A Coupled Thermo-mechanical Theory of Strain Gradient Plasticity for Small and Finite Deformations

Yooseob Song
Louisiana State University and Agricultural and Mechanical College

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A COUPLED THERMO-MECHANICAL THEORY OF
STRAIN GRADIENT PLASTICITY
FOR SMALL AND FINITE DEFORMATIONS

A Dissertation

Submitted to the Graduate Faculty of the
Louisiana State University and
Agricultural and Mechanical College
in partial fulfillment of the
requirements for the degree of
Doctor of Philosophy

in

The Department of Civil and Environmental Engineering

by

Yooseob Song
B.Sc., Hanyang University, 2006
M.Sc., Hanyang University, 2008
August 2018
TO MY BELOVED PARENTS, SOONJA AND JUSICK,

for raising me to believe that anything was possible

AND TO MY LOVELY WIFE, MINJEONG,

for making everything possible.
ACKNOWLEDGEMENTS

First and foremost I would like to express my special appreciation and thanks to my advisor professor George Z. Voyiadjis. He has been a tremendous mentor for me. I truly appreciate all his contributions of time, ideas, and funding to make my Ph.D. experience productive and stimulating. The joy and enthusiasm he has for his research was contagious and motivational for me, even during tough times in the Ph.D. pursuit.

I would like to thank my committee members, professor Dorel Moldovan, professor Wen Jin Meng, professor Suresh Moorthy, and professor Christopher G. Arges for letting my final exam be an enjoyable moment, and for their brilliant comments and suggestions. I would particularly like to acknowledge the other two professors in South Korea, Taehyo Park and Taehyun Sung, for being my reference and the financial support.

The members of the Computational Solid Mechanics Laboratory at LSU and the Computational Solid and Structural Mechanics Laboratory at Hanyang University have contributed immensely to my personal and professional time. These groups have been a source of friendships as well as good advice and collaboration. I take this time to express my sincere gratitude to all my colleagues and friends at both groups.

This dissertation would not have come to a successful completion without the help I received from the staff of the CEE department at LSU. I would like to thank Julie Mueller, Grace Mason, Jolie Préau, Madison Lane, Cindy Hukins, Dwain Dsouza and Dave Robertson for their help.

Lastly, I finish with my amazing family where the most basic source of my life energy resides. Nobody has been more important to me in the pursuit of this project than the members of my family. Words cannot express how grateful I am to my parents-in-law, Wija Park and Hyungchul Kim, my parents, Soonja Baek and Jusick Song, and my sister, Minsun Song, for all of the sacrifices that they have made on my behalf. Their prayer for me was what sustained me thus far. Most importantly, I wish to thank my loving, supportive, encouraging, and patient wife, Dr. Minjeong Kim. I need to thank them in Korean now.

어머니, 아버지 그리고 장모님, 장인어른 정말 감사합니다. 기도해 주신 덕분에 무사히 박사과정을 마쳤습니다. 믿어도 저도 지금 인생에서 중요한 발걸음을 내딛고 있는데 항상 응원해 주시고 지켜봐 주세요. 험난 사람이 될 수 있도록 노력 하겠습니다. 우리 예쁜 와이프 민정이, 그 동안 고생 많았어. 느즈막이 시작한 미국 생활이 쉽지는 않지만 지금까지 그래 왔듯 앞으로도 서로가 있어 행복할거야. 사랑해.


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ABSTRACT

In this work, a thermodynamically consistent coupled thermo-mechanical gradient enhanced continuum plasticity theory is developed for small and finite deformations. The proposed model is conceptually based on the dislocations interaction mechanisms and thermal activation energy. The thermodynamic conjugate microstresses are decomposed into energetic and dissipative components. This work incorporates the thermal and mechanical responses of microsystems. It addresses phenomena such as size and boundary effects and in particular microscale heat transfer in fast-transient processes. Not only the partial heat dissipation caused by the fast transient time, but also the distribution of temperature caused by the transition from the plastic work to the heat, are included into the coupled thermo-mechanical model by deriving a generalized heat equation. One- and two-dimensional finite element implementation for the proposed gradient plasticity theory is carried out to examine the characteristics of the proposed strain gradient plasticity model. The derived constitutive framework and the corresponding finite element models are validated through the comparison with the experimental observations conducted on micro-scale thin films. This work is largely composed of three subparts. In the first part, the proposed model is applied to the stretch-surface passivation problem for investigating the material behaviour under the non-proportional loading condition in terms of the stress jump phenomenon, which causes a controversial dispute in the field of strain gradient plasticity theory with respect to whether it is physically acceptable or not. In the second part, two-dimensional finite element implementation for small deformation is performed to investigate the size effects and the grain boundary effect of small-scale metallic materials. In the last part, two-dimensional finite element implementation for finite deformation is carried out to study the size effects during hardening as well as the mesh-sensitivity during softening of the proposed model by solving the shear band problem.
1 INTRODUCTION

This work investigates the characterizations of small-scale mechanical and thermal responses of the material in the context of the strain gradient plasticity theory. Computational continuum solid mechanics and methods are used in order to numerically investigate the capability of the models to address the small scale material responses incorporating size effects, non-equilibrium heat transfer and mesh-sensitivity.

Over the last decade, the scientific research on the mechanical behaviour of components at the micro and nano-scale have been driven by the demands of miniaturization in fields like microelectronics, nanotechnology and micro-electro-mechanical systems (MEMS). These systems form a cutting edge technology area that is predicted to have a significant impact on key market sectors such as aerospace, defense, transportation, home appliances, etc. Besides these technological motivations, describing the mechanical behaviour of metals in small scale provides a unique opportunity to investigate fundamental problems in micro-mechanics and material science.

Among these micro-scale structures, the applications of thin metal films as an integral part in several technological systems have been broadened recently. Normally the film thickness is comparable to relevant microstructural length scales such as grain size, dislocation cell sizes and particle spacing, which in turn, the mechanical properties are strongly affected by the grain size and orientation, grain size distribution and crystallographic texture. Examples of the application of these materials can be found in surface coating (e.g. thermal barrier coating in turbine blades to advance their performance above the melting point; corrosion resistant coatings), MEMS (e.g. sensors and actuators), friction reducers (e.g. medical implants and computer hard discs), electronic circuits (e.g. resistors, transistors, capacitors, and inductors).

The design and fabrication of thin films exhibit material science and engineering challenges across different length scales, from angstroms to millimeters where the integrated applications of theories such as quantum mechanics and continuum solid mechanics may be required in order to increase the knowledge and understanding of the various phenomena encountered as well as to engineer the materials in order to improve the level performance of the system.

In addition to the micro-scale material behaviour, the localization phenomena macroscopically observed in various materials is of vital importance in the performance and stability of the structures. Strain localization is a concept describing an inelastic deformation mode, in which the entire deformation of a material structure occurs in one or more narrow bands, while the rest of the structure usually exhibits unloading. The example of such phenomena can be found in adiabatic shear band in metallic materials under high speed impact, metal forming, and machining of mechanical parts. This leads to local weakness of the material due to the inhomogeneous deformations and material instability response.

However, the conventional continuum plasticity theories fail to address some of the aforementioned behaviours. The main deficiency of these theories can be summarized in modeling:

1) size dependency of the macroscopic yield strength and strain-hardening rate during the inelastic deformation observed from micro-mechanical experiments including those from nano/micro-indentation, torsion of micron-dimensioned wires, micro-bending of thin films, and bulge test;
(2) the classical (macro-mechanical) test results indicating the increase in the macroscopic yield strength and strain-hardening rate of polycrystalline metals with decrease of the particle size and the grain diameter;

(3) heat transport responses under both short time and spatial scales such as high-rate heating on thin film and microelectronic devices and pulsed-laser processing of materials;

(4) mesh dependency in finite element solution of the strain softening and width of localized shear band during the plastic deformation.

It is known that the observed size effect in macro-mechanical tests is mainly due to the interaction between statistically stored dislocations (SSDs) which increase with the plastic strain and density of geometrically necessary dislocations (GNDs), which are generated by inhomogeneous plastic flow attributable to gradients of plastic strain. The classical plasticity models normally ignore such a microstructure characteristic of materials and its evolution in the course of plasticity deformation. Moreover, the implicit assumption of the smooth variation in deformation in such theories is in contrast to the case when strain localization takes place. This leads to the ill-posedness of the standard boundary value problem and consequently discretization sensitivity in numerical simulations of localization and softening problems. Therefore, in order to preserve the well-posedness, the conventional material constitutive models are required to possess a localization limiter in order to address the strain softening ductile behaviour.

Moreover, when the medium size is of the order of or smaller than phonon mean free path, the temperature gradient cannot be established within the medium and the heat transport is partially diffusive and partly ballistic. This is caused by the activation of microstructural effects due to the small depth of the heat-affected zone or the smallness of the structures. On the other hand, if the response time in the small volume components reduces to the range comparable to the thermalization time, it leads to non-equilibrium transition of thermodynamics between electrons and phonons. The macroscale formulation of heat conduction is based on the local thermodynamic equilibrium and the continuum assumption where a set of partial differential equations are used to describe the macroscopic properties. Therefore it does not consider neither the microstructural interactions between energy carriers, nor the size and time dependency of the heat transport.

