Mesoscale simulation of grain boundary diffusion creep in the presence of grain growth

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MESOSCALE SIMULATION OF GRAIN BOUNDARY DIFFUSION
CREEP IN THE PRESENCE OF GRAIN GROWTH

A Thesis
Submitted to the Graduate Faculty of the
Louisiana State University and
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requirements for the degree of
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in
The Department of Mechanical Engineering

By
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To all who made this possible.
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ABSTRACT

Grain-boundary (GB) diffusion creep (Coble creep) is the dominant deformation mechanism for the fine-grained materials under low stress and at elevated temperature. During creep deformation the grains become elongated in the tensile direction because of atoms diffusion along GBs from places in compression to those in tension. Consequently, the GB diffusion rate depends on the normal stress gradient along the boundaries.

It is widely accepted that the GB migration generally plays two important roles during Coble creep: one leading to the decrease of the creep rate due to the increase of the grain size by GB migration mediated grain growth and the other one leading to the relaxation of the stress concentrations along the GBs and at the triple junctions.

In this study we use mesoscopic simulations to investigate the influence of the external stress and grain-boundary migration (static grain growth) on creep deformation of polycrystalline materials. Our simulation methodology is based on the variational principle of dissipated power and the simulation results reveal that the grains comprising the microstructure remain almost equiaxed during grain-boundary diffusion creep with accommodation by GB migration. In addition, the average grain size of the evolving microstructure is controlled by the interplay between the static and dynamic grain growth and depends strongly on both the externally applied stress and the strain.
CHAPTER 1 INTRODUCTION

1.1. General

“Creep” is the term given to the material deformation that occurs as a result of long term exposure to levels of stress that are below the yield or ultimate strength, often in combination with temperatures near its melting point (0.7-0.9 of the melting point). Based on the level of stress, there are two major types of creep deformations: dislocation creep and diffusional creep.

Depending on the temperature and the average grain size characterizing the microstructure diffusional creep can be also divided into two categories:

i) in the fine-grained materials the deformation occurs by the flow of atoms in the grain boundaries (GBs) separating the grains, and the deformation process is known as Coble creep. During Coble creep the strain rate is inverse proportional with \( d^3 \), where \( d \) is the average grain size [1].

ii) in the microstructures with larger grain sizes the atoms diffuse increasingly through the grain interiors and the deformation mechanisms is called Nabarro-Herring creep. During Nabarro-Herring creep the characteristic creep strain-rate is inverse proportional with \( d^2 \) [2, 3].

It is also important to notice that during diffusional creep the strain rate has a linear dependence on the externally applied stress, while during dislocation creep the strain-rate stress relationship becomes nonlinear. Due to its great relevance for various areas of engineering applications the creep phenomena has been investigated intensively over the last four decades. There are certain applications in which one would be interested in avoiding or diminishing the creep deformation. Such examples are: the collapse of the World Trade Center buildings which was credited in part to the creep of the steel structural elements, or, the turbine blades of jet engines in which the creep is minimized by making the blades from single crystals. However, in
other cases the creep deformations are useful, like in the super plasticity of fine grained metals and in metals and ceramics forming.

Stress-directed atomic diffusion in combination with GB sliding is widely recognized as the main deformation mechanism during high-temperature creep and superplastic deformation in polycrystalline materials. In general, to accommodate the continuous grain-shape change and to preserve the integrity of the material during Coble creep, accommodation processes such as GB sliding, GB migration or dislocation slip in the GBs may take place simultaneously. At an even larger grain size, a Newtonian viscous dislocation creep (known as Harper-Dorn creep [4]) may occur. Moreover, under increased applied stress, dislocation slip starts playing an increasingly important role. Given this complex interplay among various deformation processes, the dominant deformation mechanism is usually inferred from the experimentally observed power-law dependence of the strain rate as a function of stress and average grain size and compared with the exponents predicted from simple models.

During Coble creep, the atoms are transported along the GBs from regions in compression to regions in tension and the local GB diffusion flux is determined by the tensile or compressive normal-stress distribution along the boundaries and by the GB diffusivities. The macroscopic creep behavior of a polycrystal undergoing Coble creep is complex and generally governed by overall characteristics of the microstructure in which inhomogeneities play a significant role [5-10]. There are two important types of microstructural inhomogeneities: topological inhomogeneity arising from the distributions in the grain shape and grain size, and physical inhomogeneity associated with the distribution in the GB misorientations and GB-plane inclinations. These give rise to distributions in the GB energies and diffusivities, which are also strongly affected by segregation effects along the GBs. Because the lengths of the diffusion paths scale with the grain size, in order for all the grains to achieve comparable creep rates and thus to
maintain material integrity, microstructural inhomogeneity results in significantly larger normal stresses across the GBs delimiting the larger grains than those surrounding the smaller grains.

Given the inherent difficulty in measuring the stress distribution along the GBs in a polycrystal during deformation, there are no direct experimental results quantifying the relationship between microstructural inhomogeneity and GB stress distribution. However, theory and computer simulations on mostly two-dimensional models have provided valuable insights into the role of internal stresses on plastic deformation. Notable is the analytic work of Raj and Ashby [5] on diffusion-accommodated GB sliding, in which the normal-stress distribution along non-flat GBs was predicted. Later Schneibel et al. [6, 7] developed a theory for Coble creep in non-uniform grain structures to predict the stress distribution and the initial rate of movement of the GBs. This work was further extended by Ford et al. [8] who modeled the normal-stress distribution and deformation paths for different polycrystalline microstructures.

The Coble-creep equation for a polycrystal under uniaxial tension assumed to contain grains with uniform shape and size can be written as follows [8]:

\[ \dot{\varepsilon} = \beta \frac{\delta D_{GB} \Omega \sigma}{kTd^3}, \]  

(1.1)

where \( \dot{\varepsilon} \) is the strain rate, \( D_{GB} \) the GB diffusion coefficient, \( \delta \) the GB thickness, \( \Omega \) the atomic volume, \( \sigma \) the applied stress and \( k \) Boltzmann’s constant, \( T \) the absolute temperature and \( d \) the grain size. \( \beta \) is a geometrical constant that depends on the grain shape and grain-size distribution. For Coble’s idealized model of a single spherical grain, \( \beta = 18.84 \) [1]. If the spherical grain is considered as part of a microstructure, the width of the diffusion path \( \delta \) is replaced with \( 2\delta \) and \( \beta = (18.84/2) = 9.42 \). The functional form of the creep rate in Eq. (1.1) has been confirmed by Spingarn and Nix [11] for a space-filling, regular hexagonal microstructure, the only difference to Coble’s model being the magnitude of \( \beta (=36) \) for such a geometry.
Although the analytical models provide insight into the physics of creep deformation, they are too difficult to solve except for highly idealized geometries. This renders simulations as the most promising tool for the systematic investigation of the behavior of non-uniform microstructures. Two mesoscopic simulation approaches have been developed in recent years. Both discretize the microstructure by introducing nodal points along the GBs and at the triple junctions, thus describing the deformation in terms of the field of diffusional fluxes and node velocities. In the first method, pioneered by Hazzledine and Schneibel [7], the diffusional fluxes and node velocities are determined by solving a linear system of equations derived by explicitly imposing the simulation-cell border conditions, mass conservation and rate compatibility along each GB and triple junction. The second method, developed by Cocks et al. [9], uses a variational principle for dissipative systems to evolve the microstructure. Apart from being based on a fundamental physical principle governing the evolution of all dissipative systems, this approach has the advantage that any number of dissipative microstructural processes (in addition to, say, GB migration and GB sliding) can be incorporated into the general formalism.

In the present study we build on Cocks simulation methodology and try to depict more relevant characteristics of Coble creep deformation up to large tensile strains in the presence of diffusion accommodated GB sliding (with no sliding resistance) where the changes in grain shape and grain sizes occurs simultaneously due to dynamic grain growth (creep generated growth) and static grain growth (GB mediated growth). For this purpose we combine creep and the grain growth simulation in a single formalism based on the variational functional for dissipated power. The simulation of GB migration is implemented following the formalism of Weygand et al [12, 13].

The main objective of the present study is to investigate, using a mesoscopic simulation methodology, the deformation mechanisms and stress distributions in polycrystalline materials in
the presence of both GB migration and GB diffusional creep. Our studies allow us to compare the deformation behavior of polycrystalline materials with non-uniform microstructures with and without grain boundary migration present. The microstructural relaxation due to the presence of GB migration leads to a reduction of the GB stresses and can also contribute towards minimizing the overall length of the diffusion paths along the boundaries and/or to maximizing the GB sliding.

1.2. Objectives

The focus of the present work is to investigate the influence of the simultaneous presence of external stress and grain-boundary migration on creep deformation of polycrystalline materials. The specific objectives are to investigate:

a) the interplay between the microstructural characteristics (e.g. average grain size, grain boundary energy, GB mobility, etc.) and the external stress on the Coble creep deformation.

b) the effect of grain boundary migration on the strain rate during Coble creep deformation.

c) the effect of grain boundary migration on the overall stress distribution along GBs during Coble creep deformation.
CHAPTER 2 BACKGROUND

2.1. Overview of Creep Deformation

In many applications, the operating temperature is well above the room temperature and consequently when they are subjected to external stresses the materials experience straining. While at room temperature most metals and ceramics deform independent of time, at high temperatures the same materials experience plastic deformations that may increase in time [14]. This phenomenon is known in literature as “creep” and it has to be taken into consideration whenever a new system is designed, together with other materials properties, like fracture, yield, and fatigue or stress corrosion cracking. Obviously, the definition has to be narrowed because the terms “stress” and “temperature well above the room temperature” have significantly different values from one type of material to another. A widely accepted definition for creep is the following: Creep is the plastic deformation of a material that is subjected to a stress below its yield stress when that material is at a high homologous temperature. The homologous temperature is defined as the ratio of the material’s actual temperature to its melting temperature.

