at time step \( t = t_{n+1} \) unless otherwise specified. Moreover, we directly express the yield surface as a function of the viscoplastic multiplier since \( \Delta \lambda = \Delta \rho \) for von Mises plasticity/viscoplasticity. Accordingly, the dynamic yield function increment is written as follows:

\[ \Delta f_i^d = N : \Delta \sigma - N : \Delta X - h\Delta \lambda^{vp} - \theta \Delta T - y\Delta \lambda^{vp} \]  
(7.52)

where \( N \) is defined in Eq. (7.22) and \( \Delta \lambda^{vp} \) is defined as follows:

\[ \Delta \lambda^{vp} = \lambda_{n+1}^{vp} - \lambda_n^{vp} = \frac{\Delta \lambda_{n+1}}{\Delta t_{n+1}} - \frac{\Delta \lambda_n}{\Delta t_n} \]  
(7.53)

For the case of bcc metals, the scalar parameters \( h, \theta, \) and \( y \) are defined as follows:

\[ h = -\frac{\partial f_i^d}{\partial \rho} \frac{\partial R}{\partial \rho} = \frac{\partial R}{\partial \rho} = \frac{k}{2R} \left( B^2 - R^2 \right) \quad \text{for} \quad R = B \left( 1 - \exp(-kp) \right)^{1/2} \]  
(7.54)

\[ h = -\frac{\partial f_i^d}{\partial R} \frac{\partial \rho}{\partial R} = \frac{\partial R}{\partial \rho} = mR \left( B / R \right)^{1/m} \quad \text{for} \quad R = Bp^n \]  
(7.55)

\[ \theta = -\frac{\partial f_i^d}{\partial T} = -\frac{\partial f_i^d}{\partial T} \frac{\Delta T}{\Delta \lambda^{vp}} = z\hat{\gamma} \zeta \ln(\eta_o^{vp}) \frac{\Delta \lambda^{vp}}{\Delta t} \]  
(7.56)

\[ y = -\frac{\partial f_i^d}{\partial \rho} = \Delta t \hat{\gamma} T \zeta / \Delta \lambda^{vp} \]  
(7.57)

\[ \zeta = \frac{\beta}{q_1 q_2} \left( 1 - \left( -\beta_2 T \ln(\eta_o^{vp}) \frac{\Delta \lambda^{vp}}{\Delta t} \right)^{1/q_1} \right)^{1/(q_1 - 1)} \]  
(7.58)
whereas, they are defined for the case of fcc metals as follows:

\[
\begin{align*}
\dot{h} &= - \frac{\partial f^d}{\partial R} \frac{\partial R}{\partial p} = \frac{\partial R}{\partial p} = \frac{\tilde{g} k}{2\tilde{R} \sqrt{\hat{B}^2 - \tilde{R}^2}} \quad \text{for} \quad \hat{R} = \hat{B} \left(1 - \exp(-kp)\right)^{1/2} \\
\dot{h} &= - \frac{\partial f^d}{\partial R} \frac{\partial R}{\partial p} = m \tilde{g} \hat{R} \left( \hat{B} / \hat{R} \right)^{1/m} \quad \text{for} \quad \hat{R} = \hat{B} p^m
\end{align*}
\]

\[\theta = - \frac{\partial f^d}{\partial T} \frac{\Delta T}{\Delta \lambda^{vp}} = z \hat{R} \bar{\zeta} \ln(\bar{\eta}_o^{vp} \hat{p}) \]

\[y = - \frac{\partial f^d}{\partial p} = \Delta t \hat{R} T / \Delta \lambda^{vp} \]

\[\bar{\zeta} = \frac{\beta_2}{q_1 q_2} \left(1 - \left(-\beta_2 T \ln(\bar{\eta}_o^{vp} \frac{\Delta \lambda^{vp}}{\Delta t})\right)^{1/q_1} \left(-\beta_2 T \ln(\bar{\eta}_o^{vp} \frac{\Delta \lambda^{vp}}{\Delta t})\right)^{1/q_2} \right)^{-1} \]

\[\bar{\eta}_o^{vp} = \eta_o^{vp} \left(1 + C_1 \left(1 - e^{\eta_o^{vp}}\right)\right)^{-1} \]

where \(C_1\) is a material constant that is related to the microstructural physical quantities and \(\eta_o^{vp}\) represents the reference (lowest) value of the viscosity parameter proportional to the lowest value of dislocations waiting time at an obstacle (see, for more details, chapter 6). In defining Eqs.(7.59) and (7.60), the derivative of \(\bar{\eta}_o^{vp}\), which is a very small value, with respect to the plastic strain is ignored for maintaining the simplicity of the formulation, i.e. \(\partial \bar{\eta}_o^{vp} / \partial p = 0\).

Substituting Eqs. (7.19), (7.24), (7.26), and (7.53) for \(\Delta \sigma\), \(\Delta X\), \(\Delta T\), and \(\Delta \lambda^{vp}\) respectively, into the consistency condition, yields the following closed form expression for the viscoplastic multiplier

\[\Delta \lambda^{vp} = \frac{1}{\Lambda} \left(2 \mu N : \Delta \sigma + y \frac{\Delta \lambda^{vp}}{\Delta t} + f_i^d\right) \]

where

\[\Lambda = \left(\frac{y}{\Delta t} + H\right) \]

and

\[H = 3\mu + C - \gamma X : N + h + \theta \]
where \( h, \theta, \) and \( y \) were defined previously for both bcc and fcc metals. It is clear from Eq.(7.65) that the consistency parameter (viscoplastic multiplier, \( \Delta \lambda^{vp} \) ) now, not only depends on the strain (or stress), but also on the viscoplastic multiplier at the end of the previous time step. This, however, does not generate complications in the numerical procedure, as both parameters may be evaluated at each discrete time step. In other words, the incremental viscoplastic multiplier at the previous time-step, \( \Delta \lambda^{vp}_n \) and \( \Delta t_n \), need to be evaluated in order to update the consistency parameter given in Eq.(7.65).

Furthermore, taking the rate of Eq.(7.19) and making use of Eq.(7.21) along with the derived definition of the viscoplastic multiplier \( \Delta \lambda^{vp} \) given in Eq.(7.65) result in the following rate of stress equation:

\[
\Delta \sigma = \left( E - \frac{4 \mu^2}{\Lambda} N \otimes N \right) : \Delta \varepsilon - \frac{2 \mu}{\Lambda} \left( y \frac{\Delta \lambda^{vp}}{\Delta t_n} + f^d \right) N
\]

(7.68)

where the symbol \( \otimes \) represents the dyadic tensor product \((N_{ij} \otimes N_{kl} = M_{ijkl})\). Eq.(7.68) may be utilized to obtain a proper definition for the continuum elasto-viscoplastic tangent modulus, \( D^{vp} = \Delta \sigma / \Delta \varepsilon \) that is used if small time-steps are adopted. For the case of large time-steps, in contrast, an algorithmic consistent tangent stiffness modulus, \( D^{alg} = d\Delta \sigma / d\Delta \varepsilon \), is essential to preserve the quadratic rate of asymptotic convergence that characterizes the Newton-Raphson technique.

Note here that if we assign to \( N, h, \theta, \) and \( y \) their values at the beginning of the increment and use Eq.(7.51) to compute \( \Delta \lambda^{vp} \), we adopt a “forward-Euler scheme” which is bound to lead to stresses that lie outside the yield surface at the end of the increment. Accordingly, errors will accumulate such that the computed collapse load will generally be over-predicted. This, however, can be avoided by taking iterative steps to return the stresses to the yield surface or at least very close to the surface. On the other hand, Assigning to \( N, h, \theta, \) and \( y \) their values at the end of the considered discrete time step requires solving a set of nonlinear equations that is computationally complex and not preferable as mentioned earlier in this section.

**Nonlinear Scalar Equation (Radial Return Mapping)**

For isotropic elasticity with an additive decomposition of strains and associated flow, the problem of solving for \( \Delta \lambda^{vp} \) can be reduced to solving a non-linear scalar equation in the deviatoric stress space as will be explained in this subsection.

It is obvious that the hydrostatic part of the trial and the converged stresses given in Eq.(7.44) are identical, i.e. \( tr(\sigma^{*,1}) = tr(\sigma^{*,1}) \) since \( tr(\mathbf{N}^{*,1}) = 0 \) for von Mises plasticity. Thus, splitting the stresses in Eq.(7.44) into the deviatoric and hydrostatic components yields:
\[ \tau_{n+1} = \tau^*_{n+1} - 2\mu \Delta \lambda^{vp} N_{n+1} \]  

(7.69)

Combining the above relation with Eq.(7.24) gives:

\[ \xi_{n+1} = \xi_{n+1} - \Delta \lambda^{vp} \left( 2\mu + \frac{2}{3} a_{n+1} C \right) N_{n+1} \]  

(7.70)

where

\[ \xi_{n+1} = \tau_{n+1} - X_{n+1} \]  

(7.71)

\[ \xi^*_{n+1} = \tau^*_{n+1} - a_{n+1} X_n \]  

(7.72)

\[ a_{n+1} = \frac{1}{1 + \gamma \Delta \lambda^{vp}} \]  

(7.73)

In this case, the definition of the equivalent stress \( \sigma_{n+1}^{eq} \) along with \( N_{n+1} \) is rewritten as follows:

\[ \sigma_{n+1}^{eq} = \sqrt{\frac{3}{2} \xi_{n+1} \cdot \xi_{n+1}} = \sqrt{\frac{3}{2} \xi_{n+1}^{\cdot2}} \]  

(7.74)

\[ N_{n+1} = \frac{3}{2\sigma_{n+1}^{eq}} \xi_{n+1} \]  

(7.75)

Furthermore, the corresponding trial stresses can be rewritten in a similar way as in the above two relations. That is,

\[ \sigma_{n+1}^{eq*} = \sqrt{\frac{3}{2} \xi^*_{n+1} \cdot \xi^*_{n+1}} = \sqrt{\frac{3}{2} \xi^*_{n+1}^{\cdot2}} \]  

(7.76)

\[ N^*_{n+1} = \frac{3}{2\sigma_{n+1}^{eq*}} \xi^*_{n+1} \]  

(7.77)

Hence, From Eq.(7.70), \( N_{n+1} \) is determined exclusively in terms of the trial stress \( \xi^*_{n+1} \), as follows:

\[ N_{n+1} = \frac{3}{2\sigma_{n+1}^{eq*}} \xi^*_{n+1} = N^*_{n+1} \]  

(7.78)

In deviatoric stress space, the von Mises yield surface is circular and therefore the normal to the yield surface is radial (see Figure 7.2). In this regard, Eq.(7.78) represents the main principle of the return mapping algorithm as it returns the trial stress to the yield surface radially in the deviatoric stress space. This, actually, is considered as the key feature of the
radial return method as $N$ remains radial and unchanged throughout the plastic/viscoplastic corrector phase of the algorithm.

Figure 7.2 Geometric interpretation of the radial return method for von Mises plasticity/viscoplasticity with isotropic and kinematic hardening.

Next, by taking the dot product of Eq.(7.70) with $N_{n+1}$, and with the aid of Eq.(7.78) noting that $N_{n+1} : N_{n+1} = 3/2$, we obtain the following scalar equation.

$$\sigma_{n+1}^{eq} = \sigma_{n+1}^{eq} - \Delta \lambda^{vp} (3\mu + aC)$$  \hspace{1cm} (7.79)

In fact, Eq.(7.79) can alternatively be obtained by using Eq.(7.70) directly in the dot product of $\xi_{n+1}$ with itself, i.e. $\|\xi_{n+1}\| = \xi_{n+1} : \xi_{n+1}$.

Substituting Eq.(7.79) in the dynamic yield function at the end of the increment, Eq.(7.38) for bcc metals and Eq.(7.39) for fcc metals, we obtain the following nonlinear scalar relation that determines the consistency parameter $\Delta \lambda^{vp}$.

$$r(\Delta \lambda^{vp}) = \sigma_{n+1}^{eq} - \Delta \lambda^{vp} (3\mu + aC) - Y_a - R_{n+1} - \hat{Y} \left( 1 - \left( -\beta T_{n+1} \ln(\eta^{vp} \Delta \lambda^{vp} / \Delta t) \right)^{1/q_1} \right)^{1/q_2} = 0$$  \hspace{1cm} (7.80)
\[
-r(\Delta \lambda^{vp}) = \sigma^{eq}_{n+1} - \Delta \lambda^{vp} (3\mu + aC) - Y - \hat{R}_{n+1} \left(1 - \beta_2 \frac{\ln(\Delta \lambda^{vp})}{\Delta t}\right)^{1/q_1} = 0 \quad (7.81)
\]

The above relations, Eq.(7.80) for bcc metals and Eq.(7.81) for fcc metals, are the key equations for the numerical method as they represent an equivalent algorithm of the consistency condition, Eq.(7.65), for the considered internal state variables. They can be solved using the local Newton-Raphson method described in the previous section, Eq.(7.36), with one variable in each iteration, \(x_i = (\Delta \lambda^{vp})^i\). That is,

\[
(\Delta \lambda^{vp})^{i+1} = (\Delta \lambda^{vp})^i - (J(\Delta \lambda^{vp}))^i (r(\Delta \lambda^{vp}))^i \quad (7.82)
\]

in which the Jacobian in this case is a scalar quantity and defined as follows:

\[
J(\Delta \lambda^{vp}) = \left(\frac{\partial r(\Delta \lambda^{vp})}{\partial \Delta \lambda^{vp}}\right)^{-1} \quad (7.83)
\]

where for both bcc and fcc metals:

\[
\frac{\partial r(\Delta \lambda^{vp})}{\partial \Delta \lambda^{vp}} = \frac{\partial \sigma^{eq}_{n+1}}{\partial \Delta \lambda^{vp}} + \Delta \lambda^{vp} \gamma Ca_{n+1}^2 - a_{n+1}C - 3\mu - h_{n+1} - \theta_{n+1} - \frac{Y_{n+1}}{\Delta t} \quad (7.84)
\]

\[
= \frac{3\gamma a_{n+1}^2}{2\sigma_{n+1}^{eq}} \mathbf{e}_\mathbf{n} : \mathbf{X}_\mathbf{n} \quad (7.85)
\]

Herein, the scalar parameters \(h, \theta, \) and \(\gamma\), which are the same as those previously given for both bcc and fcc metals, are defined at the end of the considered time step.

Eq.(7.82) can be solved by a method similar to the successive substitution (Kobayashi and Ohno, 2002) at which the iterations are ended when an acceptable accuracy in the dynamic yield function falls within a prescribed tolerance. The convergence of the successive iteration process is guaranteed as proved by Kobayashi and Ohno (2002) since the residual \(r\) is a convex function of \(\Delta \lambda^{vp}\). For convenience, a step-by-step description of the above-mentioned implicit stress integration using the Consistency model is simply illustrated in Figure 7.3.

### 7.3.2 Radial Return Mapping (for the Perzyna Model)

The general algorithm developed in the preceding section is going to be adopted for the Perzyna viscoplastic model. This classical viscoplastic model is obtained from a rate-independent plasticity model by replacing the consistency parameter \(\hat{\lambda} > 0\) with an explicit definition for the viscoplastic multiplier. In this work, we similarly replace the consistency
parameter $\dot{\lambda}^{vp} > 0$ in the dynamic yield function by the following general definition for the viscoplastic multiplier $\Delta \lambda^{vp}$:

$$\Delta \lambda^{vp} = \frac{\Delta \lambda}{\eta^{vp}(T_{n+1})} \varphi_{n+1}(f_{n+1}, T_{n+1}, K)$$  \hspace{1cm} (7.86)$$

where $\eta^{vp}$ denotes the viscosity parameter (relaxation time) that is explicitly related to the temperature. The viscosity parameter is related to the initial dislocation density for the case of bcc metals, while, it is affected by the total dislocation density in the case of fcc metals. Thus, in contrast to bcc metals, it varies with the accumulation of the viscoplastic strain in fcc metals such that:

for bcc metals

$$\eta^{vp}_{n+1} = \eta^{vp}_0 \exp \left( \frac{1}{\beta_2 T_{n+1}} \right)$$  \hspace{1cm} (7.87)$$

for fcc metals

$$\eta^{vp}_{n+1} = \overline{\eta}^{vp}_0 \exp \left( \frac{1}{\beta_2 T_{n+1}} \right)$$  \hspace{1cm} (7.88)$$

where the plastic strain dependent parameter $\overline{\eta}^{vp}_0$ is defined in Eq.(7.64).

The overstress function, on the other hand, is defined in terms of the rate-independent yield function, which is chosen here as the athermal yield function for both bcc and fcc metals, such that:

for bcc metals:

$$\varphi_{n+1}(f_{n+1}, T_{n+1}, \hat{Y}) = \exp \left( \frac{1 - \left( 1 - \left( \frac{f_{n+1}}{\hat{Y}} \right)^{\eta} \right)^{\eta}}{\beta_2 T_{n+1}} \right)$$  \hspace{1cm} (7.89)$$

where

$$f_{n+1} = \sigma_{n+1}^{eq} - Y_a - R_{n+1}$$  \hspace{1cm} (7.90)$$

$$f_{n+1}^s = \sigma_{n+1}^{eq} - Y_a - R_n$$  \hspace{1cm} (7.91)$$

for fcc metals:

$$\varphi_{n+1}(f_{n+1}, T_{n+1}, \hat{R}) = \exp \left( \frac{1 - \left( 1 - \left( \frac{f_{n+1}}{\hat{R}} \right)^{\eta} \right)^{\eta}}{\beta_2 T_{n+1}} \right)$$  \hspace{1cm} (7.92)$$
Figure 7.3 Flow Chart of stress integration algorithm for both bcc and fcc metals using the Perzyna and the Consistency viscoplastic models.
where

\[ f_{n+1} = \sigma_{eq}^{n+1} - Y_a \]  

(7.93)

\[ f_{n+1}^* = \sigma_{eq}^{n+1} - Y_a \]  

(7.94)

Assuming that \( f_{n+1}^* > 0 \) so that viscoplastic loading takes place, then an implicit backward-Euler difference scheme yields the counterpart of the algorithm equations Eqs.(7.19)-(7.31) in which the viscoplastic multiplier in these equations is replaced by the definition given in Eq.(7.86). The nonlinear scalar relation given in Eq.(7.79) is, similarly obtained, by following the same procedure for the radial return algorithm explained in section 7.3.1 for the Consistency model, with the use of the rate-independent yield functions (Eqs.(7.90) and (7.91) for bcc metals and Eqs.(7.93) and (7.94) for the case of fcc metals) instead of the dynamic yield functions (Eqs.(7.38) and (7.42) for bcc metals and Eqs.(7.39) and (7.43) for the case of fcc metals).