In order to overcome the aforementioned problems, the thermodynamically consistent thermos-mechanical coupled higher-order strain gradient plasticity is proposed in this work and is investigated using the computational methods in order to explore the small-scale mechanical and thermal characterizations of the proposed model.

In Sections 1.2, 1.3 and 1.1, the brief literature review is addressed in the context of the experimental, theoretical and numerical and aspects of the strain gradient plasticity theory. In Section 1.4, the scope and objective of each chapter is presented.

1.1 Experimental study

The conventional plasticity theory characteristically shows the size-independent behaviour and cannot capture the size effects, in particular, when the material is subjected to the nonhomogeneous (heterogeneous) plastic deformation under the fast transient time and its size ranges in nano/microscales. After the pioneering experimental work on torsion and tension tests of the copper thin wires by Fleck et al. (1994), in which the higher flow stresses are obtained for the smaller-diameter wires when tested in torsion compared to tension, a number of researchers have been working on the developments of the strain gradient plasticity models targeting the size effects in the theoretical as well as the experimental contexts. Even before Fleck et al. (1994), the
evidence of such the size effects is found in some micro-indentation experimental observations such as De Guzman et al. (1993); Nix (1989); Poole et al. (1996); Stelmaskheno et al. (1993), but the strain gradient plasticity theories are not considered in those works.

Roughly, the experiments targeting the size effects can be divided into three categories according to the cause of size effects (Liu et al., 2012): (i) the microstructural constraints to dislocation motion such as the particle reinforcements (Lloyd, 1994), grain boundary strengthening or grain size effect (Hall-Petch effect) (Hall, 1951; Petch, 1953) and passivation layers (Nicola et al., 2006; Xiang and Vlassak, 2006), (ii) the geometrical limitations of the specimen dimensions (dislocation starvation and source exhaustion) observed in the uniaxial tests on micro-/nanopillars (Bei et al., 2007; Dimiduk et al., 2005; Feng et al., 2017; Greer et al., 2005; Kim and Greer, 2009; Uchic and Dimiduk, 2005; Uchic et al., 2004; Volkert and Lilleodden, 2006) and (iii) the strain gradient strengthening due to inhomogeneous plastic deformation presented in bending (Haque and Saif, 2003; Iliev et al., 2017; Lou et al., 2005; Shrotriya et al., 2003; Stolken and Evans, 1998), torsion (Fleck et al., 1994; Gan et al., 2014; Guo et al., 2017; Liu et al., 2013a; Liu et al., 2012; Liu et al., 2013b), and indentation (Chong and Lam, 1999; Elmustafa and Stone, 2003; Lam and Chong, 1999; Lou et al., 2003; Ma and Clarke, 1995; Mirshams and Parakala, 2004; Nix, 1997; Poole et al., 1996; Saha and Nix, 2002; Saha et al., 2001; Swadener et al., 2002; Tymiak et al., 2001). In this section, the last one (iii) will be mainly discussed. In the rest of this section, the review of the experimental investigations that have been conducted to study the size effects on the basis of the SGP models is presented according to the test types as classified in Table 1.1.

Note that some experiments exhibit an increase in the yield strength as the specimen size decreases, e.g. Fleck et al. (1994), Swadener et al. (2002), Lloyd (1994) and Kiser et al. (1996), whereas others show that the size effects mainly affect the material hardening behaviour, e.g. Xiang and Vlassak (2006). Some experiments even show the size effects on both yield strength and hardening behaviour, such as the bending tests by Haque and Saif (2003) and the torsion tests by Dunstan et al. (2009); Liu et al. (2012). What is more, in the micro-torsion tests on the copper wires with four different diameters in the range 16~180 μm by Lu and Song (2011) and in the shear test on the aluminium thin-film disks with three different thicknesses in the range 10~50 μm by Tagarielli and Fleck (2011), no size effect is observed.

Table 1.1. Experimental investigations with the aim of targeting the size effects in the context of gradient-enhanced theory (D: diameters in uniaxial, torsion tests and indent diagonal in indentation tests, h: thicknesses in uniaxial, bending, bulge, shear tests and depths in indentation tests).

<table>
<thead>
<tr>
<th>Test</th>
<th>Reference</th>
<th>Material</th>
<th>SGP model</th>
<th>Variable</th>
<th>Length scale</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Krompholz et al. (2000)</td>
<td>20 MnMoNi 55</td>
<td>Yuan et al. (2003)</td>
<td>D = 2.4~24 mm</td>
<td>0.24 mm</td>
</tr>
</tbody>
</table>

(table cont’d.)
<table>
<thead>
<tr>
<th>Test</th>
<th>Reference</th>
<th>Material</th>
<th>SGP model</th>
<th>Variable</th>
<th>Length scale</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bending</td>
<td>Stolken and Evans (1998)</td>
<td>Nickel foils</td>
<td>Fleck and Hutchinson (1993)</td>
<td>$h = 12.5\sim 50 \mu m$</td>
<td>5.3 $\pm$ 0.2 $\mu m$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Fleck and Hutchinson (1993)$^y$</td>
<td></td>
<td>6.8$\sim$10.5$\mu m$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Aifantis (1984)$^y$</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Fleck and Hutchinson (1993)$^y$</td>
<td></td>
<td>22.5$\sim$50$\mu m$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Gao et al. (1999)$^y$</td>
<td></td>
<td>4.5$\sim$7.5$\mu m$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Voyiadjis and Abu Al-Rub (2005)</td>
<td></td>
<td>Non-fixed$^e$</td>
</tr>
<tr>
<td>Bending</td>
<td>Haque and Saif (2003)</td>
<td>Aluminium foils</td>
<td>Gao et al. (1999)</td>
<td>$h = 100\sim 485$ nm</td>
<td>0$\sim$4.5 $\mu m$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Aifantis (1984)$^y$</td>
<td></td>
<td>0$\sim$10.5 $\mu m$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Fleck and Hutchinson (1993)$^y$</td>
<td></td>
<td>0$\sim$27.5 $\mu m$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Gao et al. (1999)$^y$</td>
<td></td>
<td>0$\sim$23 $\mu m$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Voyiadjis and Abu Al-Rub (2005)</td>
<td></td>
<td>Non-fixed$^e$</td>
</tr>
<tr>
<td>Bending</td>
<td>Shrotriya et al. (2003)</td>
<td>LIGA Nickel foils</td>
<td>Fleck and Hutchinson (1993)</td>
<td>$h = 25\sim 175$ nm</td>
<td>5.6 $\pm$ 0.2 $\mu m$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Aifantis (1984)$^y$</td>
<td></td>
<td>10.8$\sim$60$\mu m$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Fleck and Hutchinson (1993)$^y$</td>
<td></td>
<td>38.8$\sim$230$\mu m$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Gao et al. (1999)$^y$</td>
<td></td>
<td>7.5$\sim$40 $\mu m$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Voyiadjis and Abu Al-Rub (2005)</td>
<td></td>
<td>Non-fixed$^e$</td>
</tr>
<tr>
<td>Torsion</td>
<td>Lou et al. (2005)</td>
<td>LIGA nickel MEMS foils</td>
<td>Fleck and Hutchinson (1993)</td>
<td>$h = 25\sim 200$ $\mu m$</td>
<td>1$^{st}$ (cycle): 13.5 $\mu m$, 2$^{nd}$, 15.5 $\mu m$, 3$^{rd}$, 19.3 $\mu m$</td>
</tr>
<tr>
<td>Torsion</td>
<td>Iliev et al. (2017)</td>
<td>Indium</td>
<td>Fleck and Hutchinson (1993)</td>
<td>$h = 0.25\sim 2$ mm</td>
<td>93.34 $\mu m$</td>
</tr>
<tr>
<td>Torsion</td>
<td>Fleck et al. (1994)</td>
<td>Copper wires</td>
<td>Fleck and Hutchinson (1993)</td>
<td>$D = 12\sim 170$ $\mu m$</td>
<td>2.6$\sim$5.1 $\mu m$, mean value: 3.7 $\mu m$</td>
</tr>
<tr>
<td>Torsion</td>
<td>Liu et al. (2012)</td>
<td>Copper wires</td>
<td>Fleck and Hutchinson (1993)</td>
<td>$D = 18\sim 105$ $\mu m$</td>
<td>2.05$\sim$4.02 $\mu m$</td>
</tr>
<tr>
<td>Torsion</td>
<td>Liu et al. (2013a)</td>
<td>Copper wires</td>
<td>Fleck and Willis (2009a)</td>
<td>$D = 20\sim 50$ $\mu m$</td>
<td>4.16$\sim$4.60 $\mu m$, mean value: 4.44 $\mu m$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Fleck and Willis (2009b)</td>
<td></td>
<td>2.95$\sim$3.25 $\mu m$, mean value: 3.14 $\mu m$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Aifantis (1984, 1987)</td>
<td></td>
<td>6.80$\sim$9.65 $\mu m$, mean value: 8.27 $\mu m$</td>
</tr>
</tbody>
</table>