Creep deformation is present in both crystalline and non-crystalline solids. Moreover, it is known that during the creep, materials deform initially without formation of any cracks of voids. The capacity of plastic flow observed during creep is considered to be mediated by series of distinct physical mechanisms. Among these the most important are: the movement of dislocations, sliding at the grain boundaries and diffusional flow of atoms through the lattice and through the grain boundaries. Even if these three microstructural evolution mechanisms are considered to be independent, in practice often one process may be the accommodating process for another one. For example, it is known that the diffusional flow is the accommodating process for grain boundary sliding [15].
Usually the creep phenomenon is quantitatively described by the strain-time curve, also called creep curve. As shown in figure 2.1, creep can be subdivided into three categories: primary, secondary (or steady state), and tertiary creep.

Figure 2.1: Strain vs. Time Creep Behavior.

Normally, the creep curve starts with a region for which creep rate decreases with time. Primary creep strain is usually less than one percent of the sum of the elastic, steady state, and tertiary strains. The mechanism in the primary creep region is the climb of dislocations. The amount of initial strain of a material is caused by the initial dislocations present in the system and therefore the primary creep region is highly influenced by the history of the material. If the material had been heavily worked before the creep test, there would have been many more dislocations present and the characteristics of the primary creep region would have been much different. Also, one can note that the creep curves differ for metals and alloys. While the figure
2.1 is valid for most of the metals, the typical creep curves for alloys do not start with a primary creep regime.

The second portion of the typical strain-rate strain curve is the steady state portion. As the name itself suggests, the creep rate is almost constant in this region and has the minimum value. The increase in the strain is balanced by the recovery processes. All the creep properties of any materials are determined in this stage. During the third regime, the creep rate is larger than in the secondary creep and continues to increase exponentially till the material is fractured.

As mentioned above, creep is a plastic deformation process that occurs at temperatures well above half of the homologous temperature. Consequently, the increase in the level of the stress, or the temperature will increase the strain rate. This dependence is presented schematically in the Figure 2.2.

![Figure 2.2: Effects of temperature and stress on strain rate](image)

Depending on the type of applications, the creep might need to be avoided or enhanced. For example, the collapse of World Trade Center is credited in part to creep. Likewise the turbine blades of jet engines are made of single crystal in order to minimize or avoid the GB creep. In other situations the creep deformations are useful, like in the super plasticity of fine grained
metals and ceramics. In this case, one would like to deform the material as much as possible, using creep. It is therefore imperative in any design based on polycrystalline materials at elevated temperatures to take into consideration the creep effects and to choose accordingly both the actual materials and the microstructures.

2.2. Mechanisms of Creep Deformation

As mentioned previously, the creep can be divided, based on the level of stress, temperature and grain size into two major categories:

a) *dislocation creep*: characterized by a nonlinear strain rate stress relationship.

b) *diffusional creep*: that can be also subdivided into two groups (*note*: during diffusional creep the stress is much lower than during dislocation creep):

b.1 Coble Creep: the diffusion takes place only through the GBs and the strain rate is inverse proportional with \(d^3\), where \(d\) is the average grain size.

b.2 Nabarro-Herring Creep: the diffusion occurs through the bulk of the materials and the strain rate is inverse proportional with \(d^2\).

During diffusional creep the strain rate is proportional to the applied stress and the creep mechanism is controlled by both diffusion and GB sliding.

Dislocation creep is mediated by the nucleation and motion of dislocations. Dislocations are one-dimensional crystallographic defects within the crystal structure. Their presence highly affects the properties of materials and their movements (*slip*) through the material lattice accommodate the dislocation creep. The magnitude of the dislocation slip is characterized by the *Burger vector*. A dislocation moves in a slip plane along a slip direction. There are two major types of dislocations: *edge dislocation* and *screw dislocation*. In most crystalline materials, the majority of dislocations present are not pure edge or pure screw, but a mixture of these two
types. Figure 2.3 shows schematically the slip mechanism of an edge dislocation in a cubic lattice.

![Figure 2.3: Slip of an edge dislocation [16].](image)

The stress required to plastically deform a crystal is given by the stress necessary to move the dislocations along the various slip planes. Dislocation slip occurs by dislocation motion along the closest packed planes in the closest packed directions. Figure 2.4 shows schematically how a sequence of *climb-glide* movements can lead to creep deformation. The circle represents an obstacle (e.g. other dislocations, a defect or a precipitate particle) located on the glide plane of the dislocation. It is important to mention that the crystal lattice itself has an intrinsic resistance to a dislocation move.

![Figure 2.4: Creep generated by dislocations slip [14].](image)
The relationship between stress, $\sigma$, and strain rate $\dot{\varepsilon}$ is given by [15]:

$$
\dot{\varepsilon} = A \frac{D G b}{kT} \left( \frac{\sigma}{G} \right)^n,
$$

where $A$ is a parameter and a function of the characteristics of the microstructure, $D$ is the diffusion coefficient, $G$ is the shear modulus, $b$ is the Burger vector, $k$ is the Boltzmann’s constant, $T$ is the absolute temperature, and $n$ is the stress exponent (equal to $1/m$, where $m$ is the strain-rate-sensitivity).

The equation (2.1) can be rewritten in a similar form which includes the grain size dependence:

$$
\dot{\varepsilon} = A \frac{D G b b}{kT} \left( \frac{b}{d} \right)^p \left( \frac{\sigma}{G} \right)^n,
$$

where $d$ is the average grain size, and $A$ and $p$ are constants ($p$ is the grain size exponent). The expression given by equation (2.2) is known in the literature as power-law equation for plastic deformation and all the deformation mechanisms are described in terms of specific values of the various parameters entering in this equation. For example, the glide controlled dislocation creep is characterized by a stress exponent, $n$, that is equal to 3 whereas climb-controlled dislocation is characterized by a stress exponent $n$ equal to 4 or 5.

At high temperatures and relatively low stress levels, the deformation is due to diffusional transport of matter rather than dislocation motion. The diffusion process is started by a nonhydrostatic stress and atoms flows from compression sites to tension sites. For the diffusional creep, the value for $n$ in equation (2.2) is 1. If the diffusion takes place through the bulk of the material, the diffusional creep is called Nabarro-Herring creep. The mathematical expression (2.2) can be re-written as follows:
where $\Omega$ is the atomic volume, $D_L$ is the lattice self-diffusion coefficient and $\alpha$ is a factor that depends mainly upon the shape of the grains. The schematic representation of the Nabarro-Herring creep is presented in the figure 2.5. As we stated earlier, the controlling mechanism is vacancy diffusion or self-diffusion. If the diffusion takes place through GBs we have Coble creep deformation and the mathematical expression that relates strain rate with the stress and temperature can be written in a form similar to equation (2.2) and is given by equation (1.1) introduced in the previous section.

There are certain differences between Nabarro-Herring creep and Coble creep. First, the strain rate is inverse proportional with the square of the average grain size $d$ for Nabarro-Herring creep and with cubic of $d$, for Coble creep. This means that Coble creep has a stronger dependence on the grain size. And also, the activation energy required by diffusion trough the GBs is lower than the activation required by the diffusion trough the bulk. In addition, from the mathematical expressions (2.3) and (1.1), because $d$ appears at denominator, we can conclude that diffusional creep is much more evident in fine-grained materials.

![Figure 2.5: Schematic representation of Nabarro-Herring creep.](image)
Figure 2.6: Schematic representation of diffusional creep [15].

The diffusional flow through the GBs (Coble) was first modeled using a core and mantle mode, introduced by Gifkins [17]. This model started from experimental observation that at high temperatures the grains of a material are composed from two distinct regions, a solid core and a mantle (figure 2.7). In addition, in order to keep the grains connected during the plastic deformation this process has to be accommodated by GBs sliding. However, it is hard to separate the contributions of each process (GBs sliding and diffusional flow) and to conclude exactly which part of the total strain is produced by each process.

Figure 2.7: The core mantle model [1].
Since different creep mechanisms are dominant under various conditions and because we do not want creep in some applications or creep is desired in other applications, it is very useful to have all the deformation mechanisms summarized in a diagram. These diagrams are very common and they typically look like those presented in the figures 2.8 and 2.9.

2.3. **Grain Growth**

Grain growth is the process which takes place during the annealing of polycrystalline materials; its major feature is a systematic increase in grain size. The significance of this process comes from the profound influences of the grain size and grain-size distribution on a wide range of properties of polycrystalline materials. Grain size is a key parameter in sintered ceramic, metal and alloy microstructures and usually has to be controlled during thermo mechanical processing in order to ensure optimization of mechanical properties.

Most of the theoretical studies of grain growth in polycrystalline materials are based on soap-froth models (i.e., model with uniform GB energies and mobilities) which are considered to evolve by a similar mechanism to that which governs grain growth in metals and sintered
ceramics: the reduction of the surface energy of the network, subject to topological constraints of space-filling. In the soap-froth framework, von Neumann (1952) [18] derived the key equation,

$$\frac{dA_n}{dt} = \frac{\pi \gamma m}{3} (n - 6)$$  \hspace{1cm} (2.4)

relating the rate of area change of a grain to its number of sides, $n$, and to the product of the GB energy $\gamma$ and mobility $m$. Equation (2.4), known as the von Neumann-Mullins (VNM) relation, allows a simplified description of a coarsening network in an isotropic system in terms of only two variables: the area, $A_n$, and the topological class, $n$, i.e., number of sides, of each grain.