By substituting Eq.(7.86), with the aid of Eqs.(7.87), (7.89), and (7.90) for bcc metals and Eqs. (7.88), (7.92), and (7.93) for fcc metals, into Eq.(7.79), a non-linear scalar equation for \( \sigma_{eq}^{n+1} \) is obtained such that:

for bcc metals:

\[
r(\sigma_{eq}^{n+1}) = \sigma_{eq}^{n+1} - \sigma_{eq}^{n+1} + (3\mu + aC) \frac{\Delta t}{\eta_{eq}^{vp}} \exp \left\{ - \frac{1 - \left( (\sigma_{eq}^{n+1} - Y_a - R_{n+1}) / \hat{Y}_{2} \right)^{q_1}}{\beta_{2}T_{n+1}} \right\} = 0 
\]  

(7.95)

For fcc metals:

\[
r(\sigma_{eq}^{n+1}) = \sigma_{eq}^{n+1} - \sigma_{eq}^{n+1} + (3\mu + aC) \frac{\Delta t}{\eta_{eq}^{vp} / \hat{R}_{n+1}} \exp \left\{ - \frac{1 - \left( (\sigma_{eq}^{n+1} - Y_a / \hat{R}_{n+1}) / \hat{q}_2 \right)^{q_1}}{\beta_{2}T_{n+1}} \right\} = 0 
\]  

(7.96)

It should be mentioned here that \( T_{n+1}, R_{n+1}, \) and \( \hat{R}_{n+1} \) are also functions of \( \sigma_{eq}^{n+1} \) which increase the nonlinearity order of the above residual relations. This problem, however, may be solved iteratively using the local Newton-Raphson method described earlier with one variable in each iteration, \( x^i = (\sigma_{eq}^{n+1})^i \). That is,

\[
(\sigma_{eq}^{n+1})^{i+1} = (\sigma_{eq}^{n+1})^i - (J(\sigma_{eq}^{n+1}))^i (r(\sigma_{eq}^{n+1}))^i
\]  

(7.97)

in which the Jacobian in this case is a scalar quantity and is defined for the case of bcc and fcc metals as such

\[
J(\sigma_{eq}^{n+1}) = \left( \frac{\partial r(\sigma_{eq}^{n+1})}{\partial \sigma_{eq}^{n+1}} \right)^{-1}
\]  

(7.98)
Eq. (7.97) can similarly be solved using the successive substitution method of Kobayashi and Ohno (2002) at which the iterations are ended when an acceptable accuracy in the dynamic yield function falls within a prescribed tolerance. Once $\sigma_{n+1}^{eq}$ is calculated, the viscoplastic multiplier is determined using the following two relations for both bcc and fcc metals:

For bcc metals:

$$\Delta \lambda_{vp} = \frac{\Delta t}{\eta_o^{vp}} \exp \left\{ \frac{-\left(1-\left(\sigma_{n+1}^{eq} - Y_a - R_n\right) / \dot{\gamma}\right)^{q_1}}{\beta_2 T_{n+1}} \right\}$$ (7.99)

where

$$T_{n+1} = T_n + \frac{z_n \Delta t}{\eta_o^{vp}} \exp \left\{ \frac{-\left(1-\left(\sigma_{n+1}^{eq} - Y_a - R_n\right) / \dot{\gamma}\right)^{q_1}}{\beta_2 T_n} \right\}$$ (7.100)

$$R_{n+1} = R_n + \frac{k \Delta t \left(\bar{B}^2 - R_n^2\right)}{2 R_n \eta_o^{vp}} \exp \left\{ \frac{-\left(1-\left(\sigma_{n+1}^{eq} - Y_a - R_n\right) / \dot{\gamma}\right)^{q_1}}{\beta_2 T_n} \right\}$$ (7.101)

or

$$R_{n+1} = R_n + \frac{m \Delta t R_n \left(B / R_n\right)^{1/m}}{\eta_o^{vp}} \exp \left\{ \frac{-\left(1-\left(\sigma_{n+1}^{eq} - Y_a - R_n\right) / \dot{\gamma}\right)^{q_1}}{\beta_2 T_n} \right\}$$ (7.102)

For fcc metals,

$$\Delta \lambda_{vp} = \frac{\Delta t}{\eta_{on+1}^{vp}} \exp \left\{ \frac{-\left(1-\left(\sigma_{n+1}^{eq} - Y_a / \dot{\gamma}\right)^{q_1}}{\beta_2 T_{n+1}} \right\}$$ (7.103)

$$T_{n+1} = T_n + \frac{z_n \Delta t}{\eta_{on}^{vp}} \exp \left\{ \frac{-\left(1-\left(\sigma_{n+1}^{eq} - Y_a / \dot{\gamma}\right)^{q_1}}{\beta_2 T_n} \right\}$$ (7.104)

$$\hat{R}_{n+1} = \hat{R}_n + \frac{k \Delta t \left(\bar{B}^2 - \hat{R}_n^2\right) \bar{\gamma}_n}{2 \hat{R}_n \eta_{on}^{vp}} \exp \left\{ \frac{-\left(1-\left(\sigma_{n+1}^{eq} - Y_a / \dot{\gamma}\right)^{q_1}}{\beta_2 T_n} \right\}$$ (7.105)

or
\[
\hat{R}_{n+1} = \hat{R}_n + \frac{m\Delta t \hat{\gamma}_n \left( \hat{B} / \hat{\gamma}_n \right)^{1/m} \hat{\gamma}_n}{\hat{\gamma}^p_{on}} \exp \left\{ -\frac{\left(1 - (\sigma_{n+1}^m - Y_c) / \hat{\gamma}_n \right)^{q_i}}{\beta \hat{\gamma}_n} \right\} 
\]

(7.106)

The above-mentioned implicit stress integration process for the case of Perzyna viscoplastic model is illustrated in the flow chart presented in Figure 7.3.

Next we obtain an explicit expression for the consistent (algorithmic) elasto-viscoplastic tangent modulus in order to obtain a quadratic convergence at the system level. This modulus relates the incremental strains and incremental stresses and plays a crucial role in the overall solution strategy of a boundary value problem (Simo and Hughes, 1998).

### 7.3.3 Derivation of the Consistent (Algorithmic) Tangent Modulus

In this section, a tangent modulus consistent with the integration algorithm is developed for the proposed constitutive model. The derivation of this algorithmic stiffness matrix \( D_{alg} = d\Delta \sigma / d\Delta \epsilon \), starts by differentiating the algorithm, Eqs.(7.19)-(7.22) such that:

\[
d\Delta \sigma = E \left( d\Delta \epsilon - d\Delta \epsilon^p \right) \quad (7.107)
\]

\[
d\Delta \epsilon^p = d\Delta \lambda^p N_{n+1} + \Delta \lambda^p dN_{n+1} \quad (7.108)
\]

\[
dN_{n+1} = \frac{3}{2\sigma_{eq}} \left( I - N_{n+1} \otimes N_{n+1} \right) : d\xi_{n+1} \quad (7.109)
\]

where \( I = 1 \otimes 1 \) \((I_{ijkl} = \delta_{ij} \delta_{kl})\) is the fourth order unit tensor and \( I \) is the second-order unit tensor. Utilizing Eqs.(7.107) and (7.108), the general form for the algorithmic tangent stiffness matrix may be given as such:

\[
D_{alg} = \frac{d\Delta \sigma}{d\Delta \epsilon} = E - 2\mu \left( \frac{d\Delta \lambda^p \otimes N_{n+1}}{d\Delta \epsilon} : \Delta \lambda^p \frac{dN_{n+1}}{d\Delta \epsilon} \right) \quad (7.110)
\]

According to the above equation (7.110), the consistent tangent modulus can be easily obtained if the following two terms \( dN_{n+1} / d\Delta \epsilon \) and \( d\Delta \lambda^p / d\Delta \epsilon \) are determined. Using the chain rule, the former term can be expressed as follows:

\[
\frac{dN_{n+1}}{d\Delta \epsilon} = \frac{dN_{n+1}}{d\xi_{n+1}} \cdot \frac{d\xi_{n+1}}{d\Delta \epsilon} \quad (7.111)
\]

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In view of Eqs.(7.109) and (7.72), the two terms in the right hand side of the above equation are expressed as follows:

\[
d\frac{N_{n+1}}{\xi_n} = \frac{3}{2\sigma_{n+1}^{ep}}(1 - N_{n+1} \otimes N_{n+1}) \tag{7.112}
\]

\[
d\frac{\xi_n^*}{\Delta \xi} = \frac{d\tau_n^*}{d\Delta \xi} - \frac{d\sigma_{n+1}}{d\Delta \xi} : X_n \tag{7.113}
\]

where

\[
d\frac{d\tau_n^*}{d\Delta \xi} = \frac{d\left(\tau_n + 2\mu d\xi\right)}{d\Delta \xi} = 2\mu I^d \tag{7.114}
\]

\[
d\frac{d\sigma_{n+1}}{d\Delta \xi} = \frac{d\Delta \lambda^{vp}}{d\Delta \xi} d\Delta \lambda^{vp} = -\gamma a_{n+1} d\Delta \lambda^{vp} \tag{7.115}
\]

Herein, \(I^d = I - 1 \otimes 1\), represents the deviatoric part of the fourth-order unit tensor.

It is obvious now that \(d\Delta \lambda^{vp} / d\Delta \xi\) is the only missing term in the definition of the algorithmic stiffness matrix Eq.(7.110). This term can be determined using one of the viscoplastic multiplier definitions given in Eqs.(7.65), (7.80), and (7.99) for bcc metals and Eqs.(7.65), (7.81), and (7.103) for fcc metals. The simplest way, however, is by differentiating Eqs.(7.80) and (7.81) with respect to the strain increment, \(\Delta \xi\), such that:

\[
\frac{d\sigma_{n+1}^{ep}}{d\Delta \xi} = (3\mu + aC) \frac{d\Delta \lambda^{vp}}{d\Delta \xi} - h_{n+1} \frac{d\Delta \lambda^{vp}}{d\Delta \xi} - \theta_{n+1} \frac{d\Delta \lambda^{vp}}{d\Delta \xi} - \frac{\gamma a_{n+1} d\Delta \lambda^{vp}}{d\Delta \xi} = 0 \tag{7.116}
\]

where the scalar parameters \(h_{n+1}\), \(\theta_{n+1}\), and \(\gamma_{n+1}\) are defined in Eqs.(7.54)-(7.57) for bcc metals and Eqs.(7.59)-(7.62) for fcc metals. Using Eq.(7.74) for a similar definition of \(\sigma_{n+1}^{ep}\), the first term in the right hand side of Eq.(7.116) is given by:

\[
\frac{d\sigma_{n+1}^{ep}}{d\Delta \xi} = \frac{d\xi_n^*}{d\Delta \xi} : N_{n+1} \tag{7.117}
\]

Substituting Eq.(7.117), after making use of Eqs.(7.113)-(7.115), into Eq.(7.116) with a simple rearrangement, the differentiation of the viscoplastic multiplier with respect to the strain increment \(\Delta \xi\) is defined as follows:

\[
\frac{d\Delta \lambda^{vp}}{d\Delta \xi} = 2\mu L_{n+1}^{-1} N_{n+1} \tag{7.118}
\]

where

\[
L_{n+1} = 3\mu + aC + h_{n+1} + \theta_{n+1} + \frac{\gamma_{n+1}}{\Delta t} - \gamma C \Delta \lambda^{vp} a_{n+1}^2 - \gamma a_{n+1}^2 N_{n+1} : X_n \tag{7.119}
\]
Finally, a new expression for the algorithmic (consistent) tangent stiffness matrix is derived by substituting Eq.(7.118) for \(d\lambda^{vp}/d\Delta\varepsilon\) and Eq.(7.111) for \(dN_{n+1}/d\Delta\varepsilon\) into Eq.(7.110) with the aid of Eqs.(7.112)-(7.115) such that:

\[
D^{alg} = E - 4\mu^2 \left( \Pi_{n+1} + Z_{n+1} \left( N_{n+1} \otimes N_{n+1} \right) \right)
\]  

(7.120)

where the fourth-order tensor, \(\Pi\), and the scalar \(Z\) are defined as follows:

\[
\Pi_{n+1} = \frac{3 \Delta \lambda^{vp}}{2\sigma_{n+1}^{vp}} \left( I^d + \gamma a^2_{n+1} L_{n+1}^{-1} N_{n+1} : X_n \right) 
\]  

(7.121)

\[
Z_{n+1} = \frac{3 \Delta \lambda^{vp}}{2\sigma_{n+1}^{vp}} \left( 1 + \gamma a^2_{n+1} L_{n+1}^{-1} N_{n+1} : X_n \right) 
\]  

(7.122)

In general, the above definition of the tangent stiffness, Eq.(7.120), is not symmetric which requires some tensor multiplications and inverse calculations. However, it gives a quadratic rate of convergence with the above proposed viscoplastic model.

### 7.4 Implicit Algorithm for Finite Deformation Hypoelasto-Viscoplasticity

There exist two types of nonlinearity in the numerical modeling of finite strain plasticity/viscoplasticity: material nonlinearity (plastic/viscoplastic behavior) and geometrical nonlinearity (finite strain). In small deformation problems, the difference between the reference configuration and the subsequent configuration is assumed negligible at which the nonlinear material behavior is described by a rate-form constitutive relation, relating the rate of stress to the rate of strain and some internal variables. On the other hand, if geometrical nonlinearity is considered (i.e., large deformation problems) the aforementioned assumption is no longer valid and the choice of proper stress and strain rates is crucial in which the rigid body motion (rotation) and the objectivity should be respected and treated carefully in the constitutive formulation. One proper way to achieve a solution for such problem is by employing objective tensor quantities. The principle of material objectivity states that a constitutive relation should be independent of any rigid body motions, i.e., it should be the same for two observers in relative motions (translation and/or rotation).

In fact, the “incremental objectivity”, which is also called “material frame indifference”, is a term used for a certain methodology in which the introduced (objective) stress rate is able to properly capture the rigid body motions (that induce no straining) of a material. The formulations of an incrementally objective algorithm proceed conceptually as follows (Simo and Huges, 1998); the given spatial rate-constitutive equations are mapped to an intermediate (local) configuration, which is unaffected by the superposed spatial rigid body motions. A time-stepping algorithm is then performed in this local configuration and the discrete equations are mapped back to the Eulerian description.” In this regard, two basic
In this second approach, which is referred to as the “local rotated representation” (Simo and Marsden, 1984), the stress update is performed in a locally Cartesian rotating coordinate system, to which the evolution equations are first transformed using an orthogonal tensor, and subsequently the discrete equation is transformed back to the spatial configuration.

It is noticeable that achieving incremental objectivity or equivalently maintaining correct rotational transformation properties all along a finite element step is considered one of the major challenges in integrating a constitutive equation in the finite deformation context. In this study, we will adopt a stress integration methodology that is similar to the above second approach discussed above at which the problem can be reduced to the numerical integration of an initial value problem that generates a one-parameter subgroup of the proper orthogonal transformation. Moreover, for von Mises plasticity, it has been shown (Simo and Hughes, 1998) that the above second approach results in a return mapping essentially identical to the classical radial return algorithm of the infinitesimal theory. The proposed objective stress update algorithm is implemented, within the framework of additive plasticity, in such a way that the extension from the standard small strain finite element code to the finite strain finite element analysis is straightforward. The efficiency of the proposed algorithm relies crucially on the total uncoupling between material non-linearity and geometrical non-linearity.

In this section we outline an incremental integration scheme in which the stress objectivity is preserved for finite rotation increments to rewrite the constitutive relations in a corotational moving frame. We then summarize the radial return algorithm for integrating the material response in a way similar to that explained for the case of small deformation. A derivation of a new definition for the consistent tangent stiffness matrix that is essential to maintain the asymptotic quadratic rate of convergence is also outlined at the end of this section.

### 7.4.1 Incrementally Objective Integration Algorithm

The rate of the constitutive equation should be integrated in order to obtain a framework suitable for the application of a displacement finite element method at finite strain. A corotational formulation procedure in which all the fields of interest are transformed into the corotational system is presented here. In such a corotational system, the form of constitutive equations is treated similarly to that of the small deformation theory and is based on the additive increment of material and rotational responses. This corotational frame can be generated in the following way. Let us consider two arbitrary particles of a body connected by a unit vector \( \bar{G} \) in the undeformed configuration as shown in Fig.7.5.

The particles originally positioned at points A and B move to the position a and b, respectively, with the corresponding unit vector \( \bar{q} \). We define \( \Omega \) as an orthogonal tensor \( \Omega \cdot \Omega^T = I \) which can be used for a rotation of two unit vectors such that:
Taking the rate of the above rotation leads to the following general definition:

\[ \dot{q} = \Omega \cdot Q = W \cdot q \]  
(7.124)

where \( W \) can be any spatial second-order, skew-symmetric \( W = -W^T \), tensor field

\[ W = \dot{\Omega} \cdot \Omega^{-1} \]  
(7.125)

Using the same concept, it is possible now to generate a change of frame from the fixed Cartesian reference axes to the corresponding rotating axes (corotational axes). Thus, a family of the corotational Cushy stress tensor, denoted as \( \hat{\sigma} \), can be transformed by \( \Omega \) as

\[ \hat{\sigma} = \Omega^T \cdot \sigma \cdot \Omega \]  
(7.126)

The rate of \( \hat{\sigma} \) follows from the differentiation of the above equation with respect to time

\[ \dot{\hat{\sigma}} = \dot{\Omega}^T \cdot \sigma \cdot \Omega + \Omega^T \cdot \dot{\sigma} \cdot \Omega + \Omega^T \cdot \sigma \cdot \dot{\Omega} \]  
(7.127)

Substituting Eq.(7.125) into the above equation, the corotational objective stress rate of the Caushy stress \( \sigma^V \), that obey transformation rules for second order tensors, is defined as follows:

\[ \sigma^V = \Omega \cdot \dot{\sigma} \cdot \Omega^T = \dot{\sigma} + W^T \cdot \sigma + \sigma \cdot W \]  
\[ = \dot{\sigma} - W \cdot \sigma + \sigma \cdot W \]  
\[ = \dot{\sigma} - W \cdot \sigma - \sigma \cdot W^T \]  
(7.128)

It is obvious from the above equation, Eq.(7.128), that the Jaumann rate is recovered if the rotation tensor \( W \) coincides with the spin tensor \( \omega \). Such behavior is achieved if the unit vector \( q \) is aligned along one of the principle directions of the rate of the deformation tensor. On the other hand, the Green-Naghdi rate is obtained if \( W = R \cdot R^T \) where \( R \) is the rotation tensor in the polar decomposition of the deformation gradient tensor \( F \).

In similar way to Eq.(7.128), the rate of the backstress tensor can be written as follows:

\[ X^V = \Omega \cdot \dot{X} \cdot \Omega^T = \dot{X} + X \cdot W + W^T \cdot X \]  
(7.129)

For hypoelasto-viscplastic materials the constitutive equation is given by

\[ \sigma^V = E : d^e = E : (d - d^{vp}) \]  
(7.130)
Herein, the rate of deformation $\mathbf{d}$ represents the symmetric part of the spatial velocity gradient. Let $\hat{\mathbf{d}}$ denotes a set of corotational rate of deformation tensors such that:

$$\hat{\mathbf{d}} = \mathbf{\Omega}^T \cdot \mathbf{d} \cdot \mathbf{\Omega} \quad (7.131)$$

Substituting Eq.(7.128) into Eq.(7.130) with pre-multiplying and post-multiplying the result with $\mathbf{\Omega}^T$ and $\mathbf{\Omega}$ and the aid of Eq. (7.131) yields the following expression for the hypoelastic constitutive equation in the corotational local frame:

$$\dot{\mathbf{\sigma}} = \hat{\mathbf{E}} : \hat{\mathbf{d}} = \hat{\mathbf{E}} : (\hat{\mathbf{d}} - \hat{\mathbf{d}}^p) \quad (7.132)$$

where the corotational elastic tensor $\hat{\mathbf{E}}$ is given in the tensorial form as follows:

$$\hat{E}_{ijkl} = \Omega_{im} \Omega_{jn} \Omega_{pk} \Omega_{ql} E_{mapq} \quad (7.133)$$

It is clear from the above definitions of constitutive equations that plasticity in the corotational frame can be formulated with a structure similar to that in the small deformation theory. Moreover, the above constitutive equations are not unique depending on the various choices of rotation tensors which result in different material responses.
Since for isotropic materials the constitutive properties are rotation independent, the tensor \( \hat{\mathbf{E}} \) coincides with the one in the Cartesian frame \( \mathbf{E} \). This property plays a crucial role in numerical implementations of the von Mises flow theory which is adopted in this work. In this regard, the constitutive equation to be integrated in the corotational frame is simply reduced to

\[
\dot{\sigma} = \hat{\mathbf{E}} : (\hat{\mathbf{d}} - \hat{\mathbf{d}}^p)
\]  

(7.134)

As will be shown next, the optimal algorithm framework for hypoelastic formulations of viscoplasticity that employ “rotational” objective rates relies on the use of a corotated coordinate system. Within such a framework, the structure of the radial return method is preserved for the von Mises flow theory.