(table cont’d.)
<table>
<thead>
<tr>
<th>Test</th>
<th>Reference</th>
<th>Material</th>
<th>SGP model</th>
<th>Variable</th>
<th>Length scale</th>
</tr>
</thead>
<tbody>
<tr>
<td>Torsion</td>
<td>Liu et al. (2013a)</td>
<td>Copper wires</td>
<td>Chen and Wang (2000)</td>
<td>$D = 20\sim50 \mu m$</td>
<td>$2.72\sim3.00 \mu m$, mean value: $2.89 \mu m$</td>
</tr>
<tr>
<td></td>
<td>Guo et al. (2017)</td>
<td>Copper wires</td>
<td>Fleck and Hutchinson (1993)</td>
<td>$D = 20\sim50 \mu m$</td>
<td>$3.0 \mu m$</td>
</tr>
<tr>
<td></td>
<td>Stelmashenko et al. (1993)</td>
<td>Tungsten (W) single crystals</td>
<td>Fleck and Hutchinson (1997)*</td>
<td>surface of W: (1 0 0) $D = unknown$</td>
<td>$0.52 \mu m$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>surface of W: (1 1 0) $D = unknown$</td>
<td>$0.38 \mu m$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>surface of W: (1 1 1) $D = unknown$</td>
<td>$0.25 \mu m$</td>
</tr>
<tr>
<td>Indentation</td>
<td>Ma and Clarke (1995)</td>
<td>Silver single crystals</td>
<td>Fleck and Hutchinson (1997)*</td>
<td>$h = 0.6\sim2.0 \mu m$</td>
<td>$0.39 \mu m$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$h = 0.1\sim2.0 \mu m$</td>
<td>$0.22 \mu m$</td>
</tr>
<tr>
<td></td>
<td>McElhaney et al. (1998)</td>
<td>Copper single crystals</td>
<td>Nix and Gao (1998)*</td>
<td>$h = 0.2\sim2.0 \mu m$</td>
<td>$0.6 \mu m$</td>
</tr>
<tr>
<td></td>
<td>Nix and Gao (1998)</td>
<td>Copper (cold worked)</td>
<td>Nix and Gao (1998)</td>
<td>$h = 0.17\sim2.0 \mu m$</td>
<td>$5.84 \mu m$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Copper (annealed)</td>
<td>Nix and Gao (1998)</td>
<td>$h = 0.17\sim2.0 \mu m$</td>
<td>$12.0 \mu m$</td>
</tr>
<tr>
<td></td>
<td>Nix and Gao (1998)</td>
<td>Single crystal copper</td>
<td>Yuan and Chen (2000)</td>
<td>$h = 0.17\sim2.0 \mu m$</td>
<td>$20.0 \mu m$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Polycrystal copper</td>
<td>Yuan and Chen (2000)</td>
<td>$h = 0.17\sim2.0 \mu m$</td>
<td>$6.0 \mu m$</td>
</tr>
<tr>
<td></td>
<td>Lou et al. (2003)</td>
<td>LIGA nickel MEMS foils</td>
<td>Nix and Gao (1998)</td>
<td>$h = 0.30\sim200 \mu m$</td>
<td>$0.89 \mu m$</td>
</tr>
<tr>
<td></td>
<td>Tho et al. (2006)</td>
<td>Copper</td>
<td>Gao et al. (1999)</td>
<td>$h = 0.4\sim3.4 \mu m$</td>
<td>$2.56 \mu m$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Al-7075</td>
<td>Gao et al. (1999)</td>
<td>$h = 0.4\sim3.4 \mu m$</td>
<td>$1.35 \mu m$</td>
</tr>
<tr>
<td></td>
<td>Ro et al. (2006)</td>
<td>Al-2024 alloy</td>
<td>Nix and Gao (1998)</td>
<td>$h = 0\sim0.7 \mu m$</td>
<td>$50\sim200 \text{nm}$</td>
</tr>
<tr>
<td></td>
<td>Voyiadjis and Almasri (2009)</td>
<td>CR-1018 steel</td>
<td>Nix and Gao (1998)</td>
<td>Microhardness: $h = 0.5\sim5.0 \mu m$, Macrohardness: $h = 0.1\sim1.0 \text{mm}$</td>
<td>$15.8 \mu m$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Chong and Lam (1999)</td>
<td>$h = 10.8 \mu m$</td>
<td>$13.0 \mu m$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Abu Al-Rub and Voyiadjis (2004)</td>
<td>$h = 0.1\sim1.0 \text{mm}$</td>
<td>$3.0 \mu m$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>OFHC copper</td>
<td>Nix and Gao (1998)</td>
<td>Microhardness: $h = 0.8\sim1.5 \mu m$, Macrohardness: $h = 0.1\sim0.2 \text{mm}$</td>
</tr>
</tbody>
</table>

(table cont’d.)
The strain gradient theories can be classified into two groups based on the strategies for strain gradient dependence directly into the constitutive equations of the local type material (e.g. Acharya and Bassani (2000); Acharya et al. (2003); Acharya et al. (2004); Huang et al. (2004); Yuan and Chen (2000, 2001)) and (2) higher-order theories where higher order stresses are defined as the work conjugate of strain gradient by implying the strain energy potential incorporating the strain gradients (e.g. Aifantis (1984, 1987); Fleck and Hutchinson (1993, 1997, 2001); Fleck et al., 2014, 2015; Fleck and Willis, 2015; Gao et al., 1999; Gomez and Basaran, 2007; Gudmundson, 2004; Gurtin, 2000, 2002, 2003, 2004; Gurtin and Anand, 2005a, b, 2009; Hutchinson, 2012; Niordson and Legarth, 2010; Nix and Gao, 1998; Voyiadjis and Abu Al-Rub, 2005, 2007; Voyiadjis and Deliktas, 2009a, b; Voyiadjis and Faghihi, 2012, 2013, 2014; Voyiadjis et al., 2014; Voyiadjis et al., 2010b).

At first, strain gradient theories mainly target the mesh dependency in finite element simulation of the localization problem and width of shear band. Later, the focus in such theories has mainly directed toward the size effect and boundary layer related to plastic deformation of small volume metallic compounds.

The strain gradient theories can be classified into two groups based on the strategies for the strain gradient theory formulation: (1) lower-order theories consist of heuristically introducing the gradient dependence directly into the constitutive equations of the local type material (e.g. Acharya and Bassani (2000); Acharya et al. (2003); Acharya et al. (2004); Huang et al. (2004); Yuan and Chen (2000, 2001)) and (2) higher-order theories where higher order stresses are defined as the work conjugate of strain gradient by implying the strain energy potential incorporating the strain gradients (e.g. Aifantis (1984, 1987); Fleck and Hutchinson (1993, 1997, 2001); Gao et al. (1999); Geers (2004); Gudmundson (2004); Gurtin (2004); Gurtin and Anand (2005a, 2005b); Huang et al. (2000a); Peerlings (2007); Peerlings et al. (1996)). The main distinction between the two theories arises in the restriction of the low-order theories in term of imposing boundary conditions, which in turn, excludes the effect of boundary related size effects (e.g. surface passivation in free-standing thin films; constrained plastic flow of a thin film on a substrate subjected to uniform loading ) and grain boundary in polycrystalline from the theory that has significant factors to model a realistic material behaviour as the surface-to-volume ratio increases.

### Table: Comparison of Indentation Test, Bulge Test, and Shear Test

<table>
<thead>
<tr>
<th>Test</th>
<th>Reference</th>
<th>Material</th>
<th>SGP model</th>
<th>Variable</th>
<th>Length scale</th>
</tr>
</thead>
<tbody>
<tr>
<td>Indentation</td>
<td>Voyiadjis and Almasri (2009)</td>
<td>OFHC copper</td>
<td>Chong and Lam (1999)</td>
<td>Microhardness: $h \geq 0.8$<del>$1.5 \mu m,$ $h \leq 0.1$</del>$0.2 mm $</td>
<td>0.95 $\mu m$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Abu Al-Rub and Voyiadjis (2004)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Li et al. (2017)</td>
<td></td>
<td>Ag999 (annealed)</td>
<td>Huang et al. (2004)</td>
<td>$h \leq 0.1$~$0.56 \mu m$</td>
<td>0.976 $\mu m$</td>
</tr>
<tr>
<td>Iliev et al. (2017)</td>
<td></td>
<td>Indium</td>
<td>Nix and Gao (1998)</td>
<td>$h = 0$~$100 \mu m$</td>
<td>85.21 $\mu m$</td>
</tr>
<tr>
<td>Bulge</td>
<td>Xiang and Vlassak (2006)</td>
<td>Copper thin-films</td>
<td>Fleck and Hutchinson (2001)</td>
<td>$h = 0.34$~$0.89 \mu m$</td>
<td>0.345 $\pm 0.015 \mu m$</td>
</tr>
<tr>
<td>Shear</td>
<td>Tagarielli and Fleck (2011)</td>
<td>Aluminium foils</td>
<td>No size effect</td>
<td>$h = 10$~$50 \mu m$</td>
<td>No size effect</td>
</tr>
</tbody>
</table>

The comparison with the test data and choice of $l$ are presented in Fredriksson and Gudmundson (2005b).