All GBs in the soap-froth model of a polycrystalline microstructure have the same GB energy $\gamma$. Grain growth takes place by curvature-driven GB migration, resulting in the larger grains growing at the expense of the smaller grains. Burke and Turnbull [19] used a mean-field approach to grain growth to deduce the relationship $A(t) \sim t$ for the growth kinetics. They assumed that the surface-curvature force acts on isolated GB segments surrounding a typical grain, each moving towards its centre of curvature with a velocity

$$v = \frac{m \gamma}{r}$$  \hspace{1cm} (2.5)

where $p = \gamma/r$ is the driving force, $r$ is the mean curvature of the GB segment and $m$ is the GB mobility. Within this framework, assuming that the radius of curvature of each GB segment is proportional to the average grain radius $<R>$, the rate of change of $<R>$ is given by

$$\frac{d < R >}{dt} = k_1 \frac{\gamma m}{<R>}$$  \hspace{1cm} (2.6)

where $k_1$ is a geometric constant. Since in the soap-froth framework both $\gamma$ and $m$ are constant, equation (2.6) can be integrated directly and the time dependence of the average grain size is obtained:

$$<R>^2 - <R_0>^2 = Kt$$  \hspace{1cm} (2.7)
Here \( K = k_1 \gamma m \) is a new constant and \( <R_0> \) is the initial mean grain size. This is the well-known parabolic growth law which if written in terms of the average grain area, \( A \), and in the limit where \( <R> >> <R_0> \) reads

\[
A(t) = K t^n ,
\]
with \( n=1 \) as the growth exponent. The model proposed by Burke and Turnbull [19], although based on some very simplified assumptions, correctly predicts the growth exponent. More sophisticated and rigorous approaches to the grain-growth problem were developed later by Feltham [20], Hillert [21] and Louat [22]. Interestingly, although these models are based on quite different physical assumptions, they predict the same growth exponent of \( n=1 \).

As mentioned previously the importance of understanding the grain growth phenomena is due to the fact grain growth can affect strongly the microstructural characteristics such as grain size and grain size distribution which in turn affects strongly a whole range of properties of materials. One such property is the mechanical strength of a material. For example at low temperatures, most polycrystalline materials follow the Hall-Petch relationship, which relates the yield strength, \( \sigma_y \), to the average grain size \( d \), and is given by:

\[
\sigma_y = \sigma_0 + \frac{k_y}{\sqrt{d}} ,
\]

where \( k_y \) and \( \sigma_0 \) are materials constant for fitting parameter and starting stress for dislocation movement. At high temperatures, because the vacancies diffuse more rapidly down grain boundaries, the increase in the Coble creep is present. That is, one should consider the presence of grain growth when studying the Coble creep. In other words, as a general rule one can say that decreasing the grain size increases the strength at low temperatures while it decreases the strength at high temperatures.
Over the years many studies were focused on the grain growth phenomenon and a general set of rules was developed and summarized by Burke and Turnbull [19]. These rules are:

1. Grain growth is always mediated by grain boundary migration and not by the coalescence of neighboring grains, like water droplets do.
2. Grain boundary migration is not continuous and its direction may suddenly change.
3. One grain may grow into a neighboring grain on one side while it is being consumed from another side.
4. The rate of consumption of a grain frequently becomes more rapid as the grain is about to disappear.
5. A curved grain boundary usually migrates towards its center of curvature.
6. When grain boundaries in a single phase meet at angles other than 120 degrees, the grain included by the more acute angle will be consumed so that the angles approach 120 degrees.

Even if the grain growth occurs in any polycrystalline material, it is better observed in the annealing process of the cold worked materials. Annealing process is in fact a special heat treatment (the material is kept at high temperature for a long time and then it is cooled slowly) done in order to change the microstructure of a material. That is to change materials properties such as hardness or yield strength. Basically, this process can be subdivided into 3 phases:

1. *recovery*: during this stage, the internal stresses created due to cold-working are reduced or eliminated. There are no severe changes in the microstructure, that is the hardness or the strength are not affected very much. Even if the internal stresses are relaxed as the temperature increases, there is still an elastic deformation due to different orientations for different grains.
2. *recrystallization*: in this stage, the highly distorted structure is transformed again into a strain free structure. The driving force for recrystallization stage is the stored energy from the cold working, primarily due to the high density of dislocations. Minute crystals start to nucleate and the newly formed grains are quite small, having nucleated at sites where the local strain energies were greatest. However, once formed they can grow. It is important to mention that this process is irreversible and the distorted structure cannot be recreated anymore. The recrystallization rate in time follows the Avrami equation of any process driven by nucleation and growth [23] (figure 2.10).

![Figure 2.10: Variation of recrystallised volume fraction with time [23]](image)

3. *grain growth*: is the next stage after recrystallization and it occurs because the structure previously formed is not stable, with a large amount of energy still stored in the grain boundaries. The reduction of this energy is the driving force for the grain growth, the internal pressure into the crystal being at least two times lower at the start of the grain growth process than immediately after recrystallization (~$10^{-2}$ MPa). There are two types of grain growth: *normal grain growth* and *abnormal grain growth*.

The main difference between these two types of grain growth is given by the way in which the microstructure evolves from a state A to a state B: continuous or discontinuous. During the
normal grain growth, all the grains grow at approximately the same rate and the grain size distribution follows a log-normal plot. It is important to mention also that grains shape is independent of time, only mean radius is affected by time. In this case growth is driven only by the reduction of the total amount of grain boundary surface energy. Contributions of elastic strains, chemical and temperature gradients, etc. are neglected.

In the abnormal grain growth, the process of grow is discontinuous, because of the inhomogeneities present in the system which may lead in the end to individual grains that are much larger than the others. Because the kinetics of the abnormal grain growth is similar with the kinetics of the recrystallization, this process is called also *secondary recrystallization*. Experiments have shown that very often the grain growth is abnormal, especially in thin films where surface tensions are a key factor that influence abnormal grain growth. In addition, experiments also have shown that in some cases when the materials have second-phase particles, the abnormal grain growth is present.

![Continuous and Discontinuous Grain Growth](image)

*Figure 2.11: Normal (continuous) and abnormal grain growth*
CHAPTER 3 SIMULATION METHODOLOGY

3.1. Modeling and Simulation in Materials Science

The use of computational methods in materials science has experienced tremendous growth over the last two decades. There are certain advantages derived from this: combined with experimental observations, these techniques can help the researchers to explain some physical phenomenon and to predict the behavior of materials under given conditions. In addition, computer simulations can cut the costs required for expensive experiments, by complete inclusions of new processes and designs. But, there are also disadvantages. The main one is that even if the power of calculus is very high today comparing with 10 years ago, a gap between the real phenomenon and what simulations can model is still large.

As in any other field of sciences, modeling and simulation in materials science is based on well established general steps that one has to follow; these include:

(a) define the proper model to describe the physical system be investigated; this can be achieved by proposing a new model, by using a previous proposed model or a combination of two or more models;

(b) use the proper simulation tools (computer programs), either professional or academic, to run the simulations;

(c) define benchmark problems that would allow comparison of the simulation results with experimental results, therefore conferring credibility of the both the model and the simulation program.

Studying creep phenomena via computer simulation is also facilitated by the fact that there is a natural discretization into grains of the physical system considered. In this chapter we will
address issues such as: “what model to be used?”, “how to make the computer program as general and as portable as possible?” or “how to refine the program using experimental results”.

3.2. Creep Simulation Models

The scientific literature shows that there have been many studies over the last three decades aiming the development of creep models that are capable of predicting both the mechanical and topological features of superplastic deformation. However, despite the significant progress in this area there still is a multitude of unresolved issues. As presented in the previous chapters, one of the first proposed models aimed of explaining creep deformation is that of Gifkins [17]. According to Gifkins model the grains comprising the microstructure are composed of two regions: the grain core and the surrounding, a thin grain mantle. In addition Gifkins model assumes that the hard core is not deforming during the creep and the flow occurs only in the mantle. Another creep model was introduced by Ashby and Verrall [24]. This is based on experimental observations and assumes that during deformation the grains shapes are preserved and creep deformation can be modeled by a “grain switching” mechanism (figure 3.1).

![Figure 3.1: Grain switching in Ashby and Verrall model.](image-url)
Analytical derivations based on Ashby-Verrall models yields the following strain rate stress relationship:

\[
\dot{\varepsilon} = \left( \frac{100\Omega}{kTd^2} \right) \left( \sigma - 0.72 \frac{\gamma}{d} \right) D_L \left( 1 + \frac{3.3\delta D_{gb}}{dD_L} \right),
\]

where \( d \) is the average grain diameter, \( D \) represents diffusivities of GBs and lattice, \( \delta' \) is the width of diffusion zone, \( \Omega \) is the atomic volume and \( \gamma \) is the GB free energy. In addition to these two models, analytical results were calculated for an ideal structure formed only from identical hexagonal grains [11]. These calculations are used in the literature as a validation of any new model proposed by different researchers. The major problem of all these models is that all the topological rearrangements are not explained by physical processes but just assumed to take place.

To address this problem, new models were developed by Hazzledine and Schneibel [6-7, 25-26], respectively Cocks and Pan [27-32]. We will present much more detailed the Cocks model in the next paragraph, because this model is used in the present work. The model introduced by Hazzledine et al. takes into consideration the fact that in reality, a polycrystal has different grains, with different shapes. Starting with the assumption that the grains are rigid, GBs does not support shear stresses and the matter is conserved, they developed a model to solve the Coble creep problem for irregular, two-dimensional structures with straight GBs connected by triple points. Using this model, they also determined the stress distribution and the sliding rate. Further calculations were made for particular shapes of GBs (i.e. sinusoidal).

This model is one of the first which tried to study the effect of grains distribution and grain size over the creep. Even if this model has very good results for small structures because it does not contain any approximations and it is in perfectly concordance with the analytical models, it is
very hard to be implemented for big structures because of the high number of the equations that has to be solved for each GB.

### 3.3 Cocks Model

In this model [29], a finite element method is used to analyze the GBs diffusion, based on the variational principle introduced for the first time by Needleman and Rice [33]. According with this approach, an element is represented by the length of a GB and its degree of freedom are related to translation and rotation of the grains, the flux of vacancies across the centre line of the boundary and the chemical potential where the GB links with other GBs. The main advantage of this model is that it is capable to offer an exact solution for the stresses and relative velocities of each grain. The model was first developed assuming that all grains have an equilibrium hexagonal shape. Later on, Cocks and Pan [34] extended the analysis to a two-dimensional microstructure in which the grains can have any type of shape and any size and used a numerical technique to solve the equations that govern the diffusion process at each time step. Before explaining the equations which describe the model, it is important to mention also that few more assumptions were done: the grains were considered to satisfy the core and mantle model (that is, the diffusion takes place only through GBs), no voids or cracks are present along GBs, there is no resistance to sliding of GBs and the GBs are straight.