### 7.4.2 Radial Return Algorithm (Rotated Configuration)

Applying the same procedure described in section 7.3 to the von Mises flow theory formulated in the rotated description leads to a straightforward generalization of the radial return scheme. In this procedure the entire loading process must be divided into a sequence of loading steps at which the time interval \([0, T]\) is segmented into \([0, T] = \bigcup_{n=0}^{m} H_n\) with \(H_n = [t_n, t_{n+1}]\) denotes a time interval. Assuming that the constitutive state at \(t_n\) is given which means that we know the deformation gradient \(F_n\), the stress \(\sigma_n\), as well as all other internal variables at this instant. Further, it is assumed that the deformation gradient \(F_{n+1}\) or equivalently the increment of the displacement field \(\Delta u = x_{n+1} - x_n\) at instant \(t_{n+1}\) is known, the goal of the numerical algorithm is to determine the stress and other internal variables at time \(t_{n+1}\). With the assumption that the components of the elastic moduli in the Cartesian coordinates are constant, one can then exclude the elastic moduli from integration such that the elastic trial stress in the corotational frame is given by:

\[
\hat{\sigma}^*_{n+1} = \hat{\sigma}_n + \hat{\mathbf{E}} : \hat{\mathbf{d}} \Delta t
\]  

(7.135)

Utilizing the rotation relation Eq.(7.126), i.e.

\[
\sigma^*_{n+1} = \Omega_{n+1} \cdot \hat{\sigma}^*_{n+1} \cdot \Omega_{n+1}^T
\]  

(7.136)

\[
\sigma_n = \Omega_n \cdot \hat{\sigma}_n \cdot \Omega_n^T
\]  

(7.137)

with the following identity

\[
\Gamma_{n+1} = \Omega_{n+1} \cdot \Omega_n^T
\]  

(7.138)

One can write the trial stress (elastic predictor) in the Cartesian frame as follows:
\[ \sigma_{n+1}^* = \Gamma_{n+1} \cdot \sigma_n \cdot \Gamma_{n+1}^T + \Omega_{n+1} \cdot \left( E \cdot \dot{\Delta} \right) \cdot \Omega_{n+1}^T \]  
(7.139)

Let us now compute an increment strain tensor \( \dot{\epsilon} = \dot{\Delta} \) from a given deformation gradient tensor \( F_{n+1} \) by first introducing the relative deformation gradient

\[ f_{n+1} = F_{n+1} \cdot F_n^{-1} \]  
(7.140)

Thus, the definition of a relative increment strain tensor is given as follows:

\[ \dot{\epsilon} = \Omega^T \cdot e \cdot \Omega = \frac{1}{2} \Omega^T \left( I - \left( f_{n+1} \cdot f_{n+1}^T \right)^{-1} \right) \cdot \Omega \]  
(7.141)

Substituting Eq.(7.141) into Eq.(7.139), the trial elastic stress reduces to:

\[ \sigma_{n+1}^* = \Gamma_{n+1} \cdot \sigma_n \cdot \Gamma_{n+1}^T + E : e \]  
(7.142)

where

\[ e = \frac{1}{2} \left[ I - \left( f_{n+1} \cdot f_{n+1}^T \right)^{-1} \right] \]  
(7.143)

The above definition for the increment strain tensor is valid for any definition of \( W \) (i.e., \( \Omega \)). However an alternative definition for the increment strain tensor may be defined if we set \( \Omega = R \) which means we are adopting the Green-Naghdi rate. In this case, the strain tensor rate is written using the polar decomposition \( F = R \cdot U \) as follows:

\[ d = \frac{1}{2} R \cdot \left( \dot{U} \cdot U^{-1} + U^{-1} \cdot \dot{U} \right) \cdot R^T \]  
(7.144)

Accordingly, the increment strain tensor \( \dot{\epsilon} = \dot{\Delta} \Delta t \) is given by:

\[ \dot{\epsilon} = \dot{\Delta} \Delta t = \Omega^T \cdot d \Delta t \cdot \Omega = \frac{1}{2} \left( \Delta U \cdot U^{-1} + U^{-1} \cdot \Delta U \right) \]  
(7.145)

We can then express the trial elastic stress, Eqs.(7.135) and (7.136), as follows:

\[ \sigma_{n+1}^* = \Gamma_{n+1} \cdot \sigma_n \cdot \Gamma_{n+1}^T + \frac{1}{2} \Omega_{n+1} \cdot \left[ E : (\Delta U \cdot U^{-1} + U^{-1} \cdot \Delta U) \right] \cdot \Omega_{n+1}^T \]  
(7.146)

Next, we need to solve for \( U^{-1} \). In this regard, we use an assumed relation given first by Simo and Hughes (1998) for \( U \)

\[ U(t) = \exp \left( \frac{t - t_0}{\Delta t} C \right) \]  
(7.147)

and its increment yields
\[ \Delta U(t) = \frac{C}{\Delta t} \exp \left( \frac{t - t_n}{\Delta t} \right) \]  

(7.148)

By substituting Eq.(7.148) into Eq.(7.145), it is found that the tensor \( C \) is equivalent to the increment strain tensor between the reference and the current configurations

\[ C = \hat{d} \Delta t \]  

(7.149)

In the current configuration, \( t = t_{n+1} \), Eq.(7.147) yields

\[ U(t_{n+1}) = U_{n+1} = \exp \left( C_{n+1} \right) \Rightarrow \]
\[ C_{n+1} = \ln U_{n+1} = \frac{1}{2} \ln U_{n+1}^2 = \frac{1}{2} \ln \left( F_{n+1}^T \cdot F_{n+1} \right) \]  

(7.150)

As a result, the trial elastic stress, Eq.(7.146), reduces to

\[ \sigma_{n+1}^* = \Gamma_{n+1} \cdot \sigma_n \cdot \Gamma_{n+1}^T + \frac{1}{2} R_{n+1} \cdot (E : C_{n+1}) \cdot R_{n+1}^T \]  

(7.151)

For the above stress state Eqs.(7.142) or (7.151), the dynamic yield criterion, for the case of the Consistency model, is given by

for bcc metals,

\[ f_{n+1}^{d*} = \sqrt{\frac{3}{2} \left( \tau_{n+1}^* - X_{n+1} \right) \cdot \left( \tau_{n+1}^* - X_{n+1} \right)} - Y_a - R_n - \hat{\tau} \left( 1 - \beta_2 T_n \ln \left( \eta_{\alpha}^p \frac{\Delta \lambda_{\alpha}^p}{\Delta t} \right) \right) \right) \right)^{1/q_1/q_2} \]  

(7.152)

for fcc metals,

\[ f_{n+1}^{d*} = \sqrt{\frac{3}{2} \left( \tau_{n+1}^* - X_{n+1} \right) \cdot \left( \tau_{n+1}^* - X_{n+1} \right)} - Y_a - \tilde{R}_n \left( 1 - \beta_2 T_n \ln \left( \eta_{\alpha}^p \frac{\Delta \lambda_{\alpha}^p}{\Delta t} \right) \right) \right) \right)^{1/q_1/q_2} \]  

(7.153)

where \( \tau_{n+1}^* \) is the deviatoric part of the trial stress and kinematic hardening is defined as follows:

\[ X_{n+1} = \Gamma_{n+1} \cdot \bar{X}_n \cdot \Gamma_{n+1}^T \]  

(7.154)

\[ \bar{X}_n = aX_n \]  

(7.155)
Now, the formulation proceeds similar to that explained for the case of small deformation. If $f_{n+1}^{d*} \leq 0$, yielding does not occur in this step, i.e. the material response is elastic and \( \sigma_{n+1} = \sigma_{n+1}^* \).

In contrast, if $f_{n+1}^{d*} > 0$, the material is yielding and the stress in this state is no longer equal to the one at the trial state, i.e. \( \sigma_{n+1} \neq \sigma_{n+1}^* \). This requires a methodology to return the trial stress to the dynamic yield surface. In a similar way to the small deformation analysis, the backward-Euler algorithm and consequently the radial return algorithm is utilized here in the finite deformation context as a methodology for implicit stress integration.

The stress that lies on the yield surface should obey the following relation

\[
\sigma_{n+1} = \sigma_{n+1}^* - E : d^{vp} \Delta t = \sigma_{n+1}^* - E : N_{n+1} \Delta \lambda^{vp} = \sigma_{n+1}^* - 2\mu N_{n+1} \Delta \lambda^{vp}
\]

which, in the deviatoric space, becomes

\[
\tau_{n+1} = \tau_{n+1}^* - 2\mu \Delta \lambda^{vp} N_{n+1}
\]

The remaining part is to find a proper way of solving for the viscoplastic multiplier \( \Delta \lambda^{vp} \) in order to update the current stress and the other thermodynamic conjugate forces. The radial return mapping algorithm is performed in the same configuration as in the classical radial return algorithm of the infinitesimal theory. In this regard, the computational algorithm proposed in sub-section (7.3.1) for the case of the Consistency model and sub-section (7.3.2) for the case of the Perzyna viscoplastic model, is used in the finite deformation context such that no distinction is made between the rate-of-deformation tensor and the rate of small strain tensor and the trial stress is calculated using one of the above equations (7.142), (7.146), or (7.151). The additional computational cost for extension to a finite strain FE code only includes some geometrical manipulations.

### 7.4.3 Consistent Elasto-Viscoplastic Tangent Modulus for Finite Deformation

In the finite element implementation of a mechanical field problem, the central field equation necessarily to be solved in the spatial discrete equation derived from the weak form of the balance equation of linear momentum. In an implicit displacement field finite element formulation, equilibrium in a time step can be obtained by linearizing the nonlinear equilibrium equation at each iteration using the Newton-Raphson method. By this, one can obtain the definition of the exact or algorithmic tangent moduli. This consistent tangent modulus plays a crucial role in reducing the computation time preserving the asymptotic rate of quadratic convergence.

Since we are concerned with materials (bcc and fcc metals) that show very small elastic deformation \( U^e \approx 1 \) compared with plastic/viscoplastic deformation, the rate-additive-hyperelastic formulation reduces to the hypoelastic-corotational formulation provided that
\( \Omega = \mathbf{R} \) and \( \dot{\mathbf{E}} = \mathbf{E} \) (Beltytschko, 1973; Huges, 1983; Johnson and Bammann, 1982; Fish and Sheck, 2000). However, it should be mentioned here that using hypoplasticity in a rate form does not imply that classical hyperelasticity is recovered for zero plastic flow. Thus, in the corotational configuration, the derivation of the consistent tangent is obtained from the linearization of the incremental equation (7.134) which is rewritten as follows:

\[
\Delta \mathbf{\hat{\sigma}} = \mathbf{\hat{\sigma}}_{n+1} - \mathbf{\hat{\sigma}}_n = \mathbf{E} : (\dot{\mathbf{d}}^c \Delta t) = \mathbf{E} : (\dot{\mathbf{d}} \Delta t - \dot{\mathbf{d}}^{vp} \Delta t)
\]  

(7.158)

In a finitely deforming elasto-viscoplastic solid, it is assumed that the objective relations are governed by the above relation. Thus, differentiating Eq.(7.158) and denoting \( \Delta \mathbf{d} = \dot{\mathbf{d}} \Delta t \) and \( \Delta \dot{\mathbf{d}}^{vp} = \dot{\mathbf{d}}^{vp} \Delta t \) yield

\[
d(\Delta \mathbf{\hat{\sigma}}) = \mathbf{E} : \left( d(\Delta \dot{\mathbf{d}}) - d(\Delta \dot{\mathbf{d}}^{vp}) \right)
\]  

(7.159)

Employing the corotational transformation given in Eq.(7.131), the linearization functions of \( \Delta \dot{\mathbf{d}} \) and \( \Delta \dot{\mathbf{d}}^{vp} \) given in the last two terms in the right hand side of the above equation result in the following:

\[
d(\Delta \dot{\mathbf{d}}) = d \left( \mathbf{R}^T_{n+1} \cdot (\Delta \mathbf{d}) \cdot \mathbf{R}_{n+1} \right) = \mathbf{R}^T_{n+1} \cdot d(\Delta \mathbf{d}) \cdot \mathbf{R}_{n+1} + 2 \left( \mathbf{R}^T_{n+1} \cdot \Delta \mathbf{d} \cdot d \mathbf{R}_{n+1} \right)
\]  

(7.160)

\[
d(\Delta \dot{\mathbf{d}}^{vp}) = d \left( \mathbf{R}^T_{n+1} \cdot (\Delta \mathbf{d}^{vp}) \cdot \mathbf{R}_{n+1} \right) = \mathbf{R}^T_{n+1} \cdot d(\Delta \mathbf{d}^{vp}) \cdot \mathbf{R}_{n+1} + 2 \left( \mathbf{R}^T_{n+1} \cdot \Delta \mathbf{d}^{vp} \cdot d \mathbf{R}_{n+1} \right)
\]  

(7.161)

where the linearization of \( \mathbf{R} \) and \( \Delta \mathbf{d}^{vp} \) consistent with the integration procedure described previously is given in the following subsections for the case of hypoelastoviscoplasticity (see, for more details, the work of Fish and Sheck (2000) for the case of hyperelasoplasticity).

- **Determination of \( d\mathbf{R} \)**

Since the algorithmic stiffness matrix is calculated at the end of load step, \( n+1 \), we are going to first express the linearization of \( \mathbf{R} \) in terms of the spatial velocity gradient \( \mathbf{l} \) at \( n+1 \). Initially, and for a typical time \( t \), the velocity gradient may be written, using the tensorial notation, as follows:

\[
'\mathbf{l}_{ij} = '\mathbf{F}^{-1}_{ik} '\mathbf{F}^{-1}_{kj}
\]  

(7.162)

where

\[
'\mathbf{F}^{-1}_{kj} = '\mathbf{U}^{-1}_{kn} '\mathbf{R}^{-1}_{nj}
\]  

(7.163)

\[
'\mathbf{F}^{-1}_{ik} = '\mathbf{R}_{mk} '\mathbf{U}^{-1}_{nk} + '\mathbf{R}_{mk} '\mathbf{U}_{mk}
\]  

(7.164)

Substituting Eqs.(7.163) and (7.164) into Eq.(7.162) with pre-multiplying and post-multiplying the results by \( \mathbf{R}^{-1} \) and \( \mathbf{F} \) respectively leads to
The relation between $\dot{\mathbf{R}}$ and $\mathbf{I}$ can then be obtained by subtracting the transpose of the above equation (7.165) from itself, keeping in mind that the right stretch tensor $\mathbf{U}$ is a symmetric positive definite tensor. That is

$$
\mathbf{t}_{ij} = \mathbf{t}_{ijkl} \mathbf{R}_{kl} = \mathbf{t}_{ijkl} \mathbf{R}_{kl} - \mathbf{t}_{ijkl} \mathbf{R}_{kl}
$$

where

$$
\mathbf{t}_{ijkl} = \mathbf{t}_{ijkl} \mathbf{R}_{kl} - \mathbf{t}_{ijkl} \mathbf{R}_{kl}
$$

It should be brought to mind that the rate of deformation tensor represents the symmetric part of the velocity gradient tensor

$$
\mathbf{t}_{ijkl} = \frac{1}{2} \left( \mathbf{t}_{ij} + \mathbf{t}_{ji} \right)
$$

Using the above relation, we can then express $\dot{\mathbf{R}}$, Eq.(7.166), in terms of $\mathbf{d}$ as follows:

$$
\dot{\mathbf{R}}_{ij} = \mathbf{t}_{ijkl} \mathbf{d}_{kl}
$$

where

$$
\mathbf{t}_{ijkl} = 2 \left( \mathbf{t}_{ijkl} \mathbf{R}_{kl} - \mathbf{t}_{ijkl} \mathbf{R}_{kl} \right)
$$

Eqs.(7.166) and (7.171) may be rewritten in matrix forms as follows:

$$
d\mathbf{R}_{n+1} = \dot{\mathbf{R}}_{n+1} \mathbf{I}_{n+1} = \mathbf{T}_{n+1} \mathbf{d}_{n+1}
$$

$$
d\mathbf{R}_{n+1} = \dot{\mathbf{T}}_{n+1} \mathbf{d}_{n+1} = \mathbf{T}_{n+1} \mathbf{d}_{n+1}
$$

Considering the following identity,

$$
d(\Delta \mathbf{d}) = \Delta (d \mathbf{d}) = d d_{n+1} + d \mathbf{d}_{n+1} - d \mathbf{d}_{n+1} - d \mathbf{d}_{n+1} dt - d_{n+1} dt
$$

and multiplying both sides of Eq.(7.175) by $d \mathbf{d}_{n+1}^{-1}$, one can then obtain the following useful relation

$$
d(\Delta \mathbf{d}) = \mathbf{K}_{n+1} : d \mathbf{d}_{n+1}
$$

where

$$
\mathbf{K}_{n+1} : d \mathbf{d}_{n+1}
$$
\[ N_{n+1} = I - \frac{dd_n}{dd_{n+1}} = I - dd_n : dd_{n+1} \]  

(7.177)

Note that since the problem is driven by a given strain increment \( \Delta d \), both \( d_n \) and \( d_{n+1} \) are known and, accordingly, \( N_{n+1} \) can easily be obtained from Eq.(7.177). Hence, substituting Eq.(7.176) into Eq.(7.174) yields

\[ dR_{n+1} = Q_{n+1} : d(\Delta d) \]  

(7.178)

where

\[ Q_{n+1} = \bar{\nabla}_{n+1} : N_{n+1}^{-1} \]  

(7.179)

- **Determination of \( d(\Delta d^{vp}) \)**

It should be emphasized here that \( \Delta d^{vp} \), defined in Eq.(7.156), is determined in a similar way to the infinitesimal procedure presented previously by adopting the following associative flow rule

\[ \Delta d^{vp} = \Delta \lambda^{vp} N_{n+1} \]  

(7.180)

and, accordingly, the accumulated plastic strain increment is defined as follows:

\[ \Delta p = \Delta \lambda^{vp} = \sqrt{\frac{2}{3} \Delta d^{vp} : \Delta d^{vp}} \]  

(7.181)

Hence, differentiation of Eq.(7.180) gives,

\[ d\Delta d^{vp} = d\Delta \lambda^{vp} N_{n+1} + \Delta \lambda^{vp} dN_{n+1} \]  

(7.182)

where \( d\Delta \lambda^{vp} \) and \( dN_{n+1} \) are obtained using the same procedure explained in sub-section (7.3.3) for the infinitesimal theory. Thus, Eq.(7.182) is expressed in terms of \( \Delta d \) as follows:

\[ d\Delta d^{vp} = \mathbf{Z}_{n+1} : d\Delta d \]  

(7.183)

where

\[ \mathbf{Z}_{n+1} = 2\mu(\Pi_{n+1} + Z_{n+1} (N_{n+1} \otimes N_{n+1})) \]  

(7.184)

Note that the fourth-order tensor \( \Pi \), and the scalar \( Z \) are given in Eqs.(7.121) and (7.122) respectively.
Having defined \( dR \) and \( d(\Delta d^\nu) \) consistently, we may now proceed with the linearization of \( \Delta \dot{d} \) and \( \Delta \dot{d}^\nu \) by substituting Eqs.(7.178) and (7.183) into Eqs.(7.160) and (7.161) such that:

\[
d(\Delta \dot{d}) = \left[ (R^T_{n+1} \otimes R_{n+1}) + 2 \left( R^T_{n+1} \cdot \Delta d \cdot Q_{n+1} \right) \right] : d(\Delta d)
\]  
(7.185)

\[
d(\Delta \dot{d}^\nu) = \left[ \left( R^T_{n+1} \otimes R_{n+1} \right) \cdot Z_{n+1} + 2 \left( R^T_{n+1} \cdot \Delta d \cdot Q_{n+1} \right) \right] : d(\Delta d)
\]  
(7.186)

Hence, the linearization of \( (\Delta \sigma) \) is obtained by substituting Eqs.(7.185) and (7.186) into Eq.(7.159)

\[
d(\Delta \sigma) = \hat{D}^{alg}_{n+1} : d(\Delta d)
\]  
(7.187)

where

\[
\hat{D}^{alg}_{n+1} = E \left[ \left( R^T_{n+1} \otimes R_{n+1} \right) : \left( I - Z_{n+1} \right) + 2 \left( R^T_{n+1} \cdot \left( \Delta \lambda^\nu N_{n+1} \right) \cdot Q_{n+1} \right) \right]
\]  
(7.188)