* The comparison with the test data and choice of $l$ are presented in Begley and Hutchinson (1998).

† The comparison with the test data and choice of $l$ are presented in Yuan and Chen (2001).

‡ The comparison with the test data and choice of $l$ are presented in Voyiadjis and Abu Al-Rub (2005).

§ A non-fixed length scale parameter is proposed based on dislocation mechanics in Voyiadjis and Abu Al-Rub (2005). See Equation (44) in their work.

### 1.2 Theoretical study

The reason is that for lower-order theories the boundary conditions only can be imposed on displacement or stress and no gradient in plastic strain can be enforced for the case of homogeneous loading.

Several review articles have been published focusing on the gradient plasticity in terms of; crystal plasticity (Roters et al., 2010), theoretical development of various continuum models (Guha et al., 2015; Voyiadjis and Faghihi, 2014), Aifantis theory (Aifantis, 2003) and Fleck and Hutchinson theory (Fleck and Hutchinson, 1997). The attempts to link between the different approaches of strain gradient plasticity theories have been made by Gudmundson (2004) dealing with Acharya and Bassani (1996); Aifantis (1984, 1987); Bassani (2001); Fleck and Hutchinson (1993, 1997, 2001); Gao et al. (1999); Gurtin (2003); Huang et al. (2000a); Menzel and Steinmann (2000), Gurtin and Anand (2009) dealing with Aifantis (1984, 1987); Fleck and Hutchinson (2001), Kuroda and Tvergaard (2010) dealing with Aifantis (1984, 1987); Fleck and Hutchinson (2001); Gudmundson (2004), Kuroda (2015) dealing with Aifantis (1984, 1987); Fleck and Hutchinson (2001); Gudmundson (2004); Gurtin and Anand (2009); Kuroda and Tvergaard (2010); Muhlhaus and Aifantis (1991), and Forest and Aifantis (2010) dealing with the link between second gradient theory and the gradient elasticity model, the link between Eringen’s micromorphic model and Aifantis strain gradient plasticity.

1.3 Numerical study

Numerical solutions of the strain gradient plasticity theory by the finite element method have been used in many works as shown in Table 1.2. Aifantis (1984) and Aifantis (1987) introduce the second gradient of the effective plastic strain into the expression of the flow stress, and the effective plastic strain is used as an additional degrees of freedom by de Borst and Muhlhaus (1992) in addition to the displacement field. In their work, the higher-order boundary conditions are needed for the same or its conjugate traction. Their work focuses on the numerical stability for the strain softening materials. This can be achieved since ellipticity of the governing differential equations is maintained after entering the softening regime due to the inclusion of the gradient terms in the theory. As a consequence, mesh-dependent numerical results are avoided after localization. A drawback of this theory is that \( C^1 \)-continuity is required for the effective plastic strain field. deBorst and Pamin (1996) show that the requirement of \( C^1 \)-continuity can be avoided through a penalty formulation if the gradients of the effective plastic strain are used as another set of additional degrees of freedom. Hence three different kinds of degrees of freedom are used for this penalty formulation.

Another group of gradient plasticity theories, which introduce the first gradient of plastic strain measures, is proposed by Fleck and Hutchinson (2001) and Niordson and Hutchinson (2003a) solve the plane strain problem using the finite element method based on the Fleck and Hutchinson theory. The effective plastic strain is required as an additional degrees of freedom and the higher-order boundary conditions are needed in their theory. Only \( C^0 \)-continuity is required for the interpolation of the plastic field since no second-order gradient enter the formulation.

Meanwhile, Peerlings et al. (1998a); Peerlings et al. (1996) propose the implicit gradient plasticity theory for damage modelling of quasi-brittle materials. The application of implicit gradient plasticity theory to the softening plasticity is performed by Engelen et al. (2003). 1D and 2D finite element implementations for the geometrically linear plane strain problems are solved in Engelen et al. (2003). In Geers (2004), a finite strain logarithmic hyperelasto-plastic model with an isotropic plastic-damage variable that leads to softening and failure of the plastic material is
proposed on the basis of the implicit gradient plasticity theory. The incremental solution strategy
of the finite element implementation is highlighted in their work and the necking of axisymmetric
cylindrical bar is solved in order to emphasize the computational efficiency of the proposed
strategy.

Table 1.2. Applications of the strain gradient plasticity theory to solve the various types of
problems using finite element method.

<table>
<thead>
<tr>
<th>Application</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tension, Compression</td>
<td>Dillard et al. (2006); Feng et al. (2010); Fredriksson and Gudmundson</td>
</tr>
<tr>
<td></td>
<td>(2005a, 2005b, 2007a); Komaragiri et al. (2008); Nielsen and Niordson</td>
</tr>
<tr>
<td></td>
<td>(2013); Niordson and Hutchinson (2003b, 2011); Niordson and Redanz (2004);</td>
</tr>
<tr>
<td></td>
<td>Niordson and Tvergaard (2005); Srinivasan et al. (2008); Zhou et al. (2008)</td>
</tr>
<tr>
<td>Simple shear</td>
<td>Anand et al. (2005); Chen and Fleck (2002); Cordero et al. (2013); Fredriksson</td>
</tr>
<tr>
<td></td>
<td>and Gudmundsson (2005b); Fredriksson et al. (2009); Komaragiri et al. (2008);</td>
</tr>
<tr>
<td></td>
<td>Lele and Anand (2008); Martinez-Paneda et al. (2016a); Nielsen and Niordson</td>
</tr>
<tr>
<td></td>
<td>(2014); Niordson and Hutchinson (2003b); Panteghini and Bardella (2016);</td>
</tr>
<tr>
<td></td>
<td>Peerlings et al. (2012); Poh and Peerlings (2016); Shu and Fleck (1999);</td>
</tr>
<tr>
<td></td>
<td>Song and Voyiadjis (2018b); Voyiadjis et al. (2014); Voyiadjis and Song (2017);</td>
</tr>
<tr>
<td></td>
<td>Voyiadjis et al. (2017); Song and Voyiadjis (Under Review)</td>
</tr>
<tr>
<td>Bending</td>
<td>Feng et al. (2010); Lele and Anand (2009); Mao et al. (2013); Martinez-</td>
</tr>
<tr>
<td></td>
<td>Paneda et al. (2016a); Panteghini and Bardella (2016)</td>
</tr>
<tr>
<td>Indentation</td>
<td>Begley and Hutchinson (1998); Danas et al. (2012); Fredriksson and</td>
</tr>
<tr>
<td></td>
<td>Larsson (2008); Guha et al. (2013); Huang et al. (2000b); Hwang et al. (2002);</td>
</tr>
<tr>
<td></td>
<td>Komaragiri et al. (2008); Lele and Anand (2009); Li et al. (2017); Niordson</td>
</tr>
<tr>
<td></td>
<td>and Hutchinson (2003b); Panteghini and Bardella (2016); Poh et al. (2011);</td>
</tr>
<tr>
<td></td>
<td>Qin et al. (2009); Shu and Fleck (1998); Swaddiwudhipong et al. (2005, 2006a);</td>
</tr>
<tr>
<td></td>
<td>Swaddiwudhipong et al. (2006b); Tho et al. (2006); Yuan and Chen (2001)</td>
</tr>
<tr>
<td>Torsion</td>
<td>Bardella and Panteghini (2015); Hwang et al. (2003); Idiart and Fleck (2009)</td>
</tr>
<tr>
<td>Cyclic</td>
<td>Bardella and Panteghini (2015); Nielsen and Niordson (2014); Niordson</td>
</tr>
<tr>
<td></td>
<td>and Legarth (2010); Wulfinghoff et al. (2015)</td>
</tr>
<tr>
<td>Composite, Particle</td>
<td>Borg et al. (2006); Dahlberg and Faleskog (2013); Fredriksson et al.</td>
</tr>
<tr>
<td></td>
<td>(2009); Legarth (2015); Lele and Anand (2008); Niordson (2003); Niordson</td>
</tr>
<tr>
<td></td>
<td>and Tvergaard (2001, 2002); Poh and Peerlings (2016); Zhou et al. (2011)</td>
</tr>
<tr>
<td>Non-proportional</td>
<td>Bardella and Panteghini (2015); Martinez-Paneda et al. (2016a); Panteghini</td>
</tr>
<tr>
<td></td>
<td>and Bardella (2016); Song and Voyiadjis (2018a); Voyiadjis and Song (2017)</td>
</tr>
</tbody>
</table>

(table cont’d.)
1.4 Scopes and objectives

In Chapter 2, a new class of thermodynamic-based higher order gradient plasticity theory is proposed and applied to the stretch-surface passivation problem for investigating the material behaviour under the non-proportional loading condition. The model proposed in this chapter incorporates the thermal and mechanical responses of microsystems. It addresses phenomena such as...
as size and boundary effects and in particular microscale heat transfer in fast-transient processes. The stored energy of cold work is considered in the development of the recoverable counterpart of the free energy. The main distinction in this formulation is the presence of the dissipative higher order microstress quantity that is known to give rise to the stress jump phenomenon, which causes a controversial dispute in the field of strain gradient plasticity theory with respect to whether it is physically acceptable or not. The finite element solution for the stretch-surface passivation problem is developed and validated by comparing with three sets of small-scale experiments. Based on the validated finite element solution, the stress jump phenomenon under the stretch-surface passivation condition is investigated with the effects of the various material parameters. The evolution of the free energy and dissipation potentials are investigated at elevated temperatures. The two-dimensional simulation is also given to examine the gradient and grain boundary effect, the mesh sensitivity of the two-dimensional model and the stress jump phenomenon.