Atoms diffuse along GBs because the gradient in the stress, $\sigma$ induces a gradient in the chemical potential, $\mu$:

$$\mu = \mu_0 - \sigma \Omega, \quad (3.2)$$

where $\mu_0$ is the initial chemical potential (in the stress-free state) and $\Omega$ is the atomic volume.

Based on the Fick’s first law, the volumetric diffusional flux of atoms passing a unit length along the GBs can be expressed in the following way [16]:

$$\mu = \mu_0 - \sigma \Omega, \quad (3.2)$$

where $\mu_0$ is the initial chemical potential (in the stress-free state) and $\Omega$ is the atomic volume.
\[
J = - \frac{D_{GB} \delta_{GB}}{kT} \frac{\partial \mu}{\partial s} = \frac{D_{GB} \delta_{GB}}{kT} \frac{\partial \sigma_n}{\partial s}, \tag{3.3}
\]

where \(D_{GB}\) represents the diffusivity coefficient of the GB, \(\delta_{GB}\) is the GB thickness, \(k\) is the Boltzmann’s constant, \(T\) is the absolute temperature, \(\sigma_n\) is the normal stress on the GB and \(s\) is the coordinate along the GB.

If the atoms are deposited on the GB, the adjacent grains are forced to move apart with the velocity \(v_n\). Because the matter has to be conserved during this process, one can write the following relation:

\[
\frac{\partial J}{\partial s} + v_n = 0, \tag{3.4}
\]

From (3) and (4):

\[
v_n = - \frac{D_{GB} \delta_{GB}}{kT} \frac{\partial^2 \sigma_n}{\partial s^2}, \tag{3.5}
\]

In addition, because of the same rule of matter conservation and because we assumed that no cracks or voids appear into the GB, at each junction of the body the following relation must be satisfied:

\[
\sum_{\text{rays}} J = 0, \tag{3.6}
\]

For the GBs that intersect the free surface, the continuity of potential force \(\sigma_n\) to have the following value:

\[
\sigma_n = \gamma_s k = \sigma_c, \tag{3.7}
\]

where \(\gamma_s\) is the surface energy per unit area and \(k\) is the radius of curvature at the point of intersection with the GB.
All these equations from (2) to (7) describe the evolution of the microstructure during the Creep deformation. Cocks demonstrated that the solution of this set of equations is given by a set of velocities and fluxes that minimize the following functional:

$$\Pi = \int_{S_{\text{GB}}} \frac{kT}{2D_{\text{GB}}\delta_{\text{GB}}\Omega} jj ds - \sum_{\text{apexes}} T_{\alpha} V_{\alpha} dS + \sum_{\text{vertices}} \sigma_{\alpha} j^\alpha + \sum_{\text{rays}} (\lambda_{\alpha} \sum J)$$, \hspace{1cm} (3.8)

where $s_{\text{GB}}$ is the total length of the GBs, $S$ is the specimen length, $T_{\alpha}$ is the external traction, $V_{\alpha}$ is the velocity, $\lambda_{\alpha}$ is a Lagrange multiplier for each GBs (it is simply to consider it as the normal component of the stress at each boundary junction).

Considering suitable values for $d_0$ (average grain size) and $\sigma_0$ (average stress), one can write the following normalized relations:

$$\bar{\Sigma}_{\text{GB}} = \frac{s_{\text{GB}}}{d}, \bar{S} = \frac{S}{d}, \bar{T}_{\alpha} = \frac{T_{\alpha}}{\sigma_0}, \bar{V}_{\alpha} = \frac{V_{\alpha}}{\dot{\epsilon}_0 d}, \bar{J} = \frac{J}{\dot{\epsilon}_0 d^2}, \bar{\sigma}_{\alpha} = \frac{\sigma_{\alpha}}{\sigma_0}, \bar{\lambda}_{\alpha} = \frac{\lambda_{\alpha}}{\sigma_0}$$, \hspace{1cm} (3.9)

where

$$\dot{\epsilon}_0 = \frac{D_{\text{GB}}\delta_{\text{GB}}\Omega\sigma_0}{kT d^3}$$, \hspace{1cm} (3.10)

Then, the functional can be re-written as follows:

$$\bar{\Pi} = \frac{1}{2} \int_{S_{\text{GB}}} \bar{J} \times \bar{J} ds - \int_{S} \bar{T}_{\alpha} \bar{V}_{\alpha} dS + \sum_{\text{apexes}} \bar{\sigma}_{\alpha} \bar{J}^\alpha + \sum_{\text{vertices}} \bar{\lambda}_{\alpha} \sum \bar{J}$$, \hspace{1cm} (3.11)

Let’s consider now a particular situation: a GB between two grains, which has one end into a void and the other end into a triple junction (Figure 3.2).

When the amount of the material into the GB changes, the grains move apart with a relative velocity $\bar{v}_{\alpha}$. Because the grains are considered to be rigid, this velocity is directly related with the velocities of the grain centers:

$$\bar{v}_{\alpha} = \left[ B_0^\alpha \right] \left[ \bar{U}_0^\alpha \right]$$, \hspace{1cm} (3.12)
where \( B_0^e \) and \( \bar{U}_0^e \) represents the translational a rotational components of the velocities.

Using a similar approach, the functional can be re-written one more time:

\[
\Pi = \frac{1}{2} \sum_e \left[ U^e \right]^T K^e \left[ U^e \right] + \sum_{en} \left[ \lambda_{en} \right]^T C^{en} \left[ \bar{U}^{en} \right] + \sum_{ev} \left[ \sigma_{ev} \right]^T C^{ev} \left[ \bar{U}^{ev} \right] \cdot \left[ F \right] \left[ \bar{V} \right] \quad (3.13)
\]

where \( e \) represents the GB elements, \( en \) represents the GB which is not terminated by any void or crack, \( \left[ F \right] \) is the traction matrix, \( \left[ \bar{V} \right] \) is the boundary velocity matrix which can be related to the velocities at the centre of the grains adjacent to the specimen boundary.
As we mentioned before, the solution that we are looking for can be obtained by minimizing the functional:

$$\partial \Pi = 0$$ \hspace{1cm} (3.14)

This leads to a general matricial equation (a set of linear equations):

$$[G][U] = [F] - [C_v] [\Sigma_c]$$ \hspace{1cm} (3.15)

where $[G]$ is the generalized stiffness matrix, $[U]$ is the global matrix of degrees of freedom, $[F]$ is the external force matrix, $[C_v]$ is the matrix of constraints and $[\Sigma_c]$ is the matrix of capillarity stresses.

### 3.4. Grain Growth Simulation Models

Because of the importance of the grain growth over the internal microstructure and, in the end, over the material properties, many analytical studies tried to adequately describe grain growth kinetics. Even if these works started with more than 50 years ago and certain progresses were done, the complexity of the problem (the problem of grain growth implies not only the analysis of the kinetics of boundary energies and mobilities, but also the effect of impurities, anisotropic boundary energies and mobilities and second phase particles, and also the topological features), the main tool for investigating the phenomena of grain growth and abnormal grain growth has become computer models. Thus, each grain with its associated crystal orientation and each grain boundary with its associated five degrees of crystallographic freedom can be modeled.

In addition, if the physics behind the process is known, the evolution of the grain growth in time can be simulated.

The models that have been developed during the last 30 years can be divided into three big categories:

a) vertex models;
b) *phase field models*;

c) *Monte Carlo (MC) models*.

All the models can be also divided into two major classes, based on the nature of the procedure used for modeling:

a) *stochastic models (or Potts Models)*: are very simply to implement, but there is an uncertainty introduced in the analysis by the fact that the system definition and evolution is done not at an atomistic level; even if the relation between the probabilistic and physical phenomena is not clear, the method is sufficiently refined in order to produce acceptable results in some cases.

b) *deterministic models*: even if these models are very complex and requires a very large power of calculus, especially for the 3D case, the main advantage is that the kinetic behavior of each element in the microstructure can be introduced and analyzed.

It is important to mention that other types of models of grain growth still exists, such as those based on the finite element method.

One has to choose the model that will be used to study a particular case of grain growth based on the constraints and the limitations of the model. The model used in this work is a vertex model introduced by Kawasaki et al. [35] and further developed by Weygand et al. [12-13].

### 3.5. Kawasaki Model

In a vertex models (Figure 3.3), which is sometimes called front tracking model, grain boundaries are treated as continuous interfaces whose migration velocity $v$ is calculated in a deterministic way.

Simulations showed good agreement with theory both in terms of scaling and the parabolic growth law for the case of 2D isotropic grain growth. The move to 3D is computationally challenging since the grain boundaries must be represented by tessellated surfaces, and the
number of possible topological reactions becomes large [36]. The present work is focused on the 2D case.

![2D vertex model](image)

Figure 3.3: 2D vertex model

The entire grain structure is described by the positions of the vertices (either real or virtual, if the GBs are discretized), \( \{r\} \) and their velocities, \( \{v\} \). The entire structure has also associated a potential term \( V(r) \) which describes the total surface energy and a dissipative term \( R(\{r\},\{v\}) \) which describes the dissipation produced by the GBs movement.

\[
V(\{r\}) = \int_{GBs} \gamma(a) da , \quad (3.16)
\]

\[
R(\{r\},\{v\}) = \frac{1}{2} \int_{GBs} \frac{v(a)^2}{m_{GB}(a)} da , \quad (3.17)
\]

where \( a \) is the curvilinear coordinate along the GB, \( \gamma(a) \) is the GB energy at the position \( a \), \( v(a) \) is the normal velocity of the GB and \( m_{GB} \) is the GB mobility.
Equations (17) and (18) can be transformed into sums over the entire number of the vertices in the system.

\[
V(\{r_n\}) = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=i}^{(i)} \gamma_{ij} \|r_{ij}\|, \quad (3.18)
\]

and

\[
R(\{r_n\}, \{v_n\}) = \frac{1}{6} \sum_{i=1}^{N} \sum_{j} \left[ \frac{\|v_{ij}\|}{m_{ij}} \left[ (v_i n_{ij})^2 + (v_j n_{ij})^2 + (v_i n_{ij})(v_j n_{ij}) \right] \right], \quad (3.19)
\]

where \(ij\) is a given segment defined by two vertices with the position vectors \(r_i\) and \(r_j\), with the mobility \(m_{ij}\), the energy \(\gamma_{ij}\), and the velocities \(v_i\) and \(v_j\). The normal to the vector \(r_{ij}\) is a vector denoted by \(n_{ij}\), and the \(\|r_{ij}\|\) represents the length of the segment \(ij\). \(j\) in the second sum goes over all the vertices connected to the vertex \(i\).