Furthermore, knowing that \( d(\Delta \sigma) = \Delta (d \sigma) \), Eq.(7.187) may be equivalently written as follows:

\[
d \sigma_{n+1} = d \sigma_n + \hat{D}^{alg}_{n+1} : d(\Delta d)
\]  
(7.189)

Recalling that \( \Omega = R \), Eqs.(7.126) and (7.128) can incrementally be written as follows:

\[
\hat{\sigma}_{n+1} = R^T_{n+1} \cdot \sigma_{n+1} \cdot R_{n+1}
\]  
(7.190)

\[
d \sigma^v_{n+1} = \sigma^v_{n+1} \cdot dt = R^T_{n+1} \cdot d \hat{\sigma}_{n+1} \cdot R_{n+1}
\]  
(7.191)

By substituting Eq.(7.189) into Eq.(7.191), with the aid of Eq.(7.176), the following linearization function is derived:

\[
d \sigma^v_{n+1} = D^{alg}_{n+1} : d_{n+1}
\]  
(7.192)

or

\[
\sigma^v_{n+1} = D^{alg}_{n+1} \cdot d_{n+1}
\]  
(7.193)

where \( D^{alg} \) is the consistent stiffness tangent operator defined as follows:

\[
D^{alg} = \Gamma^v_{n+1} \cdot \frac{\sigma^v_{n+1}}{d_{n+1}} \cdot \Gamma^T_{n+1} + R_{n+1} \cdot \left( \hat{D}^{alg}_{n+1} \cdot \lambda^v_{n+1} \right) \cdot R^T_{n+1}
\]  
(7.194)
In view of \( W = \dot{R} \cdot R^T \) and \( W^T = R \cdot \dot{R}^T \), and following the first relation on the right hand side of Eq.(7.128), the objective stress rate \( \dot{\sigma}^V = d \sigma^V / dt \) can be defined at \( t = t_{n+1} \) as follows:

\[
d \sigma^V_{n+1} = d \sigma^V_n + R^T_{n+1} \cdot dR^T_{n+1} \cdot \sigma^V_{n+1} + \sigma^V_{n+1} \cdot dR_{n+1} \cdot R^T_{n+1}
\]  

(7.196)

Combining Eqs.(7.192) and Eq.(7.196) and making use of Eq.(7.174) for the definition of \( dR \), we can further relate the stress rate \( \dot{\sigma} \) to the rate of deformation \( \dot{d} \) as follows:

\[
d \sigma^V_{n+1} = \bar{D}^{alg}_{n+1} \cdot \dd d_{n+1}
\]  

(7.197)

where \( \bar{D}^{alg}_{n+1} \) is defined in matrix and tensorial forms as follows:

\[
\bar{D}^{alg}_{n+1} = D^{alg}_{n+1} - R^T_{n+1} \cdot \bar{\sigma}^V_{n+1} - \sigma^V_{n+1} \cdot \bar{R}^T_{n+1} 
\]  

(7.198)

\[
\bar{D}^{alg}_{ijkl} = D^{alg}_{pqkl} - R^T_{pqkl} \sigma_{ij} - \sigma_{iq} \bar{T}_{pqkl} R_{jq}
\]  

(7.199)

As the case in the infinitesimal theory, the algorithmic tangent stiffness defined in Eq.(7.199) is not symmetric and the formulation process needs many tensor multiplications and inverse calculations.

### 7.5 Numerical Examples

Several numerical examples are presented in this chapter in order to validate and test the proposed computational framework and numerical algorithm using both the Consistency model and the Perzyna viscoplastic model for different types of bcc and fcc metals. All numerical simulations are performed by using the Newton-Raphson iteration procedure with a fully backward Euler integration scheme. Finite element simulations are performed by implementing the proposed viscoplasticity constitutive models in the commercial finite element program ABAQUS/Explicit (2003) via a user’s material subroutine coded as VUMAT. ABAQUS/Explicit uses explicit integration algorithms and it is mainly used for high transient dynamic problems (see the reference manual of ABAQUS (2003) for further details). In the first example of this section, a uniaxial tension problem loaded with different displacement velocities and meshed with a different number of elements is considered here in order to validate the material parameters obtained previously from one-dimensional tests for Niobium, Tantalum, Vanadium and OFHC copper. The second example considers the problem of a necking in circular bar for different meshes. In the final example, the role of viscoplastic regularization in setting the character of the governing differential equations and in introducing a length scale is addressed by considering shear band development in a simple tensile plane...
strain strip subjected to low and high impact loading. In all of these examples, the effect of kinematic hardening is neglected by setting the parameters $\gamma$ and $C$ to zero. Mesh sensitivity is also investigated and illustrated for all of the aforementioned problems. Finally, the effect of strain rate and temperature on the necking and shear band development are investigated.

### 7.5.1 Verification of the Material Parameters

This example is conducted in order to demonstrate the capability of the finite element formulation to capture the effect of strain rates (displacement velocity) and temperatures on the stress-strain curves as compared with the experimental results for different bcc and fcc metals (Vanadium, Tantalum, Niobium, and OFHC Copper). In this regard, a simple uniaxial tension problem subjected to low and high displacement velocities is considered as shown in Fig. 7.6(a). Due to symmetry, only a quarter of the problem is considered and solved with a mesh of one axisymmetric element (CAX4R ABAQUS type) with the boundary conditions defined in Fig. 7.6(b). The loading history that allows for driving the test under a certain constant strain rate is defined in Fig. 7.6(c).

![Figure 7.6](image_url)

Figure 7.6 Problem description of simple uniaxial tension. (a) A specimen subjected to symmetric velocity loading. (b) A quarter of the specimen with specific boundary conditions to ensure the problem symmetry. (c) The time history for the applied velocity.
Results from the implementation of the proposed multiscale viscoplastic models are obtained for Vanadium, Tantalum, and Niobium as bcc metals and for OFHC Copper as an fcc metal for several velocities (strain rates) and initial temperatures. The material parameters are listed for the three bcc metals (V, Ta, and Nb) in Table 7.1 and for the fcc metal (OFHC Cu) in Table 7.2.

- **Vanadium (V)**

The effect of the initial temperature on the stress strain curves is studied for the case of vanadium as a bcc metal for a velocity of 25m/s that is equivalent, for the present problem dimensions, to a strain rate of 2500s⁻¹. This velocity is kept constant during a time step of 250µs (t_f =0.00025sec) in order to achieve about 50% true straining of the sample in the axial direction. The results show that the effect of the temperature is mainly captured by the yield stresses whereas the hardening stresses are almost independent of temperature as shown in Figs.7.7. These results compares very well with the experimental data given previously in chapter 2 and 5. Good comparisons also indicate that the proposed models are correctly implemented in the ABAQUS Code.

<table>
<thead>
<tr>
<th>Model Parameters</th>
<th>Nb</th>
<th>V</th>
<th>Ta</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Y_o$ (MPa)</td>
<td>60</td>
<td>60</td>
<td>50</td>
</tr>
<tr>
<td>$\bar{B}$ (MPa)</td>
<td>415</td>
<td>275</td>
<td>290</td>
</tr>
<tr>
<td>$B$ (MPa)</td>
<td>450</td>
<td>305</td>
<td>330</td>
</tr>
<tr>
<td>$m$</td>
<td>0.25</td>
<td>0.16</td>
<td>0.41</td>
</tr>
<tr>
<td>$k$</td>
<td>3.7</td>
<td>9.9</td>
<td>2.5</td>
</tr>
<tr>
<td>$\hat{Y}$ (Mpa)</td>
<td>1350</td>
<td>945</td>
<td>1125</td>
</tr>
<tr>
<td>$\eta_o^p$ (s)</td>
<td>$1.414 \times 10^{-7}$</td>
<td>$1.582 \times 10^{-7}$</td>
<td>$2.247 \times 10^{-7}$</td>
</tr>
<tr>
<td>$\beta_2$ (K⁻¹)</td>
<td>0.000149</td>
<td>0.0001392</td>
<td>0.0000937</td>
</tr>
<tr>
<td>$q$</td>
<td>3/2</td>
<td>3/2</td>
<td>3/2</td>
</tr>
<tr>
<td>$p$</td>
<td>1/2</td>
<td>1/2</td>
<td>1/2</td>
</tr>
<tr>
<td>$\rho$ (g/cm³)</td>
<td>8.57</td>
<td>6.16</td>
<td>16.62</td>
</tr>
<tr>
<td>$c_p$ (J/g.K⁰)</td>
<td>0.265</td>
<td>0.498</td>
<td>0.139</td>
</tr>
<tr>
<td>E (Mpa)</td>
<td>105</td>
<td>125</td>
<td>170</td>
</tr>
<tr>
<td>$\nu$</td>
<td>0.39</td>
<td>0.37</td>
<td>0.34</td>
</tr>
</tbody>
</table>
Figure 7.7 Stress and Strain evolution with time for Vanadium at 2500s\(^{-1}\) strain rate (V=25m/s). (a) Effect of the initial temperature (T\(\text{o}\)) on the true stress. (b) Axial true strain and equivalent plastic strain accumulated with a total time step of 250\(\mu\)s.

It is concluded from the above results (Figs. 7.7) and other results that is not reported here that the stress decreases as the temperature increases until it reaches a value where no further stress degradation is allowed indicating the initiation of the material athermal condition at a specific strain rate. This athermal temperature value is called the critical temperature, T\(_{cr}\), and it varies with the strain rates. This subject, however, was discussed in detail in chapters 2-5 for different metals.

Furthermore, the role of strain rates on the stress-strain curves is very significant particularly in metals. The yield stress strongly depends, for the case of Vanadium as a bcc metal, on the rate of loading whereas the hardening stress is almost independent of such effect. Figures 7.8(a) and 7.8(b) show the adiabatic stress-strain curves for several strain rate values (8000s\(^{-1}\)-10\(^{-5}\)s\(^{-1}\)) at initial temperatures of 296K\(^{\circ}\) and 500K\(^{\circ}\) respectively. It is obvious from these results that the static (rate-independent) condition is encountered at loading rates of 10\(^{-04}\)s\(^{-1}\) and 1s\(^{-1}\) for initial temperatures of 296K\(^{\circ}\) and 500K\(^{\circ}\) respectively. This, in fact, supports the argument discussed in the previous chapter which says that the static rate cannot be constant and erroneously set to a value of 10\(^{-05}\)s\(^{-1}\) by many authors. The static strain-rate, in fact, increases as the initial testing temperature increases. It also differs from a material to another as will be shown for the following bcc and fcc metals.
Figure 7.8 Adiabatic stress-strain curves for different strain rate of loadings for Vanadium at initial temperatures of (a) 296K [rate-independent behavior is encountered at 0.0001s\(^{-1}\) strain rate] (b) 500K [rate-independent behavior is encountered at 1s\(^{-1}\) strain rate].

Niobium (Nb)

Niobium is another bcc metal used here to test the proposed finite element formulation and its implementation in ABAQUS. A velocity of 33m/s (equivalent to 3300s\(^{-1}\) strain rate) is applied to the same problem dimension given in Fig.7.6(b) over a time step of 150\(\mu\)s to maintain around 40% of true strain in the axial direction. The effect of the initial testing temperature and the strain rate on the adiabatic stress-strain curves is similar to those shown for Vanadium at which the yield stress increases as the strain rate increases, and decreases as the temperature increases. Such effects, however, are almost negligible for the hardening stress. The true stress-strain results for the case of Niobium are illustrated in Figs.7.9 and 7.10 for a wide range of temperatures (77K-600K) and strain rates (0.0001s\(^{-1}\)-8000 s\(^{-1}\)).

In general, the numerical results for the adiabatic stress-strain curves presented here from the finite element analysis compare very well with the experimental results presented previously in chapters 2-5 for the selected temperatures and strain rates. As clearly shown in Figs.7.10(a) for initial temperature of 296K, the static (rate-independent) condition for Niobium is achieved at a strain rate of 10\(^{-2}\)s\(^{-1}\) which is slightly higher than that obtained for Vanadium. At 500K initial temperature, however, the static strain rate value is similar to that obtained for Vanadium which is 1s\(^{-1}\) as shown in Fig.7.10(b). Moreover, Niobium show higher stresses than Vanadium at low temperatures (<300K) while both metals give, nearly, similar results at high temperatures (>300K) for the indicated strain rates.
Figure 7.9 Stress and Strain evolution with time for Niobium at 3300s\(^{-1}\) strain rate (V=33m/s). (a) Effect of the initial temperature (T\(_o\)) on the true stress. (b) Axial true strain and equivalent plastic strain accumulated with a total time step of 150\(\mu\)s.

Figure 7.10 Adiabatic stress-strain curves for different strain rate of loadings for Niobium at initial temperatures of (a) 296K\(^o\) [rate-independent behavior is encountered at 0.01s\(^{-1}\) strain rate] (b) 500K\(^o\) [rate-independent behavior is encountered at 1s\(^{-1}\) strain rate].
• Tantalum (Ta)

In the case of tantalum as another bcc metal, a constant strain rate of 5000s\(^{-1}\) is maintained during the deformation process at different initial temperatures by applying a velocity of 50m/s in the axial direction of the one-element problem given in Fig.7.6(b). The velocity is applied over a total time step of 150\(\mu\)s in order to achieve over a 55% true strain. As the case for most bcc metals, the adiabatic stress-strain results illustrated in Fig.7.11(a) clearly show that the yield stress decreases with the increase of temperature at the aforementioned strain rate whereas the hardening stress is kept independent of temperature. Similar to the previous two bcc metals, the effect of strain rate on the adiabatic stress-strain results is also studied for two initial temperatures, 296K\(^0\) and 500K\(^0\), by applying different velocities (80m/s-10\(^{-7}\)m/s) as shown in Figs.7.12. The time steps used in the finite element analysis changes with the applied velocities in order to achieve around 50% true strain. The results clearly indicate that the static (rate-independent) condition is achieved at strain rates lower than those obtained for Vanadium and Niobium. Those static strain rates are found to be around 0.01s\(^{-1}\) for the case of 500K\(^0\) initial temperature and less than 10\(^{-5}\)s\(^{-1}\) at the room temperature which support the fact that using a constant value as a reference (static) strain rate in constitutive modeling is not an accurate assumption. Finally, the adiabatic stress-strain curves are in good agreement with the experimental results presented in chapters 2-5. This provides another indication for the successful finite element implementation of the proposed constitutive viscoplastic models in the ABAQUS finite element code.

Figure 7.11 Stress and Strain evolution with time for Tantalum at 5000s\(^{-1}\) strain rate (V=50m/s). (a) Effect of the initial temperature (T\(_i\)) on the true stress. (b) Axial true strain and equivalent plastic strain accumulated with a total time step of 150\(\mu\)s.
Finally, it is shown for all of the above bcc metals that the elastic strain is very small compared to the plastic/viscoplastic strain which implies no differences between the total and plastic/viscoplastic strains as clearly shown in Figs.7.7(b), 7.9(b), and 7.11(b) for V, Nb, and Ta respectively.

- **OFHC Copper**

The OFHC Copper is used here to test the finite element implementation of the proposed multiscale viscoplastic model for the case of fcc metals. Unlike bcc metals, the temperature and strain rate effects for OFHC Copper are totally controlled by the hardening stresses. The initial yield stress, on the other hand, is very small and is not affected by temperature and strain rate. This small constant yield stress value results in a very small elastic region as compared to the large plastic/viscoplastic strain region. A velocity of 40m/s, which is equivalent to a strain rate of 4000s\(^{-1}\) for the proposed problem dimensions given in Fig.7.6(b), is axially applied to the one-element (10mm×10mm) specimen to study the effect of initial temperatures on the adiabatic stress-strain curves. A total time step of 300\(\mu\)s \((t_f=0.00030\text{sec})\) is used to achieve an 80% axial true strain.

![Figure 7.12 Adiabatic stress-strain curves for different strain rate of loadings for Tantalum at initial temperatures of (a) 296K [rate-independent behavior is not encountered at 10\(^{-5}\)s\(^{-1}\) strain rate] (b) 500K [rate-independent behavior is encountered at 0.01s\(^{-1}\) strain rate].](image)

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Table 7.2 Material Parameters for OFHC Copper.

<table>
<thead>
<tr>
<th>Model Parameters</th>
<th>OFHC Cu</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Y_0$ (MPa)</td>
<td>60</td>
</tr>
<tr>
<td>$\hat{\beta}$ (MPa)</td>
<td>1175</td>
</tr>
<tr>
<td>$\hat{B}$ (MPa)</td>
<td>990</td>
</tr>
<tr>
<td>$k$</td>
<td>0.9</td>
</tr>
<tr>
<td>$m$</td>
<td>0.5</td>
</tr>
<tr>
<td>$C_f$</td>
<td>40</td>
</tr>
<tr>
<td>$\beta_2$ (K$^{-1}$)</td>
<td>0.0000351</td>
</tr>
<tr>
<td>$\eta_0^{\omega}$ (s)</td>
<td>$1.435 \times 10^{-7}$</td>
</tr>
<tr>
<td>$q$</td>
<td>3/2</td>
</tr>
<tr>
<td>$p$</td>
<td>1/2</td>
</tr>
<tr>
<td>$\rho$ (g/cm$^3$)</td>
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</tr>
<tr>
<td>$c_p$ (J/g.K$^o$)</td>
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</tr>
<tr>
<td>$E$ (Mpa)</td>
<td>115</td>
</tr>
<tr>
<td>$\nu$</td>
<td>0.34</td>
</tr>
</tbody>
</table>

Figure 7.13 Stress and Strain evolution with time for OFHC Copper at 4000s$^{-1}$ strain rate ($V=40$m/s). (a) Effect of the initial temperature ($T_o$) on the true stress. (b) Axial true strain and equivalent plastic strain accumulated with a total time step of 300$\mu$s.
Fig. 7.13(a) shows the stress evolution, for the specified velocity and time step, over a wide range of temperatures (77K-996K) at which the hardening stresses decrease with the increase of the temperature during the adiabatic deformation process. The total and the plastic/viscoplastic strain is almost identical for the case of OFHC Copper due to the very small elastic strain that is not affected by both temperature and strain rates as shown in Fig. 7.13(b).

The significant role of strain rates on the stress-strain curves is also studied for the case of OFHC Copper by applying different velocities (i.e., different strain rates) with their different corresponding time steps to approach a 60% true straining of the specimen. In this regard, a range of velocities between 80m/s and 10^9m/s with a corresponding range of time steps between 300 µs and 10^6s is utilized to show the adiabatic stress-strain curves at low and high strain rates for two different initial temperatures; 296K and 996K. The resulting adiabatic stress-strain curves are illustrated in Fig. 7.14 which shows that the hardening stresses increase with the increase of the strain rates over almost 60% true accumulated plastic strain.

The rate-independent (static) behavior of OFHC Copper is achieved when the hardening stresses are totally diminished, i.e., perfect plasticity behavior is encountered. This behavior is investigated here by studying the effect of high and low strain rates on the adiabatic stress-strain curves at a very high temperature of 996K. In this high temperature condition, the static (rate-independent or perfect plasticity) behavior is encountered at a strain rate of 10^-5s^-1 as illustrated in Fig. 7.14(b). On the other hand, the viscoplastic deformation behavior at a room temperature (296K) persists even at strain rates below 10^-7s^-1 as clearly shown in Fig. 7.14(a) at which the hardening stresses keep decreasing as the strain rates decrease.

Figure 7.14 Adiabatic stress-strain curves for different strain rate of loadings for OFHC Copper at initial temperatures of (a) 296K [rate-independent behavior is not encountered even at 10^-7 s^-1 strain rate] (b) 996K [rate-independent behavior is encountered at 10^-5 s^-1 strain rate].
In general, the stress-strain results for different temperatures and strain rates compare very well the experimental results given in the previous chapters. This, in fact, provides a good indication of the accuracy and success of the aforementioned viscoplastic model formulation and finite element implementation for the case of fcc metals. The FE implementation is further tested by using 9-element and 100-element meshing configurations for the same specimen dimensions for all of the presented metals. The results are discussed in the following subsection.