In Chapter 3, a coupled thermo-mechanical gradient enhanced continuum plasticity theory containing the flow rules of the grain interior and grain boundary areas is developed within the thermodynamically consistent framework. Two-dimensional finite element implementation for the proposed gradient plasticity theory is carried out to examine the micro-mechanical and thermal characteristics of small-scale metallic volumes. The proposed model is conceptually based on the dislocations interaction mechanisms and thermal activation energy. The thermodynamic conjugate microstresses are decomposed into dissipative and energetic components, correspondingly, the dissipative and energetic length scales for both the grain interior and grain boundary are incorporated in the proposed model and an additional length scale related to the geometrically necessary dislocations-induced strengthening is also included. Not only the partial heat dissipation caused by the fast transient time, but also the distribution of temperature caused by the transition from the plastic work to the heat, are included into the coupled thermo-mechanical model by deriving a generalized heat equation. The derived constitutive framework and two-dimensional finite element model are validated through the comparison with the experimental observations conducted on micro-scale thin films. The proposed enhanced model is examined by solving the simple shear problem and the square plate problem to explore the thermo-mechanical characteristics of small-scale metallic materials.

In Chapter 4, a thermodynamically consistent constitutive model for the coupled thermo-mechanical gradient-enhanced plasticity theory is proposed within the finite deformation framework. A corresponding two-dimensional finite element implementation is carried out to examine the micro-mechanical characteristics of small-scale metallic volumes. The proposed model is established on the basis of the implicit gradient approach and the concepts of the dislocation interaction mechanisms and thermal activation energy. The implicit gradient approach is well known for its computational strength, however, it is also commonly accepted that it cannot capture the size effect phenomenon observed in the small-scale experiments during the strain hardening regime. In order to resolve this issue, a modified implicit gradient approach which can capture the size effect under the finite deformation is constructed in this chapter. The simple shear problem is then solved to carry out the feasibility study of the proposed model on the size effect phenomenon. Lastly, the uniaxial plane strain tension problem is solved to perform the mesh sensitivity tests of the model during the strain softening regime.

In Chapter 5, the concise conclusions and some future works are presented.

It should be noted that all the terms used in each section are only valid on the relevant sections.
2 Effect of Passivation on Strain Gradient Plasticity Models for Non-proportional Loading: Energetic and Dissipative Gradient Components

2.1 Investigation on the energetic or dissipative components of the plastic strain gradients and their corresponding rates

Whether the plastic strain gradients and their corresponding rates lead to energetic or dissipative strengthening has been a fundamental issue in the field of strain gradient plasticity (SGP) theory since the early attempts that incorporate a material length scale into the conventional continuum plasticity models were proposed by Aifantis (1984, 1987). Aifantis (1984, 1987) proposed a modified flow rule for the plastic phase by including the gradient term $\beta \nabla^2 \varepsilon^p$ into the conventional flow rule as follows:

$$\tau_\varepsilon = R(\varepsilon^p) - \beta \nabla^2 \varepsilon^p$$  \hspace{1cm} (2.1)

where $\tau_\varepsilon$ is the effective stress and is calculated by $\tau_\varepsilon = \sqrt{3} \tau_{jj} \tau_{jj}/2$ with the deviatoric stress tensor $\tau_{ij}$, $R(\varepsilon^p) > 0$ is the conventional flow resistance, $\varepsilon^p$ is the accumulated plastic strain, $\beta > 0$ is a material coefficient, and $\nabla^2 = \text{div} \nabla$ is the Laplacian operator. Hereafter, a number of mechanisms associated with geometrically necessary dislocations (GNDs) have been proposed in order to explain the strengthening effect (Bardella, 2006, 2010; Bardella and Panteughini, 2015; Cermelli and Gurtin, 2001, 2002; Evers et al., 2004; Faghihi and Voyiadjis, 2014; Gurtin, 2002, 2010; Oztop et al., 2013; Voyiadjis and Abu Al-Rub, 2005). All these works are based on the SGP theory and are able to capture the size effect induced by GNDs by incorporating the gradient terms into the models with an energetic or dissipative formulation or a combination of both.

There are two different kinds of viewpoints in SGP theory in terms of the origin of the strengthening effect. Firstly, there is a specific argument that the strain gradient strengthening is purely energetic in the sense that GNDs originate in the blockage by grain boundaries and the pile-ups of dislocations has a backstress associated with the energetic strengthening (Fleck and Willis, 2015). For example, Kuroda and Tvergaard (2010) discussed the physical basis for the introduction of the nonlocal term $\beta \nabla^2 \varepsilon^p$ based on the dislocation mechanism. They argued that the term $\tau_\varepsilon + \beta \nabla^2 \varepsilon^p$ calculated in Equation (2.1) represents a total stress at the material point that activates the plastic straining, i.e. the generation and movement of dislocations. They also pointed out that the thermodynamic requirement on the plastic dissipation $D$ is evaluated by $D = (\tau_\varepsilon + \beta \nabla^2 \varepsilon^p) \varepsilon^p > 0$. This demonstration shows that the nonlocal term $\beta \nabla^2 \varepsilon^p$ is naturally interpreted as an energetic quantity, which is consistent with the interpretation in Gurtin and Anand (2009) that the nonlocal term in Aifantis’ formulation should be energetic. Secondly, there is another point of view that GNDs combine with the statistically stored dislocations (SSDs) to provide the forest hardening, which in turn, lead to the dissipative strengthening. For example, in Fleck and Hutchinson (2001), gradient term is implicitly considered as a dissipative quantity, that causes the theory to violate the thermodynamic requirement on plastic dissipation. Fleck and Willis (2009a) developed a mathematical basis for phenomenological gradient plasticity theory corresponding to both rate dependent/independent behaviour with the scalar plastic multiplier. The plastic work in Fleck and Willis (2009a) is taken to be purely dissipative in nature, and the thermodynamic microstresses are assumed to be dissipative. In their incremental form of plasticity theory, an associated plastic

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1 Reprinted with permission from Voyiadjis and Song (2017); Voyiadjis et al. (2017).
flow rule is assumed by means of the convex yield function, consequently, the positive plastic work is ensured.

Meanwhile, Fleck and Willis (2009b) developed a phenomenological flow theory version of SGP theory by extending their theory in Fleck and Willis (2009a) to isotropic and anisotropic solids with tensorial plastic multiplier. Fleck and Willis (2009b) argued that the microstress quantities should include a dissipative part, thus, it has been proposed that the term $\beta \nabla^2 \epsilon^p$ is additively decomposed into an energetic $(\cdot)_{en}$ and dissipative $(\cdot)_{dis}$ in order to develop a kinematic hardening theory. The dissipative stresses satisfy a yield condition with an associated flow plastic rule while the free energy provides the standard kinematic hardening. Reddy (2011) developed a general set of flow rules and associated variational formulations for small deformation rate independent theory based on the thermodynamically theory of Gurtin and Anand (2005a). Reddy (2011) incorporates nonlocal effects of both energetic and dissipative nature with the energetic strengthening associated with the plastic strain gradient and the size dependence increases in yield strength characterized by the dissipative strengthening associated with plastic strain gradient rates. Voyiadjis and Deliktas (2009b) also developed a strain gradient theory based on the decomposition of the state variables into energetic and dissipative components, which in turn, make the constitutive formulations to have both the energetic length scale $\ell_{en}$ and the dissipative length scale $\ell_{dis}$. The interface effect between two grains, by means of two additional length scales, was also incorporated in their work. Their results exhibit that the standard and nonlocal energetic hardening are associated with the plastic strain and the plastic strain gradients respectively, and the dissipative strengthening which characterizes the size effect in yield strength is associated with the plastic strain gradient rate.