![Figure 3.4: Schematic representation of a vertice ij](image)

The equations of movement are derived from the Lagrange function, with a dissipative term and without kinetic energy term:

\[
\frac{\partial R(\{r_n\}, \{v_n\})}{\partial v_i} + \frac{\partial v(\{r_n\})}{\partial r_i} = 0, \quad (3.20)
\]
Combining the equations (3.18), (3.19) and (3.20), one can write the general matricial equation:

\[ D_i v_i = f_i - \frac{1}{2} \sum_{j}^{(i)} D_{ij} v_j \text{, for } i=1,...,N \tag{3.21} \]

The terms involved in the equation (3.21) are given by the following relations:

\[ D_{ij} = \frac{1}{3m_{ij}r_{ij}} \begin{bmatrix} y_{ij}^2 & -x_{ij}y_{ij} \\ -x_{ij}y_{ij} & x_{ij}^2 \end{bmatrix}, \tag{3.22} \]

\[ D_i = \sum_{j}^{(i)} D_{ij}, \tag{3.23} \]

\[ f_i = -\frac{\partial V}{\partial r_i} = -\sum_{j}^{(i)} \gamma_{ij} \frac{r_{ij}}{r_{ij}} \tag{3.24} \]

In words, one can say that the implementation of the Kawasaki model has only two big steps:

a) given all the positions, GBs mobilities and energies, calculate all the constants from the relations (3.23), (3.24), (3.25);

b) solve the equation (3.22) for the new set of velocities.

### 3.6. Implementation of the Creep and Grain Growth Models

The both models, Cocks and Kawasaki, refers to a mesoscale approach of the problem of creep and grain growth. “Mesoscale” is a generic name given to an intermediate scale between the engineering scale and atomistic/molecular scale. Although today the power of calculus is very high, it is still very hard to create models using very small and numerous fundamental units, such as atoms or molecules (Figure 3.5).

In studying the creep and the grain growth, there is an advantage given by the nature: the polycrystal that has to be analyzed is already discretized into grains. As we already presented in the previous paragraphs, acceptable models can be defined and used for the simulations at this scale. The core and mantle model for grains is accepted, and a set of linear equations which
describes the evolution of the microstructure in time, in the presence of GB diffusion and GB migration was developed.

But, in addition to this, the actual implementation of the model has to address also other problems, such as: time step, topological changes, or the periodic boundary conditions.

3.6.1. Topological Transformations

During the grain boundary diffusion and grain boundary migration, the microstructure suffers topological transformations (Figure 3.6). If the GBs are considered to be straight lines, that are there are no virtual vertices, only two topological transformations can occur:

a) $T1$ process: recombination of triple points;

b) $T2$ process: annihilation of three sided grains of small area.

In the presence of virtual vertices, one more topological transformation has to be considered: $T3$ process, which is equivalent with the elimination of a grain with two triple points.

In the Figure 3.6 are schematically presented some topological transformations. “$\Delta$” represents the critical length under which the topological transformation has to be considered. Figure 3.6. (e) presents how the $T2$ process can be the result of a sequence of two processes, $T1$ process and $T2$ process.
3.6.2. Critical Length

Critical length, $\Delta$, represents the minimum distance below which two virtual vertices has to be replaced by a real vertex [39].

\[
\Delta = \frac{\alpha}{n_{\text{virtual}} + 1} < r > ,
\]

(3.25)

where $n_{\text{virtual}}$ is the number of virtual vertices between two triple points, and $\alpha$ is a simulation parameter.
< r > = \left[ \frac{2 A_{\text{total}}}{n_{\text{real}}} \right]^{1/2}, \quad (3.26)

where $A_{\text{total}}$ is the total area of the microstructure and $n_{\text{real}}$ is the total number of the triple points in the system.

### 3.6.3. Time Step

Time step is a very important parameter during the simulation. It has to be chosen such that the matricial equations can be solved (the minimum value) and no significant changes in the GBs can occur (the maximum value), that is the GB cannot modify more than a given fraction during a time step.

### 3.7. Dimensional Analysis of Characteristic Length and Time Scales

In both Coble creep and grain-growth simulations, in which the deformation or the growth occurs solely by only one mechanism (either GB diffusion or curvature-driven GB migration respectively), there is no absolute length or time scale determining the characteristics of the overall microstructural evolution. That is, if one carries on the creep or grain-growth simulation at a particular grain size it can easily extrapolate the results to a microstructure of any grain size. Typically in these single-mechanism microstructure evolution simulations the model and the corresponding codes are written and analyzed in dimensionless forms. However, as presented in this section, the simultaneous presence of both GB diffusion and GB migration introduces both physical length scales and a time scales into the system. Next, based on a dimensional analysis, we show how the various system parameters can affect the interplay between the GB diffusion and GB migration on the overall microstructure evolution mechanism.

When two or more different mechanisms are simultaneously present and are contributing to the overall evolution of the system the choice for dimensionless parameterization is not unique. For our particular problem the decision on how to set up the dimensional analysis is based on the
fact that the two physical mechanisms (GB diffusional creep and GB migration) are just loosely coupled on short time scale. Namely, if one analyses the system evolution in the presence of only one evolution mechanism, either curvature driven GB migration leading to grain growth or GB diffusional creep leading to microstructure straining one can see that each of them is characterized by a typical time scale. For example, the typical time scale, $t_{\text{diff}}$, for diffusional creep deformation can be taken as the time it takes to deform the system by, say 100%. Similarly the evolution in the curvature driven grain growth can be characterized by the time, $t_{\text{mig}}$ necessary for the system to double the average grain size.

Apart from the case when the two characteristic time scales are comparable in magnitude one can easily infer the evolution of the system in the presence of both mechanisms by simply referring to single mechanism systems. For example if $t_{\text{diff}} \gg t_{\text{mig}}$ then dominant evolution mechanism in the system is the curvature driven grain growth. Likewise when $t_{\text{mig}} \gg t_{\text{diff}}$ the GB diffusional creep dominates. The interesting case occurs when both mechanisms compete on equal footing, meaning during the same time scale we have sizable contributions from both curvature-driven GG and diffusional creep deformation.

Another way of analyzing the interplay between creep and grain growth phenomena is to compare the effective driving forces for the two processes. These are the externally applied stress, $\sigma$, for the creep and the average GB pressure (stress) for the GB migration mediated grain growth. As shown in section 2.3 (equation 2.5) the GB stress is given by $\gamma/d$ where $\gamma$ is the GB energy and $d$ is the average grain size. It is therefore expected that the relationship between these two driving forces to determine the overall evolution of the microstructure. That is, for $\sigma \gg \gamma/d$ the overall microstructural evolution will be controlled by creep whereas for $\sigma \ll \gamma/d$ the grain growth will determine the overall evolution.
In general the interdependence between the material (GB mobility, GB diffusivity, GB energy, GB width, atomic volume, etc.), microstructural (average grain size), and external parameters (external stress, temperature) is very complex and difficult to analyze by direct analysis. Dimensional analysis may therefore help de-convoluting the interdependence of various physical parameters and may give additional physical insights into the interplay between them.

Since our modeling approach of both creep and grain growth is based on the variational dissipated power functional we will formulate and expand the dimensional analysis around the variational functional. In the global functional there are two terms that account for the dissipation, one due to GB diffusion and one due to GB migration. In addition one identifies two terms that constitute the driving forces, one from the shortening of the GBs and one due to the work done by the external forces acting on the border of the simulation box (external stress). In addition we have enforced the mass conservation at the triple junctions (TJ) by introducing one Lagrange multiplier for each TJ.

Using equations (3.8), (3.16) and (3.17), without mentioning explicitly the degrees of freedom, the global variational functional reads:

\[
\Pi = \int_{\Omega} \frac{kT}{2D_{GB}} j^2 ds - \int_{\Gamma} \tilde{T} \cdot \vec{V} dS + \int_{\Gamma} \frac{1}{2m} v_n^2 ds + \sum_{GBs} \gamma \frac{\partial v_s}{\partial s} ds + \sum_{TJs} \lambda_i \sum_{rays} j , \quad (3.27)
\]

Here \(\tilde{T}\) - is the force per unit length acting along the boundary of the simulation box, i.e. the stress \(\sigma\) in our simulation system (in a two dimensional problem); \(m\) – is GB mobility; \(\gamma\) – is GB energy; \(v_n\) – the velocity component normal a GB segment; \(v_s\) - the velocity component tangential to a GB segment; \(s\)- is the length of a GB segment.
To frame the variational dissipated power functional, \( \Pi \), into dimensionless form we may choose, in addition to the reduce units introduced in section 3.3 (equation 3.9), to express: GB energy, \( \gamma \), in units of \( \gamma_0 \), the typical GB energy; the GB mobility \( m \) in units of \( m_0 \) the typical GB mobility; the functional \( \Pi \) in units of \( \Pi_0 = \gamma_0 d_0 \dot{\gamma}_0 \) and the time \( t \) in units of \( t_0 = 1/\dot{\gamma}_0 \) where \( \dot{\gamma}_0 \) is given by (see equation 3.9):

\[
\dot{\gamma}_0 = \frac{D_{GB} \Omega}{kT d_0} \sigma_0 .
\]  