- **Mesh Sensitivity**

The finite element implementation of the proposed constitutive models in the ABAQUS code is further investigated by using two other mesh configurations. The (10mm×10mm) specimen is meshed with two different numbers of elements; 9 elements and 100 elements as shown in Fig.7.15 in order to obtain the adiabatic stress-strain relationship at different initial temperatures and velocities (strain rates) for Vanadium, Niobium, and OFHC Copper. The adiabatic stress-strain results obtained from the three different mesh configurations (1-, 9-, and 100-element) at 296K° initial temperature show nearly identical results for Vanadium, Niobium and OFHC Copper at strain rates of 2500s⁻¹ (V=25m/s), 3300s⁻¹ (V=33m/s), and 4000s⁻¹ (V=40m/s) respectively as illustrated in Fig.7.16. Moreover, contour plots of the Mises stresses and the equivalent plastic strain for the aforementioned three metals are also illustrated in Figs.7.17-7.22 at different time increments. These contour results show little differences between the three different mesh configurations and also within the same mesh configuration at the early stages of deformation for both the stresses and the equivalent plastic strains. These variations, however, are within the margins of finite element analysis errors for the elasto-viscoplastic deformations at high strain rates and temperatures.

![Figure 7.15](image_url)

Figure 7.15 Two different mesh configurations for a simple tension plane strain problem with specified boundary conditions. (a) Problem meshed with 9 quadratic (CPE4R) elements. (b) Problem meshed with 100 quadratic (CPE4R) elements.
Figure 7.16 Comparisons of the adiabatic stress-strain results with 1-element, 9-element, and 100-element mesh configurations for Vanadium, Niobium, and OFHC Copper deformed at 2500s\(^{-1}\), 3300s\(^{-1}\), and 4000s\(^{-1}\) strain rates respectively with 296K\(^{\circ}\) initial temperature.

7.5.2 Necking Problem

A necking problem of a rod or a circular bar has been considered by many authors as a study to test the theoretical formulations and computational algorithms of elasto-plastic/viscoplastic constitutive models for ductile materials. In this work, a circular bar subjected to different uniaxial displacement velocities is considered to test the effectiveness of the proposed computational algorithms for both bcc metals (Niobium, Vanadium, and Tantalum) and fcc metals (OFHC Copper). The finite element program ABAQUS is used to simulate the tensile test. One fourth of the sample is modeled and meshed with three different meshes (Mesh1: 7×15, Mesh2: 10×25, Mesh3: 10×50 elements), as shown in Figs.7.23(a) and 7.23 (c), using the four-node axisymmetric element with reduced integration (CAX4R ABAQUS type).

The aforementioned three mesh configurations are considered in order to study the mesh sensitivity for the necking problem and also to assess the objectivity of the proposed thermo-viscoplastic approach used in this work. Necking is induced at the central part of the bar by introducing a geometric imperfection of 1% radius reduction as shown in Figure7.23(a). Different axial tensile displacement velocities are applied to the above circular bar, with the time history shown in Figure7.23(b), at different initial temperatures for the above-mentioned metals using the same material properties listed in Tables7.1 and 7.2.
Figure 7.17 Contour plots of the Mises stresses in Pascal for the 1-element, 9-element, and 100-element mesh configurations for Vanadium at a velocity of 25m/s (2500/s strain rate) with a 250µs total time step. (a) Stress contours at the beginning of the considered time step, 25µs. (b) Stress contours at the middle of the considered time step, 125µs. (c) Stress contours at the end of the considered time step, 250µs.
Figure 7.18 Contour plots of the Mises stresses in Pascal for the 1-element, 9-element, and 100-element mesh configurations for Niobium at a velocity of 33 m/s (3300/s strain rate) with a 150 µs total time step. (a) Stress contours at the beginning of the considered time step, 15 µs. (b) Stress contours at the middle of the considered time step, 75 µs. (c) Stress contours at the end of the considered time step, 150 µs.
Figure 7.19 Contour plots of the Mises stresses in Pascal for the 1-element, 9-element, and 100-element mesh configurations for OFHC Copper at a velocity of 40m/s (4000/s strain rate) with a 300µs total time step. (a) Stress contours at the beginning of the considered time step, 30µs. (b) Stress contours at the middle of the considered time step, 150µs. (c) Stress contours at the end of the considered time step, 300µs.
Figure 7.20 Contour plots of the equivalent plastic strain for the 1-element, 9-element, and 100-element mesh configurations for Vanadium at a velocity of 25m/s (2500/s strain rate) with a 250µs total time step. (a) Plastic strain contours at the beginning of the considered time step, 25µs. (b) Plastic strain contours at the middle of the considered time step, 125µs. (c) Plastic strain contours at the end of the considered time step, 250µs.
Figure 7.21 Contour plots of the equivalent plastic strain for the 1-element, 9-element, and 100-element mesh configurations for Niobium at a velocity of 33m/s (3300/s strain rate) with a 150µs total time step. (a) Plastic strain contours at the beginning of the considered time step, 15µs. (b) Plastic strain contours at the middle of the considered time step, 75µs. (c) Plastic strain contours at the end of the considered time step, 150µs.
Figure 7.22 Contour plots of the equivalent plastic strain for the 1-element, 9-element, and 100-element mesh configurations for OFHC Copper at velocity of 40m/s (4000/s strain rate) with a 300μs total time step. (a) Plastic strain contours at the beginning of the considered time step, 30μs. (b) Plastic strain contours at the middle of the considered time step, 150μs. (c) Plastic strain contours at the end of the considered time step, 300μs.
Figure 7.23 Problem description of necking of a circular bar. (a) A specimen subjected to symmetric velocity loading. (b) The time history for the applied velocity. (c) Five different meshes of a quarter of the sample with Mesh1:7×15, Mesh2:10×25, and Mesh3:10×50 elements.

- **Niobium (Nb)**

For the case of Niobium, an axial tensile velocity of 30m/s (equivalent to 1000s$^{-1}$ strain rate) is applied over a total time step of 135µs (equivalent to an elongation of 4.05mm=30m/s×135µs) at an initial temperature of 77K° for the three considered meshes. The corresponding initial and final deformed shapes for these meshes, at 100µs (i.e., 3mm elongation), are shown in Figure 7.24. The displacement patterns of the deformed shapes show almost the same radius reduction in all of the three meshes. The history of these patterns for the 500 elements mesh (Mesh3) at 0.06, 0.09, 0.12, and 135µs (1.8, 2.7, 3.6, and 4.05mm elongations) is illustrated in Figure 7.25(a). A three dimensional shape corresponding to half of the bar at the end of the 135µs time step is also shown in Figure 7.25(b).
Figure 7.24 Deformed (solid lines) and undeformed (dashed lines) patterns for Niobium at a strain rate of 1000s\(^{-1}\) (V=30m/s) and an initial temperature, \(T_o\), of 77K\(^o\) for the three considered meshes. Results at time step of 100\(\mu\)s (3mm elongation).

Figure 7.25 Displacement patterns for Niobium at a strain rate of 1000s\(^{-1}\) (V=30m/s) and an initial temperature of 77K\(^o\). (a) Deformation history for the 10\(\times\)50 elements (Mesh3) corresponding to total elongations of 1.8, 2.7, 3.6, and 4.05mm. (b) A three dimensional shape corresponding to half of the circular bar at a total elongation of 4.05mm.
In addition to the displacement patterns, the contours of the Cauchy stress component $\sigma_{zz}$ as well as the accumulated plastic strain show almost the same distributions over the whole area of the bar for the three considered meshes as shown in Figure 7.26(a) and Figure 7.27(a) (at 100$\mu$s, i.e., 3mm elongation). Moreover, the axial stress versus displacement curves for the three meshes show identical results over a 4mm total elongation as shown in Figure 7.26(b).

It is shown from the aforementioned results that objectivity is achieved for different meshes. This is due to the incorporation of an explicit length scale parameter in the governing equations through the viscosity definition used in the rate-dependent formulations of bcc metals constitutive relations. However, mesh dependence reappears when the accumulated plastic strains in the necking zone approaches high values as shown in Figure 7.27(b). The accumulations of the plastic strain for the three meshes are almost identical up to 70% straining. After that, the results obtained from Mesh1 ($7\times15$ elements) starts deviating from the other two meshes (Mesh2 and Mesh3). At this stage, the displacement patterns are controlled by the deformation of the last row of elements in the necking zone. This problem, however, requires further considerations in the finite element formulations and it is of the author’s interest. We should also mention here that the evolution rate of the accumulated plastic strain deviates from and exceeds the applied strain rate as soon as necking starts. This accumulated plastic strain rate increases rapidly as necking evolves as shown in Figure 7.27(b) for the curves between the accumulated plastic strain and the time.

- **Vanadium (V)**

The same applied displacement velocity and initial temperature used in the case of Niobium ($V=30m/s$, $T_o=77K^o$) are considered here for the study of the necking of a circular Vanadium bar over a total time step of 165$\mu$s which is equivalent to 5mm total elongation. The same three meshes (Mesh1: $7\times15$, Mesh2: $10\times25$, and Mesh3: $10\times50$ elements) shown in Figure 7.23 are considered. The initial and final deformed shapes for these meshes are shown in Figure 7.28 at 124$\mu$s which is equivalent to a total elongation of 3.7mm. It is obvious from the deformation patterns illustrated in Figure 7.28 that the reduction in the radius is almost the same for the three considered meshes. In Figure 7.29(a), the history of the displacement patterns for the case of Mesh3 ($10\times50$ elements) at 0.06, 0.1, 0.14, and 165$\mu$s (1.8, 3.0, 4.2, and 5.0mm total elongations) is illustrated. Moreover, a three dimensional shape corresponding to half of the bar at the end of the considered time step (165$\mu$s) is also shown in Figure 7.29(b).

Figure 7.30(a) shows the contours of the Cauchy stress component $\sigma_{zz}$ for the three considered meshes at a time step of 124$\mu$s, i.e., 3.7mm elongation. The results display the same axial stress distribution over the whole area of the bar for the three considered meshes. The variations of the axial stress over a total elongation of 5.0mm show almost identical results for the three considered meshes as shown in Figure 7.30(b). However, little deviations of the axial stresses between the three meshes are encountered at the softening region.
Figure 7.26 Necking of a circular bar for Niobium at a strain rate of 1000s\(^{-1}\) (V=30m/s) and an initial temperature of 77K\(^\circ\). (a) Contours of the Cauchy stress component in the axial direction \(\sigma_{zz}\) (Pascal) of the three considered meshes at 100\(\mu\)s (3mm elongation). (b) Axial stress versus axial displacement (elongation) curves over a total time step of 135\(\mu\)s (4.05mm total elongation) for the three considered meshes.
Figure 7.27 Necking of a circular bar for Niobium at a strain rate of 1000s$^{-1}$ ($V=30m/s$) and an initial temperature of 77K. (a) Contours of the equivalent plastic strain of the three considered meshes at 100µs (3mm elongation). (b) Equivalent plastic strain versus time curves over a total time step of 135µs (4.05mm total elongation) for the three considered meshes.
Figure 7.28 Deformed (solid lines) and undeformed (dashed lines) patterns for Vanadium at a strain rate of 1000s\(^{-1}\) (V=30m/s) and an initial temperature, \(T_0\), of 77K\(^0\) for the three considered meshes. Results at time step of 124\(\mu s\) (3.7mm elongation).

Figure 7.29 Displacement patterns for Vanadium at a strain rate of 1000s\(^{-1}\) (V=30m/s) and an initial temperature of 77K\(^0\). (a) Deformation history for the 10×50 elements (Mesh3) corresponding to total elongations of 1.8, 3, 4.2, and 5mm. (b) A three dimensional shape corresponding to half of the circular bar at a total elongation of 5mm.
In Figure 7.31(a), the contours of the equivalent plastic strain for the three considered meshes also demonstrate the same distributions in the necking zone as well as at the other parts of the bar at a time step of 124 µs, i.e., 3.7 mm elongation. The evolution of the accumulated plastic strain with the loading time history for the three considered meshes is illustrated in Figure 7.31(b) over the considered total time step 165 µs. It is also clear from Figure 7.31(b) that the rate of evolution of the accumulated plastic strain exceeds the applied axial strain rate and increases as the necking evolves throughout the deformation process.

Similar to the case of Niobium, the incorporation of an explicit length scale parameter in the governing equations through the viscosity helps in obtaining objective results for the three considered meshes for Vanadium. In this regard, mesh dependence reappears when the accumulated plastic strains in the necking zone exceed 90% as clearly shown in Figure 7.31(b) particularly for the results obtained from the coarse mesh 7×15 elements (i.e., Mesh1).

- **Tantalum (Ta)**

Similar to the other bcc metals (Vanadium and Niobium), the necking of a Tantalum circular bar is studied by applying an axial tensile displacement velocity of 30 m/s over a total time step of 165 µs (5 mm total elongation) at an initial temperature of 77 K° for the same considered meshes shown in Figure 7.23. The displacement patterns exhibit an identical radius reduction at the center of the bar for the three considered meshes (Mesh1: 7×15, Mesh2: 10×25, and Mesh3: 10×50 elements) as illustrated in Figure 7.32 at an elongation of 3.7 mm (i.e., at time step of 124 µs). The history of the deformation for the 10×50 elements mesh at total elongations of 1.8, 3.0, 4.2, and 5.0 mm along with a three dimensional shape corresponding to half of the bar at 5.0 mm elongation is shown in Figures 7.33(a) and 7.33(b).

The contours of the Cauchy stress component $\sigma_{zz}$ at a time step of 124 µs, i.e., 3.7 mm elongation show comparable stress distributions for the three considered meshes as illustrated in Figure 7.34(a). In addition, the load-displacement curves shown in Figure 7.34(b) are almost identical throughout a 5 mm total elongation. Moreover, the contours of the accumulated plastic strain displayed at 3.7 mm elongation have the same distribution over the total area of the bar for the three considered meshes as shown in Figure 7.35(a). On the other hand, the evolution of the accumulated plastic strain in the necking zone over the total considered time step show little variation between the results obtained from Mesh1 (7×15 elements) and those obtained from Mesh2 (10×25 elements) and Mesh3 (10×50 elements). The deviations between the results obtained from the three considered meshes clearly appear over 70% accumulated plastic straining as shown in Figure 7.35(b).
Figure 7.30 Necking of a circular bar for Vanadium at a strain rate of 1000 s\(^{-1}\) (V=30 m/s) and an initial temperature of 77 K. (a) Contours of the Cauchy stress component in the axial direction \(\sigma_{zz}\) (Pascal) of the three considered meshes at 124 \(\mu s\) (3.7 mm elongation). (b) Axial stress versus axial displacement (elongation) curves over a total time step of 165 \(\mu s\) (5 mm total elongation) for the three considered meshes.
Figure 7.31 Necking of a circular bar for Vanadium at a strain rate of 1000s\(^{-1}\) (\(V=30\text{m/s}\)) and an initial temperature of 77K\(^{\circ}\). (a) Contours of the equivalent plastic strain of the three considered meshes at 124\(\mu\)s (3.7mm elongation). (b) Equivalent plastic strain versus time curves over a total time step of 165\(\mu\)s (5mm total elongation) for the three considered meshes.
Figure 7.32 Deformed (solid lines) and undeformed (dashed lines) patterns for Tantalum at strain rate of 1000s\(^{-1}\) (V=30m/s) and initial temperature, T\(_o\), of 77K\(^o\) for the three considered meshes. Results at time step of 124\(\mu\)s (3.7mm elongation).

Figure 7.33 Displacement patterns for Tantalum at a strain rate of 1000s\(^{-1}\)(V=30m/s) and an initial temperature of 77K\(^o\). (a) Deformation history for the 10\(\times\)50 elements (Mesh3) corresponding to total elongations of 1.8, 3, 4.2, and 5mm. (b) A three dimensional shape corresponding to half of the circular bar at a total elongation of 5mm.
Figure 7.34 Necking of a circular bar for Tantalum at a strain rate of 1000s\(^{-1}\) (V=30m/s) and an initial temperature of 77K\(^o\). (a) Contours of the Cauchy stress component in the axial direction \(\sigma_{zz}\) (Pascal) of the three considered meshes at 124\(\mu\)s (3.7mm elongation). (b) Axial stress versus axial displacement (elongation) curves over a total time step of 165\(\mu\)s (5mm total elongation) for the three considered meshes.
Figure 7.35 Necking of a circular bar for Tantalum at a strain rate of 1000s$^{-1}$ (V=30m/s) and an initial temperature of 77K. (a) Contours of the equivalent plastic strain of the three considered meshes at 124µs (3.7mm elongation). (b) Equivalent plastic strain versus time curves over a total time step of 165µs (5mm total elongation) for the three considered meshes.
Figure 7.36 Comparisons of necking results between Niobium, Vanadium, and Tantalum at a strain rate of 1000s\(^{-1}\) (V=30m/s) and an initial temperature of 77K\(^{\circ}\). (a) Deformed (solid lines) and undeformed (dashed lines) patterns at 3.6mm elongation (time step of 120\(\mu s\)). (b) Axial stress versus axial displacement (elongation) curves over a total elongation of 5mm (time step of 165\(\mu s\)).
Figure 7.37 Comparisons of results for a necking of a circular bar between Niobium, Vanadium, and Tantalum at a strain rate of $1000 \text{s}^{-1}$ ($V=30 \text{m/s}$) and an initial temperature of $77 \text{K}$. (a) Contours of the equivalent plastic strain at 3.6mm elongation (120µs). (b) Equivalent plastic strain versus time curves over a total elongation of 5mm (time step of 165µs).
Comparisons between the results obtained for the three considered bcc metals for the same velocity and initial temperature \((V=30\text{m/s and } to=77\text{K})\) are also carried out in this work. In this regard, it is found that in spite of the differences of stress-displacement results between the three bcc metals, the displacement patterns and the evolution of the accumulated plastic strains obtained for both Vanadium and Tantalum are almost the same as compared to the results obtained for Niobium. Figure 7.36(a) and Figure 7.37(a) show a comparison between Niobium, Vanadium, and Tantalum for the displacement patterns and the accumulated plastic strains respectively obtained from Mesh3 \((10\times50\text{ elements})\) at an elongation of 3.6mm \((\text{a time step of } 124\mu\text{s})\). The variation of the axial stress and the accumulated plastic strain with a total elongation of 5mm for the three considered bcc metals is also illustrated in Figure 7.36(b) and Figure 7.37(b) respectively.

**OFHC Copper (Cu)**

Unlike bcc metals, the adiabatic viscoplastic deformation of fcc metals show a strong dependence of the temperature and strain rate on the hardening, i.e., on the plastic strain. The Oxygen Free High Conductivity Copper is used here as fcc metals to study the necking of a fcc metal bar. Like the case of all of the previous three bcc metals, a displacement velocity of 30m/s \((1000\text{s}^{-1}\text{ strain rate})\) is applied at an initial temperature of 77K over a total axial elongation of 25mm \((\text{i.e., total time steps of } 830\mu\text{s})\) using both Mesh1 \((7\times15\text{ elements})\) and Mesh2 \((10\times25\text{ elements})\) as shown in Figure 7.23. The deformation process of the necking of an OFHC Copper bar exhibits high axial straining prior to the starting time of the necking at the center of the bar as shown in Figure 7.38. The displacement patterns show almost the same radius reductions for the two considered meshes at a time step of 700\(\mu\text{s}\), which is equivalent to an elongation of 21mm.

The history of the displacement patterns for the 10\(\times\)25 elements mesh (Mesh2) at 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, and 830\(\mu\text{s} \) \((3, 6, 9, 12, 15, 18, \text{and } 25\text{mm total elongations})\), illustrated in Figure 7.39(a), clearly show that the necking of the OFHC Copper bar initiates at the center when the axial elongation exceeds a value of 18mm. Unlike the other three bcc metals, the circular OFHC Copper bar demonstrates a high radius reduction all along the axial length before the necking at the center dominates. In Figure 7.39(b), a three dimensional shape corresponding to half of the bar at the end of the 830\(\mu\text{s} \text{ time step (25mm total elongation)}\) is also illustrated.