There has been an interesting debate between Fleck, Willis, and Hutchinson (Fleck et al., 2014, 2015; Hutchinson, 2012) and Gudmundson, Gurtin, and Anand (Gudmundson, 2004; Gurtin and Anand, 2009) for the last fifteen years or so. Fleck and Hutchinson (2001) developed a phenomenological SGP theory using higher order tensors with a similar framework to that proposed by Aifantis (1984, 1987); Muhlhaus and Aifantis (1991). Higher order stresses and additional boundary conditions have been involved in the theory to develop a generalization of the classical rate-independent $J_2$ flow theory of gradient plasticity. However, they do not discuss the compatibility of their theory with thermodynamic requirements on the plastic dissipation. Gudmundson (2004) and Gurtin and Anand (2009) pointed out that the formulation of Fleck and Hutchinson (2001) violates thermodynamic requirements on the plastic dissipation. Gurtin and Anand (2009) discussed the physical nature of nonlocal terms in the flow rules developed by Fleck and Hutchinson (2001) under isothermal condition and concluded that the flow rule of Fleck and Hutchinson (2001) does not always satisfy the thermodynamic requirement on plastic dissipation unless the nonlocal term is dropped. A formulation of Fleck and Hutchinson (2001) has been modified to meet this thermodynamic requirement by partitioning the higher order microstresses into energetic and dissipative components (Hutchinson, 2012). In addition, Hutchinson (2012) classified the strain gradient version of $J_2$ flow theories into two classes: Incremental theory developed by Fleck and Hutchinson and non-incremental theory developed by Gudmundson, Gurtin, and Anand (c.f. see Fleck et al. (2014, 2015); Gudmundson (2004); Gurtin and Anand (2005a, 2009); Hutchinson (2012) for details). The specific phenomenon in the non-incremental theory that exhibits a finite stress jump due to infinitesimal changes in plastic strain that may occur under the non-proportional loading is noted and its physical acceptance is also discussed in the work of Fleck et al. (2014, 2015). Hutchinson (2012) concluded that discontinuous changes with
infinitesimal changes in boundary loads are physically suspect\(^2\). Fleck et al. (2014, 2015) have shown this phenomenon with two plane strain problems, stretch-passivation problem and stretch-bending problem, for non-proportional loading condition. In their work, it is noted that the dissipative higher order microstress quantities \(\mathbf{S}^{\text{dis}}_{ijk}\) always generate the stress jump for non-proportional loading problems. The main purpose of this dissertation is to explore the stress jump phenomenon with the stretch-surface passivation problem using the finite element method. To the best of the authors’ knowledge, no such investigations have been made yet.

In the works of Voyiadjis and co-workers (Voyiadjis and Faghihi, 2012, 2013, 2014; Voyiadjis et al., 2014), a stress jump occurs when the abrupt surface passivation, which leads to the non-proportional loading path, is introduced. As noted before, the main cause of the stress jump is the presence of the dissipative higher order microstress quantities \(\mathbf{S}^{\text{dis}}_{ijk}\). In this chapter, the formulation for two different cases of the proposed SGP theory with the dissipation potential dependent on \(\dot{\varepsilon}^P_{ij,k}\) and with the dissipation potential independent of \(\dot{\varepsilon}^P_{ij,k}\), are developed based on the new forms of the free energy and the dissipation potentials for eliminating the stress jump phenomenon. Each developed case is applied to the stretch-surface passivation problem in order to compare the behaviour of each case under the non-proportional loading condition. For this, the finite element solution for the stretch-surface passivation problem is developed by using the commercial finite element package ABAQUS/standard (2012) via the user-subroutine UEL. The proposed model and corresponding finite element code are validated by comparing with three sets of small-scale experiments, which have been conducted by Han et al. (2008); Haque and Saif (2003); Xiang and Vlassak (2006). An extensive numerical work is also carried out based on the validated code in order to compare the results from the two cases of the SGP model and to analyze the characteristics of the stress jump phenomenon. The numerical simulation part is largely composed of four subparts. In the first part, the occurrence of the stress jump phenomenon under the stretch-surface passivation condition is introduced in conjunction with the aforementioned three experiments. The second part is focused on showing the results to be contrary to each other from the two cases of the SGP model, and the parametric study in terms of the various material parameters is followed in the third part. In addition the evolution of the free energy involving the stored energy of cold work and the dissipation potentials during the plastic deformation are discussed in the third part. In the last part, the two-dimensional simulation is also given to examine the gradient and grain boundary effect, the mesh sensitivity of the two-dimensional model and the stress jump phenomenon.

2.2 Theoretical formulation of the proposed model

2.2.1 Background

There are some important issues that need to be taken into account in SGP theory for applications such as the interface and thermal effects. In both non-incremental and incremental

\(^2\) Despite the argument of Hutchinson (2012), there is another viewpoint to look at the stress jump phenomenon. The perspective taken in Fleck and Willis (2015) is that it is premature at this moment in time to judge whether a formulation associated with the stress jump is physically acceptable or not, therefore, an in-depth study of dislocation mechanism and microscale experiments with non-proportional loading history is needed.
theories which have been developed by Fleck et al. (2014, 2015); Gudmundson (2004); Gurtin and Anand (2005a); Hutchinson (2012), the thermal effect is not considered, and the interface effect is addressed only by Gudmundson (2004). In the higher order SGP theories, the higher order boundary conditions are naturally required at the free surfaces which can be sources for the defect development and its propagation toward the interior as well as at the interfaces which enhance the resistance to the plastic flow by blocking the dislocations and causing the strain gradients to accommodate the GNDs. In addition, the interfaces such as grain boundaries may act as sources of the dislocations through the transmission of plastic slip to the adjacent grains. Therefore it is needed to incorporate the modeling of the interface effect into the higher order SGP since the interfaces strongly affect the plastic flow of the materials.

Gudmundson (2004) developed a formulation of consistent boundary conditions for an expanding elastic-plastic boundary based on the modified balance law and the condition for the non-negative dissipation at the interface. Three examples, biaxially loaded isotropic thin film on a large elastic substrate, a thin wire of circular cross-section subjected to torsion, and a spherical void under remote hydrostatic tension are investigated in order to illustrate the features of the developed theory. Gudmundson (2004) concluded that there is a close connection between surface energy of an interface and boundary conditions in terms of interface plastic strains and interface moment stresses. This concept has been applied in the work of Fredriksson and Gudmundson (2005a) to analyze the size dependent yield strength of thin films subjected to biaxial strain and pure shear loading respectively. The accumulated dislocations at the interface has been modelled by a surface energy with the single length scale parameter and their numerical results have shown that the size effects with regard to yield strength of thin films for both biaxial and pure shear loading are strongly connected to the surface energy at the interface. Two types of interface models for isotropic materials have been developed by Fredriksson and Gudmundson (2007a) and used to simulate the behaviour of a thin film subjected to biaxial loading. The first model assumes that the plastic work at the interface is purely energetic in terms of the existence of surface energy with the assumption of vanishing dissipation, whereas the second model is purely dissipative in the sense that the surface energy is assumed to vanish and all plastic work at the interface is dissipated. They concluded that two types of interface models give equivalent results under monotonic and proportional loading conditions. Also, the competition between the effects of dissipative plastic strain gradient in the bulk and at the interface is investigated for a thin film, on elastic substrate by Fredriksson and Gudmundson (2007b) within a framework of small SGP. Fredriksson and Gudmundson (2007b) carried out the theoretical study with respect to the effects of interface yield strength and hardening and concluded that the yield strength of the film is determined by the weakest link of the bulk and the interface. The interface models developed by Borg and Fleck (2007); Cermelli and Gurtin (2002); Gurtin (2008); Gurtin and Needleman (2005); Sun et al. (2000) are classified in the identical category as that of Fredriksson and Gudmundson (2005a, 2007a, 2007b). Cermelli and Gurtin (2002) proposed a gradient theory of small deformation single crystal plasticity with a focus on the influence of grain boundaries on the evolution of GNDs in the interior of the grains. Cermelli and Gurtin (2002) concluded that in the initial stages of plastic deformation, where the density of GNDs is small, the grain boundary acts as a barrier for plastic slip, which in turn results in an increase in the density of GNDs. This boundary layer effect is consistent with the results of experiments of Sun et al. (2000), who determined the geometric dislocation tensor in a bicrystal through measurements of lattice rotations. Numerical analysis of a bicrystal for in-plane tensile loading is investigated in Borg and Fleck (2007) by using a strain gradient crystal plasticity theory and an isotropic phenomenological gradient plasticity theory. An internal length scale and
interfacial potential to account for the grain boundary resistance to dislocations are included and the numerical results show that the surface profile adjacent to a grain boundary in a bicrystal is very sensitive to the choice of this internal length scale and interfacial potential. In this regard, interface plays a significant role for the plastic deformation at the micron scale where there exists relatively high ratio of surface area to volume.

Also, in the nano and micro systems, the effect of the higher order gradient on temperature needs to be considered for the fast transient behaviour. When the phonon mean path is in the order of or no fewer than the medium size, the heat transport is partly ballistic rather than purely diffusive. This is caused by the activation of microstructural effects due to the small depth of the heat affected zone or the smallness of the structure and the non-equilibrium transition of thermodynamic circumstances related to reducing the response time (Tzou and Zhang, 1995). If the response time in small volume compounds reduces to the range comparable to the thermalization time, which is the time required for the metal lattice to reach thermodynamic equilibrium states, it results in non-equilibrium transition of thermodynamic states between electrons and phonons (Brorson et al., 1990; Tzou, 1995; Tzou and Zhang, 1995). The classical heat equation is not able to capture the effect of phonon-electron interaction in this time frame, therefore, the microscopic generalized heat equation has to be employed to interpret these phenomena.