(3.28)

That is, we have the additional dimensionless quantities:

\[
\bar{\gamma} = \frac{\gamma}{\gamma_0} ; \quad \bar{m} = \frac{m}{m_0} ; \quad \bar{t} = \frac{t}{\dot{\gamma}_0} ; \quad \bar{\Pi} = \frac{\Pi}{\dot{\gamma}_0 \gamma_0 d_0}
\]  

(3.29)

Using the normalized physical quantities given by equations (3.9) and (3.29) in equation (3.27) the reduced units variational functional becomes:

\[
\bar{\Pi} = \frac{\Pi}{\dot{\gamma}_0 \gamma_0 d_0} = \int_{\Gamma_{GB}} \frac{1}{2} \bar{J}^2 d\bar{s} - \int_{\Gamma} \bar{T} \cdot \bar{V} d\bar{S} + \sum_{\xi_{GB}} \bar{\lambda}_i \sum_{\text{rays}} J_i + \zeta \sum_{\text{GBs}} \int_{\Gamma_{GB}} \bar{\gamma} \frac{\bar{\nabla} S}{\bar{\nabla} \bar{S}} d\bar{s} + \eta \int_{\Gamma_{GB}} \frac{1}{2 \bar{m}} \bar{V}_{\text{a}2} d\bar{s} ,
\]  

(3.29)

where we have introduced two dimensionless parameters \( \zeta \) and \( \eta \) given by:

\[
\zeta = \frac{\gamma_0}{\sigma_0 d_0} = \frac{(\gamma_0/d_0)}{\sigma_0}
\]  

(3.30)

and

\[
\eta = \frac{\dot{\gamma}_0 d_0}{m_0 \sigma_0} = \frac{D_{GB} \Omega \delta}{m_0 kT} \frac{1}{d_0^2} = \frac{1}{m_0 \gamma_0} \left( \frac{d_0^2}{\dot{\gamma}_0} \right) = \zeta \frac{t_{\text{migr}}}{t_{\text{creep}}} ,
\]  

(3.31)

In equation (3.30) the dimensionless parameter, \( \zeta \), represents the ratio between the typical GB pressure (stress) on a grain of average size \( d_0 \) and the typical value of the externally applied
stress $\sigma_0$. It therefore characterizes the interplay between the driving forces for the two microstructure evolution phenomena present simultaneously in the system.

The second characteristic dimensionless parameter $\eta$ characterizes the time response of the two physical phenomena present and it can be expressed as the ratio of two characteristic time scales. In equation (3.31),

$$t_{\text{migr}} = \frac{d_0^2}{m_0 \gamma_0},$$  \hspace{1cm} (3.32)

defines a characteristic time for curvature-driven grain growth, and it represents the time over which a certain fraction of grains have disappeared during grain growth while the average grain size has increases by an amount of the order of $d_0$ (let’s say the grain size has doubled).

Moreover,

$$t_{\text{creep}} = \frac{1}{\dot{\varepsilon}_0},$$  \hspace{1cm} (3.33)

defines a characteristic time for the diffusional creep deformation, and it represents for example the time it takes for the system to reach a 100% straining under a constant strain rate $\dot{\varepsilon}_0$.

It is important to notice that when observed individually the two physical phenomena, curvature-driven grain growth and diffusional creep deformation, are indeed characterized by only one of the two typical driving forces ($\sigma_0$ and $\gamma_0/d_0$) and by only one of the two typical time scales ($t_{\text{migr}}$ and $t_{\text{creep}}$). However when the two physical phenomena are simultaneously present in a system which is characterized by certain physical properties such us: GB energies, GB mobilities, GB diffusivities, temperature, average grain size, and, externally applied stress the one that dominates the microstructure evolution is the one that has the largest driving force and/or the smallest characteristic time scale. That is, for example, if $\zeta \gg 1$ one would expect that
system evolution to be dominated by GB migration grain growth whereas if $\zeta \ll 1$ Cobble creep would be the controlling mechanisms. A similar qualitative analysis can be given in terms of the values of the parameter $\eta$. For example if $\eta = \zeta \frac{t_{\text{migr}}}{t_{\text{creep}}} \ll 1$ the system evolution is expected to be dominated by GB migration whereas if $\eta = \zeta \frac{t_{\text{migr}}}{t_{\text{creep}}} \gg 1$ the evolution would be dominated by GB diffusional creep deformation. The interesting evolutions of systems are those for values of $\zeta$ and $\eta$ around unity when both mechanisms compete on equal footing; and this is the region we plan to map and characterize thoroughly in our research. Of course the two extreme cases, Coble creep only and grain growth only will also be analyzed for reference and comparison of the overlapping mechanisms regimes.
CHAPTER 4 PROBLEM FORMULATION

Diffusional creep is the primary deformation mechanism at high temperature and low stresses. As mentioned in the introduction the deformation mechanism is known as Coble creep when the deformation is controlled by GB diffusion. The current understanding of Coble creep is mostly derived from single grain models in the presence of some averaged external mean stress. According to these models the atoms diffuse on the grain surface from regions under compression to those under tension. In addition, these models are developed by using various simplifying assumes. Among these the most important are:

- grain boundaries are assumed to be flat.
- grains are considered to be rigid, i.e. no elastic strains are present.
- diffusion occurs only through the GBs; i.e. there is no transport through grain interiors
- grain boundary diffusion is the rate-controlling process.
- grain boundary sliding occurs without any energy dissipation.

These assumptions help us to simplify the implementation of the creep model. However, in realistic polycrystalline aggregates, the deformation mechanism is more complex and in addition to GB diffusion it involves GB sliding with finite sliding resistance and GB migration. For such complex behavior there are currently no analytical models and therefore computer modeling and simulation can provide valuable insights. Indeed at temperatures typical for both creep deformation and grain growth (i.e., about 0.7 – 0.9 of the melting point), the grain sliding resistance is believed to play a minor role. Moreover, experimental results have also shown that most of the above mentioned assumptions lead to reasonable models for creep and grain growth.

In the present study, we analyze the relevant features of deformation in a two-dimensional
polycrystalline microstructure in the presence of both GB diffusion and GB migration where the
grain size and grain shapes changes occur simultaneously.

For the grain growth component we have implemented in our simulation codes the algorithm
developed by Kawasaki [35] and Weygand [12-13]. This model is based on the variational
formulation for the dissipated power and is indeed a very flexible modeling approach in which
the only ingredients are the GB energies and GB mobilities. Moreover, the Kawasaki model has
the advantage that it can be easily coupled directly with the model for the GB diffusional creep.
In our simulations the GB creep is simulated using the Pan and Cocks model [27].
CHAPTER 5 RESULTS AND DISCUSSION

In the present simulation study we focus on the GB creep in the presence of both GB diffusion and GB migration. As shown by dimensional analysis in section 3.7 the presence of both GB diffusion and GB migration combined with the typical microstructural characteristics such as: average grain size, GB mobility, GB energy and the external parameters, applied stress and temperature, can have a complex effect on the overall microstructure evolution. The description of the complex behavior of the system has been shown by dimensional analysis to reduce to a model system that depends on two dimensionless parameters, $\zeta$ and $\eta$. Therefore by exploring the two dimensional parameter space allows us to map all the possible microstructure evolution paths of the system.

As presented in equation (3.31) the dimensionless parameter $\eta$ given by $\eta = \frac{D_{gb} \Omega \delta}{mkT d^2}$ is determined by material characteristics (GB diffusivity, GB mobility, GB width, and atomic volume), temperature and the average grain size. The other dimensionless parameter $\zeta$, given by $\zeta = \frac{\gamma}{\sigma d}$ (see equation (3.30)) is controlled mainly by external factors such as the applied stress and the average grain size. In the present study we will investigate the various microstructure evolution paths for fixed $\eta$ (here we chose $\eta = 1$) and variable $\zeta$. As discussed in section 3.7 the increased value of the parameter $\zeta$ signifies an increase of the role of GB migration during the creep deformation. One can see that the extreme values $\zeta = 0$ characterizes the creep only evolution whereas $\zeta = \infty$ characterizes the evolution by grain growth only.
5.1 Coble Creep Deformation of a Homogeneous Regular-Hexagonal Grain Structure

As a baseline, we first consider deformation creep in the regular hexagonal microstructure. In our model system the constant tensile stress is applied in the vertical direction and, for simplicity, the GBs will be constrained to be straight. Moreover in our model the GB properties are assumed isotropic, that is, all the GBs have the same GB energies and mobilities.

5.1.1. Deformation in the Presence of Only GB Diffusional Creep

Deformation of a homogeneous regular hexagonal microstructure containing 247 grains in the presence of creep only was investigated. Figure 5.1 shows the evolution of the microstructure at various levels of strain. The overall evolution is in good agreement with the simulations of Pan and Cocks [34] and Spingarn and Nix [11]. Therefore one can observe that with the increasing strain the grain boundaries perpendicular to the stress direction shorten while those oriented at 30° elongate.

![Figure 5.1 Snapshots of the regular hexagonal microstructure deforming by GB creep only](image)

\[ \varepsilon = 0 \% \]
\[ \varepsilon = 20.31 \% \]
\[ \varepsilon = 40.05 \% \]
\[ \varepsilon = 50.50 \% \]
\[ \varepsilon = 60.44 \% \]
\[ \varepsilon = 80.16 \% \]
\[ \varepsilon = 100.7 \% \]
Since in our simulation model the GBs can slide freely without and resistance they do not support shear stress and therefore most of the applied stress has to be supported by the perpendicular boundaries. As the system evolves the shortening of perpendicular leads to a continuous increase of the tensile normal stress along these boundaries. In turn this leads to faster creep rates. At around 60% straining the perpendicular boundaries undergo T1 switching events and the strain rate starts decreasing.

Figure 5.2 shows that up to about 60% straining the strain rate increase continuously with the straining. Moreover our numerical simulations predict the same strain-rate response as the analytical result of Spingarn and Nix [11].