In addition to the displacement patterns, the contours of the Cauchy stress component \(\sigma_{zz}\) at a time step of 700\(\mu\text{s} \), i.e., 21mm elongation show the same distributions over the whole area of the bar for the two considered meshes as shown in Figure 7.40(a). Moreover, the axial stress versus displacement curves for the two meshes show also identical results over a 25mm total elongation as shown in Figure 7.40(b). The identical results of the stress-displacements curves for the case of OFHC Copper extend further to the softening regions. The comparable results between the two considered meshes are also observed for the distributions of the equivalent plastic strain over the total area of the bar. Figure 7.41(a) show the contours of the equivalent plastic strain for the two considered meshes at a 21mm elongation \((700\mu\text{s time step})\). The evolution of these equivalent plastic strains in the necking zone over a total time step of 830\(\mu\text{s} \)
(25mm elongation) is also illustrated, for the two meshes, in Figure7.41(b). The results obtained from the two considered meshes show excellent comparisons over a 140% plastic straining. Moreover, the time evolution rate of the equivalent plastic strain in the necking zone is equivalent to the applied loading rate up to 50% straining. This equivalent plastic strain rate, however, exceeds the applied loading strain rate and increases rapidly as soon as the necking process at the center of the bar evolves in which the plastic strain exceeds a value of 0.5.

Figure 7.38 Deformed (solid lines) and undeformed (dashed lines) patterns for OFHC Copper at a strain rate of 1000s⁻¹ (V=30m/s) and an initial temperature, T₀, of 77K° for Mesh1 (7×15 elements) and Mesh2 (10×25 elements) at time step of 700µs (21mm elongation).

It is obvious from the above necking results of the OFHC Copper circular bar that the effect of mesh refinement is almost negligible. These achieved objective results point toward a successful incorporation of an explicit length scale parameter in the governing equations through the viscosity parameter used in the rate-dependent formulations of fcc metals constitutive relations. However, mesh dependence reappears when the accumulated plastic strains in the necking zone approach very high values (over 150% plastic straining) as shown in Figure7.41(b). At this stage, the displacement patterns are controlled by the deformation of the last row of elements in the necking zone as clearly shown in Figure7.39(a) at a time step of 830µs. As mentioned earlier, this problem needs further consideration in the rate-dependent finite element formulation.
For the case of OFHC Copper, inducing a necking at the center of the circular bare requires a very high axial displacement (over 20mm elongation) in spite of the 1% radius reduction of the introduced geometric imperfection. In contrast, the initiation of necking at the center of the three considered bcc metals starts after less than 2mm of total elongation as shown in Figure 7.43. In other words, the softening of the bcc metals at the considered temperature and loading rates starts shortly after passing the yielding limit whereas it prolongs up to more than 70% straining for the case of OFHC Copper. This, however, indicates that most fcc metals maintain their high ductility behavior even at very low temperatures in which bcc metals behave as brittle materials (less ductility).

Further investigation of the necking process for a circular bar is also conducted in this work for the above bcc and fcc metals at different initial temperatures and loading rates. The results, which are not reported in this dissertation, obtained from this investigation show the same comparisons between fcc and bcc metals and between the three considered bcc metals themselves. Moreover, the dimension of the specimen along with the introduced geometric imperfection (1% radius reduction) affects largely the results and the shape of the necking at the center of the bar. The authors are currently investigating the necking problem of different geometric imperfections for different types of bars.

Figure 7.39 Displacement patterns for OFHC Copper at a strain rate of 1000s\(^{-1}\) (V=30m/s) and an initial temperature of 77K\(^{\circ}\). (a) Deformation history for the 10×25 elements (Mesh2) corresponding to total elongations of 3, 6, 9, 12, 15, 18, and 25mm. (b) A three dimensional shape corresponding to half of the circular bar at a total elongation of 25mm.
Figure 7.40 Necking of a circular bar for OFHC Copper at a strain rate of 1000s$^{-1}$ ($V=30$m/s) and an initial temperature of 77K$^\circ$. (a) Contours of the Cauchy stress component in the axial direction $\sigma_{zz}$ (Pascal) of the two considered meshes at 21mm elongation (700$\mu$s). (b) Axial stress versus axial displacement (elongation) curves over a total elongation of 25mm (total time step of 830$\mu$s) for the two considered meshes.
Figure 7.41 Necking of a circular bar for OFHC Copper at a strain rate of 1000s$^{-1}$ ($V=30$m/s) and an initial temperature of 77K$^\circ$. (a) Contours of the equivalent plastic strain of the two considered meshes at 700$\mu$s (21mm elongation). (b) Equivalent plastic strain versus time curves over a total time step of 830$\mu$s (25mm total elongation) for the two considered meshes.
Figure 7.42 Comparisons of necking results between bcc (Niobium, Vanadium, and Tantalum) and fcc (OFHC Copper) metals at a strain rate of 1000s\(^{-1}\) \( (V=30\text{m/s}) \) and an initial temperature of 77K\(^\circ\). Axial stress versus axial displacement curves over a total elongation of 25mm (total time step of 830\(\mu s\)).

Figure 7.43 Comparisons of necking results between bcc (Niobium, Vanadium, and Tantalum) and fcc (OFHC Copper) metals at a strain rate of 1000s\(^{-1}\) \( (V=30\text{m/s}) \) and an initial temperature of 77K\(^\circ\). Equivalent plastic strain versus axial displacement curves over a total elongation of 25mm (time step of 830\(\mu s\)).
Effect of Temperature on Necking

The effect of temperature and loading rates on the adiabatic stress-strain results was investigated in the previous chapters for both bcc and fcc metals. In this subsection, however, the initiation and development of a necking at the center of the circular bar at different initial temperatures and a specific loading rate is presented for Niobium and OFHC Copper as bcc and fcc metals, respectively.

For the case of Niobium, the same tensile displacement velocity of 30m/s is applied in the axial direction at additional four different initial temperatures 190K°, 296K°, 400K°, and 500K° over a total time step of 150µs that is equivalent to a total elongation of 4.5mm using the 10×25 element mesh (Mesh2). The corresponding displacement patterns and the contours of the equivalent plastic strain at the end of the considered time step are shown in Figure7.44(a) and Figure7.44(b) respectively. It is found that at the end of the considered time step, the considered bcc metals exhibit a larger radius reduction at low initial temperatures than that obtained at high initial temperatures. In other words, the radius reduction at the center of the bar decreases as the initial temperature increases as clearly shown in the deformed patterns given in Figure7.44(a). This may be attributed to the high value of stresses encountered due to the high yielding stresses at low temperatures. The yield stresses of most bcc metals are strongly affected by the temperature whereas the hardening is almost independent of such effect. Thus, at the very early stages (initial yielding), stresses encountered inside the material increases as the initial temperature decreases. This, in turn, helps in earlier initiation and faster development of the material necking. Since the viscosity and accordingly the introduced length scale is related to temperature as defined in Chapter6, the effect of initial temperature on the necking process is a reflection of the effect of different initial length scale on the deformation process.

Once the material passes the yield limit, the evolution of the plastic strains along with the high yielding stresses provides a very large amount of plastic work that will, consequently, be converted into heat and stored inside the material due to the adiabatic condition. As a result, the deformation temperature inside the material increases rapidly and leads to a faster material softening. Figure7.45(a) shows the stress variation with time for the considered initial temperatures (including the 77K° initial temperature adopted previously). The results obviously indicate that the softening which is a precursor of the necking initiation starts earlier at low initial temperatures whereas it is delayed as the initial temperature increases. This behavior may also be concluded from the evolution of the equivalent plastic strain in the necking zone of the deformed bar illustrated in Figure7.45(b). It is clear that the trends of the equivalent plastic strain evolution with time are almost the same for the five considered initial temperatures. Moreover, the amount of plastic straining at which the initiation of necking starts is about the same for all of the considered initial temperatures. However, the time required for such plastic strains differs from one to another. It should be pointed out here that not only the amount of temperature affects and controls the material softening or the development of necking but also its evolution rate during the total time of adiabatic deformation as shown in Figure7.46.
Figure 7.44 Necking of a circular bar for Niobium at a strain rate of 1000 s\(^{-1}\) (\(V=30\) m/s) and initial temperatures of 190 K\(^\circ\), 296 K\(^\circ\), 400 K\(^\circ\), and 500 K\(^\circ\) for Mesh2 (10\(\times\)25 elements) at the end of total time step of 150 \(\mu\)s (4.5mm total elongation). (a) Deformed (solid lines) and undeformed (dashed lines) patterns. (b) Contours of the equivalent plastic strains.
Figure 7.45 Results for a necking of a Niobium circular bar at a strain rate of 1000s\(^{-1}\) (V=30m/s) and initial temperatures of 190K\(^o\), 296 K\(^o\), 400 K\(^o\), and 500K\(^o\) for Mesh2 (10×25 elements). (a) Curves of the axial stresses versus time (b) Curves of the evolution of equivalent plastic strain with time in the necking zone.
Figure 7.46 Evolution of temperatures in the necking zone during a total time step of 150\(\mu\)s of a Niobium circular bar at a strain rate of 1000\(s^{-1}\) (V=30m/s) and initial temperatures of 190K\(^\circ\), 296 K\(^\circ\), 400 K\(^\circ\), and 500K\(^\circ\) for Mesh2 (10×25 elements).

In the case of fcc metals, the plastic hardening is strongly affected by the deformation temperature whereas, the yielding is almost independent of temperature. Thus, the deformation behavior during the necking process of an OFHC Copper (fcc metal) circular bar differs from that shown in Niobium (bcc metal). To investigate such an effect, the same velocity and initial temperatures used previously for Niobium are adopted over a total time step of 1000\(\mu\)s which is equivalent to 30mm total elongation using the 7×15 elements mesh (Mesh1). The corresponding displacement patterns and the contours of the equivalent plastic strains at a time step of 766\(\mu\)s (23mm) are shown in Figure7.47(a) and Figure7.47(b) respectively. The stress and equivalent plastic strain variations with time for the five considered initial temperatures (including the 77K\(^\circ\) initial temperature adopted previously) are also illustrated in Figure 7.48(a) and Figure7.48(b) respectively. As in the case of Niobium, the radius reduction of OFHC Copper bar at the end of the considered time step for the case of low initial temperatures is higher than that obtained for the case of higher initial temperatures. However this radius reduction takes place after the deformed bar exhibiting large amount of plastic straining.

Figure7.48(a) clearly shows that the softening which is considered here a precursor of the initiation of necking starts earlier in the case of the lower initial temperature whereas it is delayed as the initial temperature increases. Like the case of bcc metals, the trends of the equivalent plastic strain evolution with time are almost the same for the five considered initial temperature as illustrated in Figure7.48(b).
Figure 7.47 Necking of a circular bar for OFHC Copper at a strain rate of $1000\text{s}^{-1}$ ($V=30\text{m/s}$) and initial temperatures of $190\text{K}^\circ$, $296\text{K}^\circ$, $400\text{K}^\circ$, and $500\text{K}^\circ$ for Mesh1 ($7\times15$ elements) at a total time step of $760\mu\text{s}$ (23mm total elongation). (a) Deformed (solid lines) and undeformed (dashed lines) patterns. (b) Contours of the equivalent plastic strains.
Figure 7.48 Results for a necking of an OFHC Copper circular bar at a strain rate of 1000 s⁻¹ (V=30 m/s) and initial temperatures of 190 K, 296 K, 400 K, and 500 K for Mesh1 (7×15 elements). (a) Curves of the axial stresses versus time (b) Curves of the evolution of equivalent plastic strain with time in the necking zone.
Furthermore, the amount of plastic straining at the time of necking initiation is nearly the same for all of the considered initial temperatures. However, the time required for such plastic strains differs from one to another.

The amount of stresses at the early stages of deformation (yielding limit) is almost the same for all of the considered initial temperatures since there is no effect of such temperatures on the yield stresses. As the material deforms, plastic strains start accumulating throughout the adiabatic deformation process and, accordingly, the hardening stresses, resulted from such deformation, increase. At this stage, the amount of plastic work inside the material increases and mostly converts into heat causing a considerable rise of the deformation temperature. This increase of temperature continues gradually until the material softens indicating the initiation process of a necking at the center of the bar. Since the hardening stress of fcc metals increases as the temperature decreases, the deformation of an OFHC Copper bar with a low initial temperature shows a higher stress hardening than those obtained at high initial temperatures. The large stress encountered at the low temperatures, in turn, causes a high evolution rate of temperature due to the high evolution rate of plastic strain leading to a faster initiation of material necking. The evolution rate of the deformation temperature increases as soon as the necking starts (see Figure 7.49) due to the considerable increase of the equivalent plastic strain.

Figure 7.49 Evolution of temperatures in the necking zone during a total time step of 1000µs of an OFHC Copper circular bar at a strain rate of 1000s⁻¹ (V=30m/s) and initial temperatures of 190K°, 296 K°, 400 K°, and 500K° for Mesh1 (7×15 elements).
• Effect of Loading Rate on Necking

In this subsection, the effect of the applied displacement velocity on the initiation and development of necking at the center of the Niobium and OFHC circular bar is presented. Displacement velocities of 3m/s, 10m/s, 50m/s as well as the previous 30m/s velocity are considered at a specific initial temperature of 77K° for both metals. For the case of Niobium, time steps of 1500µs, 450µs, 150µs, and 90µs are employed to ensure a total elongation of 4.5mm for the aforementioned velocities respectively, using the 7×15 elements mesh (Mesh1). Figure7.50(a) shows the displacement patterns of the deformed and undeformed bar at an elongation of 3mm for three different velocities. The corresponding contours of the equivalent plastic strains are also illustrated in Figure7.50(b). The results clearly indicate that the radius reduction and accordingly the equivalent plastic strain encountered at the center of the bar for a certain amount of elongation increases as the rate of loading decreases. This, in fact, is due to the larger amount of time provided for low velocities than that available for high velocities for the specified amount of elongation. In other words, an elongation of 3mm requires a total of 1000µs time step for the lower velocity (3m/s), whereas, only 6% (60µs) of that time is needed to initiate the same amount of elongation for the case of the higher velocity (50m/s).

Figure7.51(a) and Figure7.51(b) show, for the four considered velocities and over a total elongation of 4.5mm, the adiabatic curves of axial stress-axial displacement and the evolution of the equivalent plastic strain over the total applied elongation respectively. The results show that the amount of elongation needed to initiate a necking at the center of the bar (starting point of material softening) increases as the rate of loading increases. However, the amount of time required for the initiation of necking decreases as the rate of loading increases as clearly shown in Figure7.52 at which the equivalent plastic strain is plotted versus the total considered time step in the logarithmic scale for the four considered loading rates.

Once the necking initiated at the center of the circular bar, the evolution rate of the equivalent plastic strain in the necking zone increases rapidly producing very high plastic strain values. Although this evolution rate (i.e, the reduction rate in the radius at the center of the deformed bar) is almost the same for the four considered displacement velocities as noticed from Figure7.51(b) and Figure7.52. The amount of the final equivalent plastic strain (total radius reduction) differs from one velocity to another due to the fact that the amount of time available for the development of necking (i.e., remaining time after the initiation of necking) is higher for the lower velocity than that for the higher velocity since necking is initiated earlier in the case of the lower velocity.

In the case of an OFHC Copper circular bar, a total elongation of 30mm is achieved by considering time steps of 10000µs, 3000µs, 1000µs, and 600µs for velocities of 3m/s, 10m/s, 30m/s, and 50m/s respectively using the 7×15 elements mesh (Mesh1). The displacement patterns of the deformed and undeformed shapes are presented in Figure7.53(a) for the four considered velocities at a total elongation of 18mm. Their corresponding equivalent plastic strain contours are also presented in Figure7.53(b).
Figure 7.50 Necking of a Niobium circular bar at initial temperature of 77K° and velocities of 3m/s, 10m/s, and 50m/s for Mesh1 (7×15 elements) at a total elongation of 3mm. (a) Deformed (solid lines) and undeformed (dashed lines) patterns. (b) Contours of the equivalent plastic strains.
Figure 7.51 Results for a necking of a Niobium circular bar at an initial temperature of 77K° and velocities of 3m/s, 10m/s, 30m/s and 50m/s for Mesh1 (7×15 elements). (a) Curves of the axial stresses versus elongation (b) Curves of the evolution of equivalent plastic strain with elongation in the necking zone.
The results obtained at the end of the considered elongation demonstrate that the amount of radius reduction and its corresponding equivalent plastic strain at the center of the bar is larger for the lower velocity than that obtained for the higher velocity. This fact coincides with the result obtained for a Niobium bar indicating that the reduction (necking) in the radius at the center of the bar decreases as the rate of loading increases. This, as explained earlier, is attributed to the small amount of time available for the initiation and development of necking at high displacement velocities.

The time or the amount of elongation required to initiate a necking in the center of the bar is also affected by the rate of loading as shown in the axial stress-elongation and axial stress-time curves illustrated in Figures 7.54(a) and (b) respectively. In these two Figures, it is clear that the material softening starts at different displacements and different times for the four considered loading rates. Higher displacement velocities require a higher amount of elongation to initiate a certain necking. Such an amount of elongation, however, is achieved in a lower time. This behavior is clearly shown in the evolution of the equivalent plastic strain in the necking zone with the applied elongation over the four different time steps presented in Figures 7.55(a) and (b). It is noticed from these two figures that the evolution rate of the equivalent plastic strain in the necking zone increases rapidly as soon as the necking initiated producing very high plastic strain values. The amount of such strains is higher for the case of lower velocity due to the higher amount of loading time that is required for such development.
Figure 7.53 Necking of an OFHC Copper circular bar at an initial temperature of 77K° and velocities of 3m/s, 10m/s, 30m/s, and 50m/s for Mesh1 (7×15 elements) at a total elongation of 18mm. (a) Deformed (solid lines) and undeformed (dashed lines) patterns. (b) Contours of the equivalent plastic strains.
Figure 7.55 Results for a necking of an OFHC Copper circular bar at an initial temperature of 77K and velocities of 3m/s, 10m/s, 30m/s and 50m/s for Mesh1 (7×15 elements). (a) Curves of the axial stresses versus time. (b) Curves of the axial stresses versus elongation.
Figure 7.54 Results for a necking of a Niobium circular bar at an initial temperature of 77K° and velocities of 3m/s, 10m/s, 30m/s and 50m/s for Mesh1 (7×15 elements). (a) Curves of the evolution of equivalent plastic strain in the necking zone with time (logarithmic). (b) Curves of the evolution of equivalent plastic strain in the necking zone with the applied elongation.
7.5.3 Shear Bands in Plane Strain Tensile Deformation

In the classical rate-independent plasticity theory, the onset of strain softening results in the mathematical ill posedness of the field equations. Since there is no length scale involved in the evolution of the shear band, the localization zone stays confined to the size of one element. As a result, a finer element size leads to a smaller shear band thickness with higher peak strains. This mesh sensitivity can be solved by introducing a viscosity term that helps in keeping the field equation well posed. Needleman (1988), Loret and Prevost (1990) and Sluys (1992) have shown that the material rate dependence introduces a length scale effect into the initial value problem, even though the constitutive equations do not explicitly contain a parameter with the dimension of length. Sluys (1996) has demonstrated that this viscous length scale effect can be related to the spatial attenuation of waves that have real wave speeds in the softening regime. Wang et al. (1996) found an expression for the internal length scale and examined the influence of a material imperfection on shear band formation. In this work (Farid and Voyiadjis, 2005), another expression for the length scale parameter that enters the constitutive equations through the viscoplastic multiplier is presented as explained in the previous chapter. This length scale is related to the microstructural physical quantities such as distance between obstacles (grain size) and distance between dislocations or in other words dislocation density.