Meanwhile, the stored energy of cold work is considered in the present work in the development of thermo-mechanical coupled heat equation. The extensive literature review on the theoretical and experimental developments in terms of the stored energy of cold work has been investigated by Bever and co-workers (Bever et al., 1973; Titchener and Bever, 1958). A main issue in the very early publications was on the determination of experimental values, and it then moved to the interpretation of the stored energy, particularly regarding its dependence on variables and its relation to other property changes due to cold work (Bever et al., 1973). Rosakis and co-workers (Hodowany et al., 2000; Rosakis et al., 2000) have discussed the notion of stored energy of cold work within a conventional theoretical framework, and a number of experimental works regarding the stored energy of cold work have been carried out since the pioneering experiments of Taylor and co-workers (Farren and Taylor, 1925; Quinney and Taylor, 1937; Taylor and Quinney, 1934). Recently, Anand et al. (2015) proposed a single crystal gradient thermo-plasticity theory that accounts for the stored energy of cold work and thermal annealing. The numerical implementation of this work using the finite element method was conducted by (McBride et al., 2015). In the present work, the functional form of the stored energy of cold work is postulated in order to derive the thermo-mechanical coupled heat equation.

A coupled thermo-mechanical and thermodynamic consistent higher order SGP theories including the interface effect and the thermal effect have been developed by Voyiadjis and co-workers to investigate the behaviour of small-scale metallic materials (Faghihi and Voyiadjis, 2012, 2014; Faghihi et al., 2013; Voyiadjis and Deliktas, 2009a, b; Voyiadjis and Faghihi, 2012, 2013, 2014; Voyiadjis et al., 2014). All the works of Voyiadjis and co-workers considered the effects of interface energy that are incorporated into the formulation to address various boundary conditions, strengthening, and formation of the boundary layers as well as the thermal effects that are crucial, for instance, for simulating the behaviour of high speed machining for metallic materials using the SGP models. In this section, two different cases of the high order SGP theory proposed by the authors are studied with and without the dissipative higher order microstress quantities $S_{ijk}^{dis}$ based on the new forms of the free energy and the dissipation potentials for eliminating an elastic loading gap.
2.2.2 Principle of virtual power for the bulk and interface

![Figure 2.1](image)

The principle of virtual power is used to derive the equations for the local equation of motion and the nonlocal microforce balance for volume $V$ as well as the equations for local traction force and nonlocal microtraction condition for the external surface $S$ respectively. In the presence of varying temperature fields at the microstructure level, the formulation should incorporate the effects of the temperature gradient on the thermo-mechanical behaviour of the material due to the micro-heterogeneous nature of material (Forest and Amestoy, 2008). In this sense, it is assumed here that the plastic strain, plastic strain gradient, temperature and temperature gradient contribute to the power per unit volume.

Moreover, as it is mentioned in the previous section, the effect of the interface plays a crucial role for the plastic behaviour of the material at the microscale. An interface (grain boundary) separating grains $G_1$ and $G_2$ is taken into account here and it is assumed that the displacement field is continuous, i.e. $u_{i}^{G_1} = u_{i}^{G_2}$, across the grain boundary (Figure 2.1). As shown in this figure, a dislocation moving toward the grain boundary in grain $G_1$ cannot pass through the grain boundary but it is trapped and accumulated at the grain boundary due to the misalignment of the grains $G_1$ and $G_2$ that are contiguous to each other. In this sense, the grain boundary acts as an obstacle to block the dislocation movement, therefore the yield strength of the material increases as the number of grain boundaries increases. By assuming that the interface surface energy depends on the plastic strain rate at the interface of the plastically deforming phase, the internal part of the principle of virtual power for the bulk $P_{int}$ and for the interface $P_{int}^I$ are expressed in terms of the energy contributions in the arbitrary subregion of the volume $V$ and the arbitrary subsurface of the interface $S^I$ respectively as follows:

$$P_{int} = \int_{V} \left( \sigma_{ij} \dot{\varepsilon}_{ij} + X_{ij} \dot{\varepsilon}_{ij} + S_{ijk} \dot{\varepsilon}_{ij,k} + \mathcal{A} \dot{T} + \mathcal{B} i \dot{T} \right) dV$$

(2.2)
\[ P_{\text{int}}^i = \int_{S^i} \left( M_{ij}^{G_1} \dot{\varepsilon}_{ij}^{pG_1} + M_{ij}^{G_2} \dot{\varepsilon}_{ij}^{pG_2} \right) dS^i \]  \hspace{1cm} (2.3)

where the superscripts ‘e’, ‘p’, and ‘I’ are used to express the elastic state, the plastic state, and the interface respectively. The internal power for the bulk in the form of Equation (2.2) is defined using the Cauchy stress tensor \( \sigma_{ij} \), the backstress \( \chi_{ij} \) conjugate to the plastic strain rate \( \dot{\varepsilon}_{ij}^p \), the higher order microstress \( S_{ijk} \) conjugate to the gradients of the plastic strain rate \( \dot{\varepsilon}_{ij,k}^p \), and the generalized stresses \( \mathcal{A} \) and \( \mathcal{B}_i \) conjugate to the temperature rate \( \dot{T} \) and the gradient of the temperature rate \( \dot{T}_i \) respectively. The terms \( \mathcal{A} \) and \( \mathcal{B}_i \) are also called microforces according to Gurtin’s terminology (Gurtin, 1996). The internal power for the interface in the form of Equation (2.3) is defined using the interfacial microscopic moment tractions \( M_{ij}^{G_1} \) and \( M_{ij}^{G_2} \) expending power over the interfacial plastic strain rates \( \dot{\varepsilon}_{ij}^{pG_1} \) at \( S_{ij}^{G_1} \) and \( \dot{\varepsilon}_{ij}^{pG_2} \) at \( S_{ij}^{G_2} \) respectively.

Moreover, since the plastic deformation, which is accommodated by the generation and motion of the dislocation, is influenced by the interfaces, Equations (2.3) results in higher order boundary conditions generally consistent with the framework of a gradient type theory. These extra boundary conditions should be imposed at internal and external boundary surfaces or interfaces between neighboring grains (Aifantis and Willis, 2005; Gurtin, 2008). The internal power for the bulk is balanced with the external power for the bulk expended by the tractions on the external surfaces \( S \) and the body forces acting within the volume \( V \) as shown below:

\[ P_{\text{ext}} = \int_V b_i v_i \, dV + \int_S \left( t_i v_i + m_{ij} \dot{\varepsilon}_{ij}^p + \alpha \dot{T} \right) dS \] \hspace{1cm} (2.4)

where \( t_i \) and \( b_i \) are traction and the external body force conjugate to the macroscopic velocity \( v_i \) respectively. It is further assumed here that the external power has terms with the microtraction \( m_{ij} \) and \( \alpha \), conjugate to the plastic strain rate \( \dot{\varepsilon}_{ij}^p \) and the temperature rate \( \dot{T} \) respectively since the internal power in Equation (2.2) contains the terms of the gradients of the plastic strain rate \( \dot{\varepsilon}_{ij,k}^p \) and the gradients of the temperature rate \( \dot{T}_i \) respectively.

Making use of the principle of virtual power that the external power is equal to the internal power (\( P_{\text{int}} = P_{\text{ext}} \)) along with the integration by parts on some terms in Equation (2.2), and utilizing the divergence theorem, the equations for balance of linear momentum and nonlocal microforce balance can be represented respectively, for volume \( V \), as follows:

\[ \sigma_{ij,j} + b_i = 0 \] \hspace{1cm} (2.5)

\[ \chi_{ij} - \tau_{ij} - S_{ij,k} = 0 \] \hspace{1cm} (2.6)

\[ \text{div} \mathcal{B}_i - \mathcal{A} = 0 \] \hspace{1cm} (2.7)

where \( \tau_{ij} = \sigma_{ij,j} - \frac{1}{3} \sigma_{kk} \delta_{ij} \) is the deviatoric part of the Cauchy stress tensor and \( \delta_{ij} \) is the Kronecker delta.