![Figure 5.2 Strain rate versus strain for the regular hexagonal microstructure deforming by GB creep only](image)

Figure 5.3 (b) shows the periodic distribution of the normal stress along GBs indicated in figure 5.3(a) by the bold line. The microstructure considered is the homogeneous un-strained
regular hexagonal structure. One can clearly distinguish two sets of GBs; those normal and those that are inclined at 30° with respect to stress direction. As seen from Figure 5.3(b) the perpendicular boundaries are under tension (i.e. the normal stress $\sigma_n>0$) over the entire GB length with a maximum stress of $2\sigma_o$ in the middle of each GB. By contrast, along certain regions of the inclined boundaries the stress is tensile whereas along other regions it is compressive; the compressive stress reaches its maximum in the middle.

![Figure 5.3](image)

Figure 5.3 (a) A regular hexagonal grain structure subjected to uniaxial tensile stress and (b) the stress distribution in the microstructure along the selected path

The stress profiles at 50% and 80% straining respectively along the corresponding median paths are presented in Figures 5.4 and 5.5. Interestingly at 50% the stress is mostly tensile along the entire path and the maximum tensile stress drops below $\sigma_o$. A further decrease of the maximum tensile stress is also observed in 80% strained microstructure (see figure (5.5)).
Figure 5.4 (a) Snapshot of a regular hexagonal microstructure subjected to uniaxial stress after 50% straining in the presence of Coble creep only. (b) The stress distribution in the center of the strained microstructure along the selected path.

Figure 5.5 (a) Snapshot of a regular hexagonal microstructure after 80% straining in the presence of Coble creep only. (b) The stress distribution in the center of the strained microstructure along the selected path.
5.1.2. Deformation in the Presence of Both GB Diffusional Creep and GB Migration

Next we consider the creep deformation of the homogeneous regular hexagonal microstructure in the presence of both GB creep and GB migration. As shown by dimensional analysis, the relative weight of creep or GB migration on the overall microstructure evolution is “tuned” by adjusting the dimensionless parameter $\zeta$. Large values of $\zeta$ translate into an increased role of the GB migration. Figures 5.6 and 5.7 show the evolution of four microstructures characterized by $\zeta = 0.01, 1, 100$ and 1000 at various levels of strain. The GB migration induces the movements of GBs and triple junctions which, in turn leads to a relaxation of the microstructure. The grain switching and the grain aspect ratio are also strongly influenced by the presence of GB migration. Our simulation results show that for large values of the parameter $\zeta$ (i.e. $\zeta = 100$ and $\zeta=1000$) the deformed microstructure is more relaxed after the grain switching events. That is, the grain aspect ratio is closer to one and the grains look more equiaxed when the deformation occurs in the presence of GB migration.

In figure 5.8 the related plots of the strain rate versus total strain for the four systems with $\zeta = 0.01, \zeta = 1, \zeta = 100$ and $\zeta =1000$ are compared with the regular hexagonal system. These plots show that the increased role of GB migration (i.e. larger values of $\zeta$) leads to a decrease of both the peak height and peak width of the corresponding strain rates. This can be rationalized by noticing that the GB migration has the tendency to drive the system away from the highly unphysical grain configurations, characterized by highly elongated grains that are present at the switching time.
Figure 5.6 Two sets of snapshots of a regular hexagonal microstructure deforming by GB creep in the presence of GB migration. The interplay between GB creep and GB migration in the two systems is characterized by the system parameter $\zeta$ (see Equation (3.30)). (a) System with $\zeta = 0.01$ and (b) System with $\zeta = 1$. 
Figure 5.7 Two sets of snapshots of a regular hexagonal microstructure deforming by GB creep in the presence of GB migration. The interplay between GB creep and GB migration in the two systems is characterized by the system parameter $\zeta$ (see Equation (3.30)). (a) System with $\zeta = 100$ and (b) System with $\zeta = 1000$. 

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5.2. Coble Creep Deformation in Regular Microstructures with Inhomogeneities

In this section we describe our investigations into the role of inhomogeneities on the strain rate and stress distributions in systems deforming by GB creep. The role of GB migration on the overall evolution is also investigated.

5.2.1. Deformation in the Presence of Only GB Diffusional Creep

Next we consider two regular hexagonal microstructures with single inhomogeneities close to their centre deforming by GB creep only. The inhomogeneous microstructures were obtained by performing separate grain growth simulations on the corresponding regular hexagonal microstructures. In order to achieve the abnormal grain growth that would favor the growth of only the central grain the GB properties (GB energies and mobilities) of all GBs surrounding the biased grain were modified (i.e. a decrease of GB energy favors the growth of the biased grain).

Figure 5.8 Strain rate versus strain for a regular hexagonal microstructure deforming by GB creep in the presence of GB migration for various values of the parameter $\zeta$. 
The selected grain grows abnormally, allowing us to generate microstructures with inhomogeneities of various sizes. In this study we focused on two systems with single inhomogeneities of areas $A_1 = 4A_0$ for the first system and $A_2 = 10A_0$ for the second system. $A_0$ is the area of a hexagonal grain.

Figures 5.9 and 5.11 show two set of snapshots of the deforming microstructures with larger grains close to their center. By close inspection of these snapshots we can see that in both microstructures at about 60% strain the regular hexagonal grains close to the larger grain have already undergone T1 switches whereas the grains relatively far away have not yet begun switching.

The reason for the early switches in the vicinity of the larger grain is the presence of larger stresses along these boundaries and therefore larger diffusional fluxes which in the end leads to higher rates for the change of the GBs lengths.

Figure 5.9  Snapshots of the regular hexagonal microstructure containing a large grain in the middle deforming by GB creep only. The area of the large grain is about 4 times that of a regular-hexagonal grain

The reason for the early switches in the vicinity of the larger grain is the presence of larger stresses along these boundaries and therefore larger diffusional fluxes which in the end leads to higher rates for the change of the GBs lengths.
According to figures 5.10 and 5.12, in the presence of the inhomogeneity the time evolution of the microstructure is less symmetric with respect to the strain at which the creep rates exhibit maxima. Moreover the variability of the magnitude of the diffusive fluxes is larger in the presence of inhomogeneity and consequently the GB switching events will not take place simultaneously for all the GBs perpendicular to the tensile direction. This in turn leads to the decrease of the peak in the strain rate vs. strain curve.

Figure 5.10  Strain rate versus strain for the regular hexagonal microstructure containing a larger grain in the middle deforming by GB creep only. The area of the large grain is about 4 times that of a regular-hexagonal grain.
Figure 5.11 Snapshots of the regular hexagonal microstructure containing a large grain in the middle deforming by GB creep only. The area of the large grain is about 10 times that of a regular-hexagonal grain.

Figure 5.12 Strain rate versus strain for the regular hexagonal microstructure containing a larger grain in the middle deforming by GB creep only. The area of the large grain is about 10 times that of a regular-hexagonal grain.
Figure 5.13 (a) A regular hexagonal grain structure with a large inhomogeneity in the centre subjected to uniaxial tensile stress. The area of the large grain is about 10 times that of a regular-hexagonal grain. (b) The stress distribution in the microstructure along the selected path.

Figure 5.14 (a) Snapshot of a regular hexagonal microstructure with a large inhomogeneity in the centre subjected to uniaxial tensile stress after 50% straining in the presence of Coble creep only. The area of the large grain is about 10 times that of a regular-hexagonal grain. (b) The stress distribution in the center of the strained microstructure along the selected path.
The presence of inhomogeneity has also strong impact on the stress distribution in the microstructure. Figures 5.13, 5.14 and 5.15 give the stress distribution along the indicated paths by the bold line; particularly along about half of the boundaries surrounding the inhomogeneity. By comparing these stress profiles with the stress along a path in uniform regular microstructure one can see that at certain GBs around the larger inhomogeneity the normal stress reaches values as high as three times the externally applied stress.

The presence of inhomogeneity has also strong impact on the stress distribution in the microstructure. Figures 5.13, 5.14 and 5.15 give the stress distribution along the indicated paths by the bold line; particularly along about half of the boundaries surrounding the inhomogeneity. By comparing these stress profiles with the stress along a path in uniform regular microstructure one can see that at certain GBs around the larger inhomogeneity the normal stress reaches values as high as three times the externally applied stress.

Figure 5.15 (a) Snapshot of a regular hexagonal microstructure with a large inhomogeneity in the centre subjected to uniaxial tensile stress after 80% straining in the presence of Coble creep only. The area of the large grain is about 50 times that of a regular-hexagonal grain. (b) The stress distribution in the center of the strained microstructure along the selected path.
5.2.2. Deformation in the Presence of Both GB Diffusional Creep and GB Migration

Next we focus on the deformation creep of the regular microstructures with inhomogeneities in the presence of GB migration. Figures 5.16 and 5.17 show the evolution of the microstructures, with a small inhomogeneity close to their centers, in the presence of GB migration. Systems with $\zeta = 0.01$, $\zeta = 1$, $\zeta = 10$ and $\zeta = 100$ were analyzed. Our simulation results clearly show a more relaxed straining of the microstructure for the systems in which the GB migration plays a significant role (i.e. systems with larger values of $\zeta$). This is clearly seen by comparing the snapshots of the deforming microstructure at 80% and 100% strains in the absence of GB migration (see figure 5.9) with those in the presence of GB migration (see figure 5.17). Notable is the overall relaxation of the microstructure around the inhomogeneity in the presence of significant GB migration. The presence of GB migration has also a significant impact on the overall strain-rate dependence on the strain (see Figure 5.18). For larger values of $\zeta$ both the peaks heights and peaks width are reduced significantly. Again this can be rationalized in terms of GB migration effect of grain switching events as well as on the relaxation of the microstructure.