In this study, however, the new developed physically based constitutive viscoplastic model is utilized in investigating the initiations and growths of the shear bands for the same above-mentioned metals using the verified material parameters listed in Tables 7.1 and 7.2. The plastic deformation of polycrystalline solids incorporates microscopically localized deformation modes that can be precursors to shear localization or in another word narrow bands of intense straining. These shear bands are very important as they dominate the deformation process and/or fracture modes in many materials particularly in metals. The initiation and development of adiabatic shear bands are investigated at different strain rates and temperatures. Different initial value boundary problems (inducing different geometrical nonlinearities) modeled using different mesh configurations are also considered.

- Simple Tension Plane Strain Problem

A simple uniaxial plane strain tension problem, with dimensions and loading history given in Figures 7.55(a) and (b) respectively, is considered in this example to study the initiation and development of the adiabatic shear bands in tensile deformation of several metals. The finite element program ABAQUS is used to simulate the tensile test. The theoretical formulations and computational algorithms of the proposed elasto-viscoplastic constitutive models are tested by studying the mesh sensitivity problem using different mesh configurations. In this regard, the considered problem is modeled and meshed with five different mesh discretizations (Mesh1:10×20, Mesh2:15×30, Mesh3:20×40, Mesh4:25×30, Mesh5:30×60 elements) as shown in Figure 7.56 using the four-node plane strain element with reduced integration (CPE4R ABAQUS type).
Figure 7.55 Problem description of tensile plane strain deformation. (a) A specimen subjected to certain displacement velocity loading with a specified boundary condition. (b) The time history for the applied impact tensile loading.

Figure 7.56 Five different mesh configurations used for the considered problem. Mesh1:10×20, Mesh2:15×30, Mesh3:20×40, Mesh4:25×50, and Mesh5:25×50 elements.
In this example, we will first investigate the differences between the rate-independent and rate-dependent plasticity constitutive equations by applying certain displacement velocities at certain initial temperatures using the five considered meshes. For this type of problem, shear bands may be developed and formed in different directions as there is no certain imperfection or defects induced in the sample. Deformations of a homogenous body with uniform initial conditions become inhomogeneous because of the interaction with the incident waves reflected from the boundaries and corner. This may happen at different instants in the considered metals due to the differences in their material properties. Moreover, it may also encounter at different instants within the same metal if different displacement velocities (different waves) are considered. However, this problem should be not affected by the mesh refinement. (i.e., by using different mesh configurations).

First we analyzed a rate-independent problem by applying a displacement velocity of 33m/s at an initial temperature of 77K° for Niobium using the same material parameters listed in Table7.1. The analysis is performed over a total time step of 100µs to ensure a total elongation of 3.3mm for all of the five considered meshes. The effect of viscosity is ignored by setting a constant value for the yield stress that corresponds to the applied rate of loading.

In Figure7.57 (a), the deformed and undeformed patterns for the five meshes are illustrated at a time step of 70µs (2.1mm elongation). It is obvious from these patterns that the observed width of shear bands is determined by the element size such that the deformation is localized along a line of integration points. The von Mises stresses at the localized regions over the total elongation of the specimen (3.3mm) clearly show the mesh dependency of the considered rate-independent analysis as shown in Figure7.57(b). The inclusion of geometrical nonlinearities in the description of strain softening cannot solve the discretization dependency since the dissipated energy decreases as the mesh is refined (Wang and Sluys, 2000).

Figures7.58(a) and (b) show the deformed and undeformed shapes of the corresponding contours of the equivalent plastic strains for the aforementioned displacement patterns. It is clearly shown in these figures that the width of the shear bands decreases as the element mesh size decreases. Moreover, the peak values of the accumulated strains increases rapidly as the localizations evolve as clearly shown in the curves plotted in Figure7.59 for the considered five mesh discretizations. Therefore, viscosity should be included in the constitutive equations to solve such mesh dependency. This viscosity effect, however, has a regularization effect not only on in the high strain rates (dynamics) loads but also in the low strain rates (quasi-static) case as will be shown later on.
Figure 7.57 Mesh-dependent results for Niobium using the 10×20, 15×30, 20×40, 25×50, 30×60 elements discretizations. (a) Deformed (solid lines) and undeformed (dashed lines) patterns at 70µs time step (2.1mm elongation). (b) Load-displacement curves over the total considered time step (100µs).
Figure 7.58: Mesh-dependent results for Niobium at 70µs time step (2.1mm elongation). Contours of the equivalent plastic strains (showing the shear bands) using rate-independent analysis for the 10×20, 15×30, 20×40, 25×50, 30×60 elements discretizations. (a) Deformed shape. (b) Undeformed shape.
Figure 7.59 Evolution of the equivalent plastic strains over the total time step (100µs) at the localized regions for Niobium using the 10×20, 15×30, 20×40, 25×50, 30×60 elements discretizations.

The rate-dependent analysis is performed, using the developed physically based constitutive viscoplastic model, by applying the same axial displacement velocity (V=33m/s) and initial temperature (77K) over a total time step of 100µs (3.3mm total displacement) using three mesh discretizations (Mesh1, Mesh2, and Mesh3). The corresponding deformed and undeformed deformation patterns are illustrated in Figure7.60(a) at a time step of 83µs (2.7mm displacement). The load (Mises)-displacement curves over the total time step is also plotted in Figure7.60(b). The deformed and undeformed shapes for the contours of the equivalent plastic strain are illustrated in Figures7.61(a) and (b) respectively at the same time step for the three considered meshes. By comparisons with the results obtained from the rate-independent analysis (Figures7.57(a), and 7.58(a, and b)), one observes that the shear band has a finite width that is independent of the finite element size. Moreover, the load-displacement curves (Figure7.60(b)) show almost identical results for all of the considered meshes as compared to those obtained for the rate-independent analysis.
Figure 7.60 Mesh-independent results for Niobium using the 10×20, 15×30, 20×40 elements discretizations. (a) Deformed (solid lines) and undeformed (dashed lines) patterns at 83µs time step (2.7mm elongation). (b) Load-displacement curves over the total considered time step (100µs).
Figure 7.61: Mesh-independent results for Niobium at 83µs time step (2.7mm elongation). Contours of the equivalent plastic strains (showing the shear bands) using the proposed viscoplastic constitutive relations for the 10×20, 15×30, 20×40, 25×50, 30×60 elements discretizations. (a) Deformed shape. (b) Undeformed shape
The peak strain values evolved during the localization process is investigated by plotting the evolution of the equivalent plastic strain at the localized region (shear band position) over the total considered time step as shown in Figure 7.62. The results show generally the same evolution rates and accordingly similar peak strain values are demonstrated for Mesh2 and Mesh3. However, little variation is encountered from the results obtained using the 10×20 element discretization (Mesh1) as compared to the other two meshes (Mesh2 and Mesh3). It is therefore concluded that coarse meshes are not preferred for such kind of deformations. In other words, results stabilize and become identical beyond a certain limit of mesh refinement.

This is also verified by applying another displacement velocity of 66m/s value at the room temperature (300K) using four element mesh discretizations (Mesh2, Mesh3, Mesh4, and Mesh5). The corresponding displacement patterns and equivalent plastic strain contours, shown in Figures 7.63(a) and (b) respectively, illustrate clearly the identical results (the same width of shear bands) obtained from the further refinement of meshes. Furthermore, the stress (Mises)-displacement curves as well as the evolution of the equivalent plastic strains at the localized regions show nearly the same results over the total considered time step obtained using the four considered meshes as shown in Figures 7.64(a) and (b) respectively.
Figure 7.63: Mesh-independent results for Niobium at V=66m/s (3300s\(^{-1}\) strain rate) and To=300K\(^o\) for the 15×30, 20×40, 25×50, 30×60 elements discretizations at 87\(\mu\)s time step. (a) Displacement patterns (b) Contours of the equivalent plastic strain.
Figure 7.64 Mesh-independent results for Niobium at \( V=66\text{m/s} \) (3300s strain rate) and \( T_\circ=300\text{K} \) at the shear bands for the 15×30, 20×40, 25×50, 30×60 elements discretizations. (a) Load-displacement curves (6.6mm total displacement). (b) Evolution of the equivalent plastic strain (100\( \mu \text{s} \) total time step).
Investigation of the initiation and development of shear bands is extended to the other bcc metals (Vanadium and Tantalum) using the same material parameters listed in Table 7.1. In the case of Vanadium, a velocity of 50m/s (2500s^{-1}) is applied at initial temperature of 300K over a total time step of 150\mu s to ensure a total axial displacement of 7.5mm. Like the case of Niobium, the corresponding displacement patterns and equivalent plastic strain contours, illustrated in Figures 7.65(a) and (b) respectively, show clearly the formation of a neck and a pronounced shear band of almost the same for the four considered mesh configurations; Mesh2, Mesh3, Mesh4, and Mesh5. Moreover, the stress (Mises)-displacement curves as well as the evolution of the equivalent plastic strains at the localized regions show nearly the same results over the total considered time step as shown in Figures 7.66(a) and (b), respectively.

The mesh-independent results are also obtained for the case of Tantalum for the 20×40 (Mesh3), 25×50 (Mesh4), 30×60(Mesh5) elements discretizations. In this case, a velocity of 60m/s (3000s strain rate) is applied at an initial temperature of 300K over a total time step of 150\mu s which provides a total elongation of 9mm. Figures 7.67(a) and (b) display the displacement patterns and the contours of the equivalent plastic strains respectively whereas, Figures 7.68(a) and (b) illustrate the load (Mises)-displacement curves and the evolution of the equivalent plastic strains, respectively at the shear bands positions over the total considered time step. The results generally indicate the successful incorporation of the viscosity parameter in the theoretical formulations and computational algorithms of the proposed elasto-viscoplastic constitutive models.

For the case of OFHC Copper as fcc metals, a displacement velocity of 33m/s (1650s^{-1} strain rate) is applied at initial temperature of 77K using the 10×20 (Mesh1), 15×30 (Mesh2), 20×40(Mesh3) elements discretizations. The above-mentioned displacement velocity is applied over a total time step of 500\mu s ensuring about 16.5mm displacement in the axial direction. In the adiabatic deformation process of this metal and after large amount of strains, the localization is controlled by a necking at one of the four corners. In Figure 7.69(a), the deformed and undeformed displacement patterns are illustrated at a time step of 470\mu s (15.5mm applied displacement) for the three considered meshes. The corresponding contours of the equivalent plastic strain are shown in Figure 7.69(b). Although the material localization is dominated by the necking process (no pronounced shear bands), mesh-independent results are obtained from almost all of the three mesh discretizations. Moreover, objectivity can also be observed from the load-displacement curves presented in Figure 7.70(a) over the total applied displacement (16.5mm). It is obvious from the stress-displacement curves that the hardening stresses increase with the applied displacement due to the accumulation of the plastic strains. Also, the material show high ductility as compared to the three bcc metals used in this work. In other words, material softening is encountered after a large amount of elongation. Figure 7.70(b) shows the evolution of the accumulated plastic strain at the necking region over the total considered time step (500\mu s). The results obtained using the three above-mentioned mesh configurations show almost an identical evolution rate and accordingly identical peak strains. However, there is little variation between the results obtained from the coarse mesh (Mesh1) and the other two meshes (Mesh2 and Mesh3) particularly after 100% plastic straining.
Figure 7.65: Mesh-independent results for Vanadium at $V=50\text{m/s}$ ($2500\text{s}^{-1}$ strain rate) and $T_0=300\text{K}$ for the $15\times30$, $20\times40$, $25\times50$, $30\times60$ elements discretizations at $125\mu\text{s}$ time step. (a) Displacement patterns (b) Contours of the equivalent plastic strain.
Figure 7.66 Mesh-independent results for Vanadium at $V=50m/s$ (2500s strain rate) and $T_o=300K$ at the shear bands for the $15\times30, 20\times40, 25\times50, 30\times60$ elements discretizations. (a) Load-displacement curves (7.5mm total displacement). (b) Evolution of the equivalent plastic strain (150$\mu$s total time step).
Figure 7.67: Mesh-independent results for Tantalum at $V=60m/s$ (3000$s^{-1}$ strain rate) and $T_0=300K$ for the $20\times40$, $25\times50$, $30\times60$ elements discretizations at $150\mu s$ time step. (a) Displacement patterns. (b) Contours of the equivalent plastic strain.
Figure 7.68 Mesh-independent results for Tantalum at $V=60\text{m/s}$ (3000s strain rate) and $T_0=300\text{K}$ at the shear bands for the $20\times40$, $25\times50$, $30\times60$ elements discretizations. (a) Load-displacement curves (9.0mm total displacement). (b) Evolution of the equivalent plastic strain (150$\mu\text{s}$ total time step).
Figure 7.69: Mesh-independent results for OFHC Copper at $V=33\text{m/s}$ ($1650\text{s}^{-1}$ strain rate) and $T_0=77\text{K}$ for the $10\times20$, $15\times30$, $20\times40$ elements discretizations at $470\mu\text{s}$ time step (15.5mm elongation). (a) Displacement patterns. (b) Contours of the equivalent plastic strain.
Figure 7.70 Mesh-independent results for OFHC Copper at $V=33\text{m/s}$ ($1650\text{s}^{-1}$ strain rate) and $T_0=77^\circ\text{K}$ for the $10\times20$, $15\times30$, $20\times40$ elements discretizations. (a) Load-displacement curves (9.0mm total displacement) away from the necking zone. (b) Evolution of the equivalent plastic strain (150µs total time step) in the necking zone.
It should be emphasized that, unlike the case in bcc metals, the initial yield stress for the considered fcc metal is small and almost constant, whereas, the hardening stress evolves with the accumulation of plastic strains. This results in delaying the material softening and consequently, necking process dominates the material localization from the time of initial softening till the final stage of material failure. For this reason and the fact that there is no geometric imperfection or material defects imposed in this example, shear banding is not prominent. Figure 7.71 shows the development of the magnitude and the distribution of the equivalent plastic strain obtained from the 20×40 mesh discretization (Mesh3) at different loading times. It’s clear that, for the considered simple tensile plane strain problem, the localization region appears through the necking at the final stages of deformation, i.e., after a large amount of plastic strains.

Figure 7.71 The magnitude and the contours of the equivalent plastic strains for OFHC Copper at V=33m/s and To=77K at different times. Results are obtained from the 20×40 mesh discretization (Mesh3).
Effect of Initial Temperature on Shear Banding

The effect of initial temperature on the initiation and development of shear bands for the considered tensile plane strain problem is investigated. In this regard, a displacement velocity of 66m/s (3300s⁻¹ strain rate) is applied at initial temperatures of 77K, 150K, 200K, 250K, 300K, and 400K using the material parameters of Niobium (Table 7.1). A total axial displacement of 6.6mm is achieved over a total time step of 100μs using the 20×40 element mesh discretization (Mes3). The corresponding displacement patterns at the end of the considered time step are shown in Figure 7.72. The magnitude and the distribution of the equivalent plastic strain at the end of the considered time step are also illustrated in Figure 7.73 for the six considered initial temperatures. It is interesting to note that the width of the shear band increases as the initial temperature increases. This is, however, attributed as the case in bar necking to the high initial yield stress values encountered at low initial temperatures. These initial high stresses cause an earlier material softening and accordingly a faster rate of evolution of the equivalent plastic strain at the initial localized regions. These high plastic strains along with the high stresses offer a large amount of plastic work that will, in turn, be converted into heat causing a considerable increase in the deformation temperature (since the deformation is adiabatic, i.e., no outside transfer of temperature).

The resulting curves of the load (Mises)-displacement and the evolution of the equivalent plastic strain in the localized regions (shear band positions) for the six initial temperatures are illustrated in Figures 7.74(a) and (b) over the total considered time step. It is obvious that the material softening, which may be considered as a precursor of shear band initiation, starts earlier at low initial temperatures whereas it is delayed as the initial temperature increases. This delay in the material softening results in material necking at the further stages of deformation as shown in the adiabatic deformation at 400K initial temperature. Such behavior, however, is similar to that shown in the adiabatic deformation of OFHC Copper (Figure 7.69). It should also be emphasized that the variation in the shear band width at different initial temperatures is controlled by the increasing rate of the evolution of the equivalent plastic strains at the localized regions. This increasing rate is accompanied with an increase in the evolution rate of temperature causing, in turn, a finer width of the shear band. On the other hand, the amount of the equivalent plastic strain at a certain time has a slight if no effect on the shear band width. This negligible effect is clearly shown from the contours of the equivalent plastic strain at about 60% peak strains. This specific peak plastic strain is achieved at a different time for each of the six considered initial temperatures as illustrated in Figure 7.75.

Figure 7.76 shows the evolution of material temperature over the total considered time step for the different initial temperatures. It is clearly shown that the rate evolution of the adiabatic deformation temperature in the localized regions is increasing rapidly at the lower initial temperatures (e.g., 77K) and approaches very high relative values. This evolution rate, however, is almost constant during the total considered time step in the case when higher initial temperature is considered (e.g., 400K). In the absence of defects (no initial damage), the deformation behavior of bcc metals in general and Niobium in particular at the initial stages of deformation is almost brittle for the case of very low initial temperature whereas, in the case of very high initial temperature, ductility is observed from the early stages of deformation.
Figure 7.72 Deformed (solid lines) and undeformed (dashed lines) displacement patterns for Niobium at a strain rate of 3300s⁻¹ (V=66m/s) and initial temperatures of 77K, 150K, 200K, 250K, 300K, and 400K for Mesh3 (20×40 elements). Variations of the shear band width at the end of a total time step of 100µs (6.6mm total displacement).
Figure 7.73 Contours and Magnitudes of the equivalent plastic strain for Niobium at a strain rate of 3300s\(^{-1}\) (V=66m/s) and initial temperatures of 77K\(^{\circ}\), 150K\(^{\circ}\), 200K\(^{\circ}\), 250K\(^{\circ}\), 300K\(^{\circ}\), and 400K\(^{\circ}\) for Mesh3 (20×40 elements). Variations of the shear band width at the end of a total time step of 100\(\mu\)s (6.6mm total displacement).
Figure 7.74 Resulting curves for Niobium at $V=66\text{m/s}$ (3300s$^{-1}$ strain rate) and initial temperatures of 77K, 150K, 200K, 300K, 400K in the localized regions (shear band positions) and over the total considered time step (100µs, 6.6mm). (a) Load-displacement curves. (b) Evolution of the equivalent plastic strain.
Figure 7.75 Contours and Magnitudes of the equivalent plastic strain for Niobium at a strain rate of 3300s\(^{-1}\) (V=66m/s) and initial temperatures of 77K, 150K, 200K, 250K, 300K, and 400K for Mesh3 (20×40 elements). Variations of the shear band width at an amount of about 60% accumulated plastic strain at the peak regions.
• **Effect of Displacement Velocity on Shear Banding**

The effect of the applied displacement velocity on the initiation and development of necking at the center of the Niobium and OFHC circular bar is investigated in this work. In this regard, several displacement velocities of the range between 10m/s to 100m/s (500s\(^{-1}\) to 5000s\(^{-1}\) strain rate) considered at a specific value of initial temperature (150K\(^\circ\)). The material parameters for Niobium (Table7.1) are considered using the 20×40 element discretization (Mesh3). Different time steps corresponding to different applied velocities are used to ensure a total axial displacement of 5mm at the end of each time step. Unlike for the case of the different initial temperatures, a unique position for the shear band can not be achieved at different applied displacement velocities unless a certain geometric nonlinearity or material defect is imposed in the present simple tensile plane strain problem. As mentioned earlier, for the considered uniform initial conditions, the deformation of Niobium becomes inhomogeneous because of the interaction with the incident waves reflected from the boundaries and corners. This inhomogeneous behavior results in different positions of localization as appeared in the present investigation after applying different velocities (different waves). This non-uniqueness solutions are clearly shown in the displacement patterns of Niobium at velocities of 10m/s, 30m/s, 50m/s, 60m/s, 70m/s, 80m/s, 90m/s, and 100m/s displayed in Figure7.77.
Figure 7.77 Deformed (solid lines) and undeformed (dashed line) displacement patterns for Niobium at initial temperature of 150K° and velocities of 10m/s, 30m/s, 50m/s, 60m/s, 70m/s, 80m/s, 90m/s and 100m/s at the end of a total displacement of 5mm.
Although the width of shear bands are almost the same, the position and the shape of the pronounced shear bands at the end of the 5mm total displacement vary from an applied velocity to another. This behavior can also be noticed in Figure 7.78 in which the magnitudes and the contours of the equivalent plastic strain are illustrated for velocities of 10m/s, 30m/s, 50m/s, 60m/s, 70m/s, 70m/s, and 80m/s. Since there exist more than one solution for the considered problem, comparisons between the different applied velocities for the stress-displacement and the evolution rate of the equivalent plastic strain are not representative. Such results, therefore, are not presented in this work.

![Figure 7.78 Contours and Magnitudes of the equivalent plastic strain for Niobium at initial temperature of 150K° and velocities of 10m/s, 30m/s, 50m/s, 60m/s, 70m/s, and 80m/s at the end of s total displacement of 5mm.](image)
CHAPTER 8

SUMMARY, CONCLUSIONS AND FUTURE CONSIDERATIONS

8.1 Summary and Conclusions

This dissertation may be classified into three interrelated parts: (a) Microstructure and physical basis for the new derived flow stress models; (b) Thermodynamic formulation of the multiscale models; and (c) Algorithmic treatment and numerical issues for the proposed models applications.

(a) Physically based flow stress models for metals and steel alloys (Chapters 2-5).

The concept of thermal activation energy along with the dislocation interactions mechanism is used here in modeling the flow stress for metals with different crystal structures (body centered cubic (bcc), face centered cubic (fcc), and hexagonal closed-packed (hcp)) as well as steel alloys under low and strain rates and temperatures. In bcc metals, the thermal yield stress, due to the short-range barriers (Peierls barriers), shows a strong dependency on the strain rate and temperature while the plastic strain hardening which represents the athermal stress is independent of them. In contrary, the thermal stress in fcc metals is strongly dependent on the plastic strain due to the domination of the dislocation intersections on the mechanisms behavior of the thermal activation analysis. For the case of hcp metals, the thermo-mechanical behavior shows a combination between the plastic deformation behavior of both bcc and fcc structures. Thus, the thermal component as well as the athermal component of the flow stress for the proposed hcp model strongly depends on the plastic strain. Besides, both yielding and hardening stresses are strain rate and temperature dependent. In steel alloys, both thermal and athermal flow stresses are plastic strain dependent, however due to the high percentage of Iron, the majority of the thermal part of the flow stress belongs to the yield stress, whereas, the plastic hardening dominates the athermal flow stress. This indicates that the resistance to the Peierls’ barriers mostly controls the thermal activation analysis of most steel alloys.

The effect of dislocation density multiplications (chapter 2) as well as its evolution with the plastic strain (chapter 5) is incorporated in modeling the thermo-mechanical response of different structure types of metals. Two different definitions for modeling the hardening stresses are employed. The first definition uses the experimental power law fitting, whereas the second one is derived using the plastic strain evolution of the dislocation density. The simulation of the adiabatic and isothermal plastic flow stresses for different bcc, fcc and hcp metals is achieved at low and high strain rates and temperatures. The predicted results, generally, show a good agreement as compared with different experimental results conducted by several authors for niobium, vanadium, molybdenum and tantalum for bcc metals, titanium for hcp metals and OFHC copper for fcc metals. In fact, the predicted results using the proposed models are in some cases closer to the experimental results than those estimated by the Zerilli and Armstrong model and the Nemat-Nasser and his co-workers’ model.
The modeling of the adiabatic and isothermal plastic flow stresses of AL-6XN stainless steel is achieved (chapter 3) at low and high strain rates and over a wide range of temperatures using a combination of both bcc and fcc models. True stress-true strain modeling is achieved for different strain rates and temperatures by incorporating the classical secant method for the case of uniaxial loading. However, the temperature effect on the elastic modulus is not considered in this work. The model predictions, in general, are in good agreement with the experimental results.

The dynamic strain aging (DSA) phenomenon is clearly encountered in titanium for most temperatures and strain rates while it activates only at low strain rates and over a narrow range of high temperatures for most bcc metals. For OFHC copper, the DSA effect is not observed for the present temperature and strain rate range of experimental data. In fact, the dynamic strain aging encountered in some metals at certain temperatures is strain rate dependent. Its effect, however, is not included in the present modeling where the dislocation movement as well as the dislocation evolution controls the plastic deformation in the absence of diffusion and creep.

In investigating the derivation of the Z-A model (chapter 4), two crucial points are noticed. First, the model parameters are modified after making use of the evolution equation of the mobile dislocation density. Second, the use of the approximation $\ln(1 + x) \approx x$ in obtaining the Z-A model into its final form, is not an accurate assumption since this expansion is not valid when the variable $x$ is close to a value of 1.0. The percentage of the differences between the exact and approximated values affects significantly the prediction of the flow stresses because these values are due to an exponential term which is multiplied by a large numerical quantity. These differences, however, have been overcome through the fitting techniques of the experimental data. This causes the model parameters to be more phenomenologically based rather than physically interpreted. Consequently, the Z-A physically based relations for bcc and fcc metals are modified here (chapter 4) such that the material parameters are physically deduced and accurately related to the nano/micro-structure physical parameters. The nonlinear stress-temperature relationship derived in this work shows very good correlations with the experimental results for OFHC copper, Tantalum, vanadium, and Niobium. Besides, the adiabatic stress-strain relations computed using the proposed relations show relatively very good correlations over wide ranges of temperatures and strain rates. In contrast, the results predicted by the Z-A model show a wide deviation from the experimental results of the OFHC copper and tantalum particularly at higher temperatures.

Finally, the numerical identification of the physical parameters in the nano/micro-scale is presented for all of the considered metals. In general, most metals contain an initial amount of dislocations which are naturally exited or generated through the manufacturing process. These dislocation densities, however, help metals deform plastically until a level where no further dislocation generation is allowed. This indicates that the saturation limit of dislocation densities is reached. The initial and saturated values of the dislocation densities, however, differ from metal to metal. The numerical values of the physical nano- and micro-quantities used in defining the proposed models that are obtained for the considered metals are listed in chapter 5. Although these quantities are defined based on the model parameters that are fitted experimentally, their values are found to be reasonable when compared to those available in
the literature. The initial dislocation density values are fixed and set around $5 \times 10^{12} \text{m}^{-2}$ for the case of bcc metals and a little higher value for fcc and hcp metals. Consequently, the saturated values of these dislocation densities are found to be in the order of $10^{15} \text{m}^{-2}$ for all metals. The main conclusions for this part of the dissertation include:

- The effect of initial dislocation density enters the proposed models through the thermal component of the flow stress. This effect, however, is expected to be higher for bcc metals than other metal structures due to the fact that the thermal stress of bcc metals is nearly related to the yield stress (Peierls stress) and not affected by the dislocation density evolution with plastic strain. That is to say, the yielding strength is less when the material contains a high initial dislocation density and vice versa. Once the material yields, the evolution of dislocation density along with the initial dislocation density contribution plays a crucial role in determining the flow stress and particularly the thermal stress as in the case for most fcc metals and slightly less for hcp metals.

- The contribution of the generation of the mobile dislocation density during the plastic deformation in the proposed model shows a considerable effect on the prediction of the flow stress particularly in the case of high strain rates and temperatures. Excluding the mobile dislocation density increment from the present formulation causes additional hardening that over-predicts the experimental data.

- Although, the hardening and yielding of AL-6XN stainless steel are strain rate and temperature dependent, the microstructure of the material evolves mainly with temperature history.

- In the proposed model, the following typical values; of 1.5 and 0.5 are used for the exponents $p$ and $q$, respectively. Unfortunately, the value of the threshold yield stress in the component of the thermal stress is sensitive to the choice of $p$ which characterizes the tail of the obstacle. This sensitivity, however, is less for the threshold hardening stress term in the thermal hardening component.

- There should be different definitions for the evolution equations of the dislocation density for each of the bcc and fcc metals metal. The evolution relations in general should consider the history effect of the dislocation density during plastic deformation for the hardening component whereas it does not require the history effect in the case of thermal yielding.

- The Z-A model assumed an exponential stress-temperature relationship in modeling the thermal stress component based on experimental observations. This exponential form is inappropriate for all types of metals particularly at elevated temperatures. This, in turn, causes the thermal stress component of the Z-A model to never vanish at any temperature which is inconsistent with the considered mechanisms that become athermal when $G \rightarrow G_o$ at certain critical temperatures.

- Finally, the numerical identification of the physical parameters in the nano/micro-scale demonstrates reasonable quantities as compared to those specified in the literature.
A general consistent thermodynamic framework for small and large deformations of both bcc and fcc metals is presented in this study. A coupled temperature and strain rate microstructure physically based yield function, derived in (a), along with a Clausius-Duhem inequality (first and second laws of thermodynamics), the additive decomposition of the total strain rate into elastic and viscoplastic parts, the maximum dissipation principle, generalized normality, the thermomechanical heat equation, and an appropriate and consistent free energy definition are incorporated in deriving the proposed three dimensional kinematical model. This constitutive model, however, takes into consideration small and large deformation analyses and is applicable for both low and high strain rates at different elevated temperatures. The evolution equations are expressed in terms of the material time derivatives of the elastic strain, accumulated plastic strain (isotropic hardening), and the back stress conjugate tensor (kinematic hardening). Similar to the static and dynamic yield surfaces, two equivalent yield surfaces are introduced; the athermal yield surface and the thermal yield surface. The choice of the form of the Helmholtz free energy function is very important since it constitutes the basis for deriving the constitutive equations. In this work, the absolute temperature and the strain rate are considered as internal state variables in the definition of the Helmholtz free energy function.

The temperature effect is considered very crucial in thermo-viscoplastic deformation particularly in adiabatic conditions. Therefore, an explicit viscosity-temperature relationship is derived to impose the effect of the accumulated heat on the adiabatic deformation. A proper definition for the magnitude of the viscoplastic flow is also achieved in order to characterize the dynamic behavior of the material. The viscoplastic multiplier is found to be equivalent to the accumulated plastic strain for the von Mises plasticity. Two different definitions for the viscoplastic multiplier are introduced: the first relation is obtained analogous to the one defined in the well-known viscoplastic model of Perzyna whereas, the second definition is derived after utilizing the same concept used in the Consistency model.

It is known that the viscosity parameter, also known as the relaxation time, is considered the most important parameter in the finite element implementation of viscoplasticity. This helps in introducing a physical length scale that helps in regularizing some problems encountered in finite element computations. It allows the spatial difference operator in the governing equations to retain its ellipticity. In this work, an explicit definition of the length scale in terms of the microstructural physical quantities is achieved. In the Perzyna model, both the static yield function and the athermal yield function may be used to check whether viscoplasticity occurs. Moreover, the two models show different responses during unloading process.

As for bcc metals, the viscosity of fcc metals is also proportional to the dislocations waiting time at an obstacle. It is affected by both the temperature and the accumulative plastic strain. The rise of the heat inside the material diminishes the strength of the obstacles such that the mobile dislocations overcome these barriers in a lesser amount of time at which the viscosity of the material decreases. Moreover, the large amount of accumulated plastic strain
that evolves during the viscoplastic deformation gives an indication of obstacle weakness, i.e., viscosity degradation. A further rise in temperature \((T \to T_c)\) makes the thermo-visco-stress completely vanish at which the yield surface is reduced to its athermal rate-independent state. This kind of deformation, however, is achieved at extremely high temperatures. In the case of fcc metals, the accumulated plastic strain plays a significant role in the viscoplastic deformation. This effect is extended to the definition of the proposed length scale which varies with the accumulation of the plastic strain during the viscoplastic deformation.

The main conclusions of this study are:

- It should be clearly stated here that the definition of the specific free energy function should take into consideration the deformation condition (rate independent/rate dependent and/or isothermal/adiabatic) as well as the material type (bcc metals, fcc metals, steel alloys, concrete, etc.). Thus, introducing a unique form of the free energy definition for all types of materials and loading conditions is not an accurate assumption in the thermodynamic consistent formulation for constitutive relations.

- In the Consistency model, the material always unloads elastically regardless of the size and the position of the yield surface, while, in the Perzyna model, viscoplasticity occurs during the first stages of the unloading process. After a sufficient time of unloading, the overstress becomes exhausted, the Perzyna model unloads elastically. This is, however, not the case for bcc metals at which the yield stress controls the viscoplastic deformation. That is to say, the assumption for the Consistency model to unload elastically may be accepted for a material with viscoplastic behavior similar to bcc metals.

- It is found that the introduced length scale through the viscosity parameter shows high values for bcc metals than those obtained for fcc metals. Moreover, the proposed length scale decreases as the plastic strain increases. The effect of the plastic strain accumulation is clearly observed in fcc metals and slightly in bcc metals.

- The use of the thermal and athermal yield surfaces instead of the static and dynamic yield functions in the thermodynamic formulation is found to be satisfactory.

- The static yield surface coincides with the athermal yield surface at the critical (athermal) temperatures \((T=T_{cr})\).

(c) Computational aspects and applications for the proposed models (Chapters 7).

A consistent algorithmic treatment for the developed viscoplasticity constitutive relations within the context of small strain deformation is developed. The algorithm is then extended to account for the objectivity of stress integration in finite strain viscoplasticity. Implementing the developed thermo-viscoplastic models in the finite element code (ABAQUS) using the material subroutine VUMAT is also achieved. Computational aspects of the proposed model are addressed through the finite element implementation with an implicit stress integration algorithm. The radial return algorithm which is a special case of the backward-Euler method is
used to introduce a nonlinear scalar equation in terms of the viscoplastic multiplier for the case of the Consistency viscoplastic model and in terms of the equivalent stress for the case of the Perzyna viscoplastic model. Consistent algorithmic tangent stiffness matrices are derived for both small and finite strain viscoplastic models. In this work, an incremental integration scheme in which the stress objectivity is preserved for finite rotation increments to rewrite the constitutive relations in a corotational moving frame is presented.

In the finite element implementation of a mechanical field problem, the central field equation necessarily to be solved in the spatial discrete equation is derived from the weak form of the balance equation of linear momentum. In an implicit displacement field finite element formulation, equilibrium in a time step may be obtained by linearizing the nonlinear equilibrium equation at each iteration using the Newton-Raphson method. By this, one can obtain the definition of the exact or algorithmic tangent moduli. This consistent tangent modulus plays a crucial role in reducing the computation time preserving the asymptotic rate of quadratic convergence.

Several numerical examples are presented in this work in order to validate and test the proposed computational framework and numerical algorithm for different types of bcc and fcc metals. All numerical simulations are performed by using the Newton-Raphson iteration procedure with a fully backward Euler integration scheme. Finite element simulations are performed by implementing the proposed viscoplasticity constitutive models in the commercial finite element program ABAQUS/Explicit (2003) via a user’s material subroutine coded as VUMAT. Numerical implementation for a simple tension problem meshed with different numbers of elements is used for testing the proposed model for tantalum, niobium, and vanadium as bcc metals and for OFHC Copper as fcc metals at low and high strain rates and temperatures. The numerical results of the isothermal and adiabatic stress-strain curves compare very well with the experimental data for most of the above-mentioned metals. Furthermore, a set of numerical examples under strict deformation conditions are presented in order to check the effectiveness and the performance of the proposed framework and its finite element implementation in the ABAQUS code at different loading conditions. Results obtained for different boundary conditions show, generally, mesh independency. Finally, the effect of temperature and loading rates on the initiation and development of a necking at the center of the circular bar and shear band development is presented for different types of metals. Conclusions of the above numerical issues include:

- The static strain rate value (at which the material becomes rate-independent) is not a constant as advocated by many authors. This value changes with the change in the deformation temperature. It also differs from a metal to another.

- Objectivity is achieved for different meshes. This is due to the incorporation of an explicit length scale parameter in the governing equations through the viscosity definition used in the rate-dependent formulations of the constitutive relations. The proposed computational algorithms introduce properly the localization limiting of a scale-dependent continuum: the results of finite element simulations are almost insensitive to mesh refinement.
Mesh independence reappears when the accumulated plastic strains in the localized regions approaches high values. The width of the localization zone needs to be many times larger than the element size for the proper calculation of the viscoplastic strain. This means that the meshes used in localization problems must be fine enough. Upon further mesh refinement convergence to a meaningful solution is guaranteed.

Introducing realistic definitions for the material parameters of the proposed constitutive relations helps in achieving a proper understanding of the localization behavior of metals under different loading conditions.

It is found that at the end of the considered time step, the considered bcc metals exhibits a larger radius reduction at low initial temperatures than that obtained at high initial temperatures. In other words, the radius reduction at the center of the bar decreases as the initial temperature increases. Similarly, the width of the shear band increases as the initial temperature increases. The effect of initial temperature is a reflection of the effect of a different initial length scale on the deformation process. The softening starts earlier at low initial temperatures whereas it delays as the initial temperature increases.

The results show that the amount of elongation needed to initiate a necking at the center of a bar (starting point of material softening) increases as the rate of loading increases. However, the amount of time required for the initiation of necking decreases as the rate of loading increases.

Unlike for the case of the different initial temperatures, a unique position for the shear band may not be achieved at different applied displacement velocities unless a certain geometric nonlinearity or material defect is imposed. The deformation becomes inhomogeneous because of the interaction with the incident waves reflected from the boundaries and corners. This inhomogeneous behavior results in different positions of localization.

8.2 Future Directions

The following issues and research directions are found necessary such that they deserve further considerations:

In the dissertation, the thermodynamic formulation of the proposed multiscale modeling is derived for bcc and fcc metals only. The formulations should be extended to include hcp metals as well as different types of steel alloys.

Similar to the viscoplastic behavior, a micromechanical basis for introducing the effect of damage on the localization is needed.

Since the localization problems involve high strain gradients, adaptive meshing techniques are encouraged to be used.
• The dynamic strain aging phenomenon needs to be addressed and included in the viscoplastic characterization of some metals.

• Since all of the material parameters of the proposed constitutive relations are related to the microstructural physical quantities, a parametric study considering the effect of each of these parameters is very important in order to show the significance of each parameter.

• Applications should be extended to include three dimensional problems and higher velocities are encouraged to use.

• Characterization and modeling of the coupling between viscoplasticity and damage is required particularly for the problem of impact damage in metals and composite structures.


BIBLIOGRAPHY PART II: BY OTHER AUTHORS


VITA

Farid Hamid Abed was born in Iraq on January 15, 1970. Farid received his primary and secondary education in various public schools in Baghdad, Iraq. He subsequently graduated from the University of Technology in Baghdad with a Bachelor of Science degree in building and construction engineering in May 1992. After a break of two years, working as a site and design engineer in different projects in Iraq, he traveled to Jordan to join the Jordan University of Science and Technology (JUST), pursuing a master degree in structural engineering under the guidance of Professor Ghazi Abu-Farsakh. In JUST, he worked as teaching and research assistant for four years. Farid left Jordan in 1998 and traveled to Dubai in the United Arab Emirates (UAE) to work as a material and geotechnical engineer in a private technical laboratory for two years. After that, he joined the University of Sharjah working as a lecturer in the department of Civil Engineering. Mr. Abed began his doctoral study in 2001 at Louisiana State University (LSU) in the United States under the supervision of Boyd Professor George Z. Voyiadjis. Four years later he completed the research presented in this dissertation with a 4.0 GPA. He has been involved in researches in several areas, such as computational mechanics, mechanics of solids and structures, structural dynamics, mechanics of materials, fracture and damage mechanics, and multiscale modeling of metals and steel alloys at low and high strain rates and temperatures. He has several publications that have been published in several prestigious journals in the field of structural engineering and engineering mechanics. He has also participated in a number of international and national conferences. Mr. Abed got married (Asma’a) in May, 2000, in Dubai, UAE, and he has currently a four year girl (Heba) and a two year boy (Bara’a).