GB migration seems to be even more important on the overall creep straining of microstructures containing larger inhomogeneities. Comparison of figures 5.19 and 5.20 with figure 5.11 shows that indeed at larger strains (80% to 100%) the GB migration mechanism promotes much more relaxed microstructure. Again notable is the relaxation of the microstructure around the inhomogeneity. The relaxation process has also strong impact on both the strain rates (see figure 5.21) and the stress distribution along the GBs surrounding the inhomogeneity (see figures 5.22, 5.23, 5.24 and 5.25).
Figure 5.16 Two sets of snapshots of a regular hexagonal microstructure containing a large grain in the middle deforming by GB creep in the presence of GB migration. The area of the large grain is about 5 times that of a regular-hexagonal grain. The interplay between GB creep and GB migration in the two systems is characterized by the system parameter $\zeta$ (see Equation (3.30)). (a) system with $\zeta = 0.01$ and (b) system with $\zeta = 1$. 
Figure 5.17 Two sets of snapshots of a regular hexagonal microstructure containing a large grain in the middle deforming by GB creep in the presence of GB migration. The area of the large grain is about 5 times that of a regular-hexagonal grain. The interplay between GB creep and GB migration in the two systems is characterized by the system parameter $\zeta$ (see Equation (3.30)). (a) system with $\zeta = 10$ and (b) system with $\zeta = 100$. 
Figure 5.18 Strain rate versus strain for the regular hexagonal microstructure containing a larger grain in the middle deforming by GB creep in the presence of GB migration. The area of the large grain is about 5 times that of a regular-hexagonal grain. For reference and comparison the creep only curve is also given in addition to those characterizing the systems with $\zeta = 0.01; 1; 10$ and 100.
Figure 5.19 Two sets of snapshots of a regular hexagonal microstructure containing a large grain in the middle deforming by GB creep in the presence of GB migration. The area of the large grain is about 10 times that of a regular-hexagonal grain. The interplay between GB creep and GB migration in the two systems is characterized by the system parameter $\zeta$ (see Equation (3.30)). (a) system with $\zeta = 0.01$ and (b) system with $\zeta = 0.1$. 
Figure 5.20 Two sets of snapshots of a regular hexagonal microstructure containing a large grain in the middle deforming by GB creep in the presence of GB migration. The area of the large grain is about 10 times that of a regular-hexagonal grain. The interplay between GB creep and GB migration in the two systems is characterized by the system parameter $\zeta$ (see Equation (3.30)). (a) system with $\zeta = 10$ and (b) system with $\zeta = 100$. 
Figure 5.21 Strain rate versus strain for the regular hexagonal microstructure containing a larger grain in the middle deforming by GB creep in the presence of GB migration. The area of the large grain is about 50 times that of a regular-hexagonal grain. For reference and comparison the creep only curve is also given in addition to those characterizing the systems with $\zeta = 0.01; 0.1; 10$ and 100.

Figure 5.22 (a) Snapshot of a regular hexagonal microstructure with a large inhomogeneity in the centre subjected to uniaxial tensile stress after 50% straining in the presence of both Coble creep and GB migration and characterized by the parameter $\zeta = 10$. The area of the large grain is about 10 times that of a regular-hexagonal grain. (b) The stress distribution in the center of the strained microstructure along the selected path.
Figure 5.23 (a) Snapshot of a regular hexagonal microstructure with a large inhomogeneity in the centre subjected to uniaxial tensile stress after 80% straining in the presence of both Coble creep and GB migration and characterized by the parameter $\zeta = 10$. The area of the large grain is about 10 times that of a regular-hexagonal grain. (b) The stress distribution in the center of the strained microstructure along the selected path.

Figure 5.24 (a) Snapshot of a regular hexagonal microstructure with a large inhomogeneity in the centre subjected to uniaxial tensile stress after 50% straining in the presence of both Coble creep and GB migration and characterized by the parameter $\zeta = 100$. The area of the large grain is about 10 times that of a regular-hexagonal grain. (b) The stress distributions in the strained microstructure along two paths selected close to the center and close to one end respectively.
5.3. Coble Creep in the Presence of Grain Boundary Migration in a Non-Uniform Grain Structure

In this section we describe our investigations on a non-uniform grain structure in systems deforming first by GB creep only, and then by both GB creep and GB migration.

5.3.1. Deformation in the Presence of Only GB Diffusional Creep

In figure 5.26 we present five consecutive snapshots of the evolution of a non-uniform structure subjected to a constant stress. As can be seen, the structure becomes very unstable even for relatively low level of strains. In fact even over the relatively low level of straining the grain aspect ratio changes significantly. The grains are highly elongated in the direction of the applied stress.
Figure 5.26  Snapshots of non-uniform microstructure deforming by GB creep only.

Figure 5.27 shows the corresponding strain rate versus strain. The evolution of the strain rate is relatively constant as the strain increases. This is an expected result as opposing the regular microstructures the grain switch events responsible for the presence of peaks are not occurring all of them at the same time in the non-uniform microstructures.

Figure 5.27  Strain rate versus strain for the non-uniform microstructure deforming by GB creep only.
5.3.2. Deformation in the Presence of Both GB Diffusional Creep and GB Migration

Next we present the evolution of the non-uniform microstructure in the presence of both GB creep and GB migration, for systems with $\zeta = 10$ and $\zeta = 100$. As can be seen in the figures 5.28, not only the microstructure responded well for higher level of stresses, but the deformation did not change the aspect ratio of the grains.

(a)

Figure 5.28 Two sets of snapshots of a non-uniform microstructure deforming by GB creep in the presence of GB migration. The interplay between GB creep and GB migration in the two systems is characterized by the system parameter $\zeta$ (see Equation (3.30)). (a) system with $\zeta = 10$ and (b) system with $\zeta = 100$. 

(b)
The corresponding figure 5.29 presents the strain rate versus strain in the presence of the GB creep only, and in the presence of GB creep and GB migration. One can see that the presence of GB migration produces a decrease of the values of strain rate at the same levels of strain. This is reduction in the strain rate can be attributed to the increase of the average grain size due to the grain growth that takes place during the deformation process.

![Figure 5.29](image.png)

**Figure 5.29** Strain rate versus strain for the non-uniform microstructure deforming by GB creep in the presence of GB migration. For reference and comparison the creep only curve is also given in addition to those characterizing the systems with $\zeta = 10$ and 100.

Figures 5.30, 5.31, 5.32 and 5.33 show the stress distribution along paths close to the center of the microstructures. One can see that indeed the stress distributions are affected by the presence/absence GB migration during the creep deformation. The GB creep only and GB creep plus GB migration are analyzed in systems with $\zeta = 10$ and $\zeta = 100$. 
Figure 5.30 presents the normalized normal stresses along the indicated path for the non-uniform structure subjected to creep deformation only. The stress profile is given for the original non-strained microstructure. Interestingly our simulations show that although there are certain periodic variations of the stress profile similar to the regular microstructure the stress can reach values much larger than in the regular microstructures. For example along the GB marked by an arrow in figure 5.30 the normal stress reaches values as high as 4.3 $\sigma_0$. Next we analyzed the stress distribution for the same microstructure, in the presence of both GB creep and GB migration (system with $\zeta = 10$) after 50% straining. One can clearly see that now the structure is much more relaxed and the maximum value of the normal stress along the same path GB is only 1.6 times larger than the applied external stress.
Next we present the stress distribution in microstructures that evolve in the presence of both GB creep and GB migration, (for systems with $\zeta = 10$) after 100% straining. As can be seen in the Figure 5.32, the maximum values of the normal stresses along certain GBs is higher than in the previous case, with a maximum value of normal stress approximately 2.5 times larger then the applied tensile stress, these values are smaller than the values obtained when the non-uniform structure was subjected only to creep.
Figure 5.33 (a) Snapshot of a non-uniform microstructure subjected to uniaxial tensile stress after 22% straining in the presence of both Coble creep and GB migration and characterized by the parameter $\zeta = 100$. (b) The stress distribution in the center of the strained microstructure along the selected path.

Figure 5.33 presents the stress distribution in the presence of both GB creep and GB migration, for $\zeta = 100$ and after a 22% straining. The microstructure is much more relaxed this time, and for the maximum value the normal stress along a GB is approximately only 1.1 times larger than the tensile stress.

Figure 5.33 (a) Snapshot of a non-uniform microstructure subjected to uniaxial tensile stress after 22% straining in the presence of both Coble creep and GB migration and characterized by the parameter $\zeta = 100$. (b) The stress distribution in the center of the strained microstructure along the selected path.
CHAPTER 6 CONCLUSIONS

In this study using the mesoscale simulations based on the variational principle of dissipated power we have investigated the GB diffusional creep in the presence of GB migration. The overall microstructural evolution, strain rate dependence on the strain and the stress distribution during straining were investigated on three sets of typical microstructures. We considered regular hexagonal microstructures, regular hexagonal structures with inhomogeneities and non-uniform grain structures.

Our studies indicate that in the absence of GB migration as an accommodation process, the more complex topology of the evolving microstructure has to be carefully monitored in order to avoid unphysical triple junctions’ crossings. In addition in the absence of GB migration the microstructures become highly distorted at large strains.

When GB migration is considered the evolution of the microstructure follows a more physical trajectory with fairly equiaxed grain structures even at larger strains. Moreover the presence of GB migration during creep leads to microstructures characterized by much lower internal stresses.
REFERENCES


VITA

Lucian Zigoneanu graduated from Polytechnic University of Bucharest, Romania. He received a bachelor’s degree in Electronics, Telecommunications and Information Technology, with a major in Applied Electronics, in 1996 and a master’s degree with a major in Quality and Reliability Engineering, in 1997. He worked for three years as customer service engineer for Excel Comp, Bucharest and five years as field service engineer in the Cluj-Napoca branch for Romsys SA, Bucharest. During these years, he also was exchange student at Ecole Nationale Supérieure d’Arts et Métiers, Paris, France for three months (1997), visiting engineer for a software-hardware engineer training at Wincor Nixdorf, Paderborn, Germany (2003) and visiting engineer for a software-hardware training at Dell Europe, Bracknell, United Kingdom (2004). In fall 2005, he was accepted in the department of Mechanical Engineering for a Master of Science degree, Louisiana State University in Baton Rouge, Louisiana.