On the external surface \( S \), the equations for local surface traction conditions and nonlocal microtraction conditions can be written respectively with the outward unit normal vector to \( S \), \( n_k \), as follows:

\[ t_i = \sigma_{ij} n_i \] \hspace{1cm} (2.8)

\[ m_{ij} = S_{ij,k} n_k \] \hspace{1cm} (2.9)

\[ \alpha = B_i n_i \] \hspace{1cm} (2.10)

In addition, the interfacial external power \( P_{\text{ext}}^I \), which is balanced with the interfacial internal power \( P_{\text{int}}^I \), is expended by the macrotractions \( \sigma_{ij}^{G_1}(-n_i^f) \) and \( \sigma_{ij}^{G_2}(n_i^f) \) conjugate to the
macroscopic velocity \( \rho_i \), and the microtractions \( \mathbf{S}_{ijkl}^{G_1} (n_k^l) \) and \( \mathbf{S}_{ijkl}^{G_2} (n_k^l) \) that are conjugate to \( \dot{\varepsilon}_{ij}^{G_1} \) and \( \dot{\varepsilon}_{ij}^{G_2} \) respectively as follows:

\[
P_{\text{ext}}^I = \int_{S^I} \left\{ (\sigma_{ij}^{G_2} n_j^l - \sigma_{ij}^{G_1} n_j^l) \rho_i + \mathbf{S}_{ijkl}^{G_2} n_k^l \dot{\varepsilon}_{ij}^{G_2} - \mathbf{S}_{ijkl}^{G_1} n_k^l \dot{\varepsilon}_{ij}^{G_1} \right\} dS^I \tag{2.11}
\]

By equating \( P_{\text{int}}^I = P_{\text{ext}}^I \) with considering the arbitrary variation of the plastic strain at the interface, the interfacial macro- and microforce balances can be obtained as follows:

\[
(\sigma_{ij}^{G_1} - \sigma_{ij}^{G_2}) n_j^l = 0 \tag{2.12}
\]
\[
\mathbf{M}_{ij}^{G_1} + \mathbf{S}_{ijkl}^{G_2} n_k^l = 0 \tag{2.13}
\]
\[
\mathbf{M}_{ij}^{G_2} - \mathbf{S}_{ijkl}^{G_1} n_k^l = 0 \tag{2.14}
\]

The microforce balance conditions in Equation (2.13) and Equation (2.14) represent the coupling behaviour in the grain interior at the interface to the behaviour of the interface, since the microtractions \( \mathbf{S}_{ijkl}^{G_1} n_k^l \) and \( \mathbf{S}_{ijkl}^{G_2} n_k^l \) are the special cases of Equation (2.8) for the internal surface of the interface.

### 2.2.3 Thermodynamic formulation with higher order gradients for stress and temperature

The first law of thermodynamics, which encompasses several principles including the law of conservation of energy, is taken into account in the present work in order to develop a thermodynamically consistent formulation accounting for the thermo-mechanical behaviour of small-scale metallic volumes during the fast transient process. Viscoelastic adiabatic deformation of metals is not only influenced by the rate of loading but also by the initial testing temperature as well as its evolution due to conversion of the plastic work into heat. In order to consider micromechanical evolution in the first law of thermodynamics, the enhanced SGP theory with the plastic strain gradient is employed for the mechanical part of the formulation, whereas the micromorphic model is employed for the thermal counterpart as follows (see the work of Forest and co-workers (Forest and Aifantis, 2010; Forest and Amestoy, 2008; Forest and Sievert, 2003)):

\[
\rho \dot{\mathbf{E}} = \sigma_{ij} \dot{\varepsilon}_{ij}^{ex} + \mathbf{X}_{ij} \dot{\varepsilon}_{ij}^{pl} + \mathbf{S}_{ijkl} \dot{\varepsilon}_{ij,k}^{pl} + \mathbf{A} \dot{T} + \mathbf{B}_{ij} \dot{T}_{,i} - \text{div} \mathbf{q}_i \tag{2.15}
\]
\[
\dot{\mathbf{E}}^T = \mathbf{M}_{ij}^{pl} \dot{\varepsilon}_{ij}^{pl} + \mathbf{q}_i^T n_i^l \tag{2.16}
\]

where \( \rho \) is the mass density, \( \mathbf{E} \) is the specific internal energy, \( \dot{\mathbf{E}} \) is the internal surface energy density at the contacting surface, and \( \mathbf{q}_i \) and \( \mathbf{q}_i^T \) are the heat flux vectors of the bulk and the interface respectively.

The second law of thermodynamics, or entropy production inequality as it is often called, yields a physical basis that accounts for the distribution of GNDs within the body along with the energy carrier scattering and requires that the free energy increases at a rate not greater than the rate at which work is performed. Based on this requirement, entropy production inequalities for the bulk and the interface can be expressed respectively as follows:

\[
\rho \dot{s} - \rho \dot{\mathbf{E}} - \sigma_{ij} \dot{\varepsilon}_{ij}^{ex} - \mathbf{X}_{ij} \dot{\varepsilon}_{ij}^{pl} - \mathbf{S}_{ijkl} \dot{\varepsilon}_{ij,k}^{pl} - q_i \frac{T}{T} + \mathbf{A} \dot{T} + \mathbf{B}_{ij} \dot{T}_{,i} \geq 0 \tag{2.17}
\]
\[
\dot{s}^T - q_i^T n_i^l \geq 0 \tag{2.18}
\]

where \( s \) is the specific entropy, and \( s^T \) is the surface density of the entropy of the interface.
2.2.4 The energetic and dissipative components of the thermodynamic microstresses

Internal energy $\Theta$, temperature $T$, and entropy $s$ describing the current state of the material can be attributed to the Helmholtz free energy $\Psi$ (per unit volume) such as

$$\Psi = \Theta - Ts$$

(2.19)

By taking the time derivative of Equation (2.19) for the bulk and the interface and substituting each into Equation (2.17) and Equation (2.18) respectively, the nonlocal free energy (i.e. Clausius-Duhem) inequality for the bulk and the interface can be obtained as follows:

$$\sigma_{ij}\dot{\varepsilon}_{ij}^e + X_{ij}\dot{\varepsilon}_{ij}^p + S_{ijk}\dot{\varepsilon}_{ij,k}^p + \mathcal{A}\dot{T} + B_i\dot{T}_i - \rho\dot{\Psi} - \rho s\dot{s} - q_i\frac{T_i}{T} \geq 0$$

(2.20)

$$\mathcal{M}_{ij}^l\dot{\varepsilon}_{ij}^{pl} - \dot{\Psi}^I - s^I\dot{T} \geq 0$$

(2.21)

In order to derive the constitutive equations within a small-scale framework, an attempt to account for the effect of non-uniform distribution of the microdefection with temperature on the homogenized response of the material is carried out in the present work with the functional forms of Helmholtz free energy in terms of state variables. By assuming the isothermal condition for the interface (i.e. $T^I = 0$), the Helmholtz free energy for the bulk and the interface are given respectively by

$$\Psi = \Psi(e_{ij}^e, e_{ij}^p, e_{ij,k}^p, T, T_i)$$

(2.22)

$$\Psi^I = \Psi^I(e_{ij}^{pl})$$

(2.23)

where the function $\Psi$ is assumed to be smooth and the function $\Psi^I$ is assumed to be convex with respect to a plastic strain at the interface $e_{ij}^{pl}$.

During the process of establishing the constitutive equations, the thermodynamic requirement that the plastic dissipation work must be non-negative has to be preserved. Taking time derivative of the Helmholtz free energy for the bulk $\dot{\Psi}$ and the interface $\dot{\Psi}^I$ give the following expressions respectively

$$\dot{\Psi} = \frac{\partial \Psi}{\partial e_{ij}^e}\dot{e}_{ij}^e + \frac{\partial \Psi}{\partial e_{ij}^p}\dot{e}_{ij}^p + \frac{\partial \Psi}{\partial e_{ij,k}^p}\dot{e}_{ij,k}^p + \frac{\partial \Psi}{\partial T}\dot{T} + \frac{\partial \Psi}{\partial T_i}\dot{T}_i$$

(2.24)

$$\dot{\Psi}^I = \frac{\partial \Psi^I}{\partial e_{ij}^{pl}}\dot{e}_{ij}^{pl}$$

(2.25)

By substituting Equation (2.24) into Equation (2.20) for the bulk and Equation (2.25) into Equation (2.21) for the interface, and factoring out the common terms, one obtains the following inequalities:

$$\left(\sigma_{ij} - \rho \frac{\partial \Psi}{\partial e_{ij}^e}\right)\dot{e}_{ij}^e + \left(X_{ij} - \rho \frac{\partial \Psi}{\partial e_{ij}^p}\right)\dot{e}_{ij}^p + \left(S_{ijk} - \rho \frac{\partial \Psi}{\partial e_{ij,k}^p}\right)\dot{e}_{ij,k}^p$$

$$+ \left(\mathcal{A} - \rho s - \rho \frac{\partial \Psi}{\partial T}\right)\dot{T} + \left(B_i - \rho \frac{\partial \Psi}{\partial T_i}\right)\dot{T}_i - q_i T_i \geq 0$$

(2.26)

$$\mathcal{M}_{ij}^l\dot{e}_{ij}^{pl} - \frac{\partial \Psi^I}{\partial e_{ij}^{pl}}\dot{e}_{ij}^{pl} \geq 0$$

(2.27)

Guided by Equations (2.26) and (2.27), it is further assumed that the thermodynamic microstress quantities $X_{ij}, S_{ijk}, \mathcal{A}$ and $\mathcal{M}_{ij}^l$ are decomposed into the energetic and the dissipative components such as

$$X_{ij} = X_{ij}^{en} + X_{ij}^{dis}$$

(2.28)
\[ S_{ijk} = S_{ijk}^{en} + S_{ijk}^{dis} \quad (2.29) \]
\[ \mathcal{A} = \mathcal{A}_{ij}^{en} + \mathcal{A}_{ij}^{dis} \quad (2.30) \]
\[ M_{ij}^l = M_{ij}^{l,en} + M_{ij}^{l,dis} \quad (2.31) \]

The components \( M_{ij}^{l,en} \) and \( M_{ij}^{l,dis} \) represent the mechanisms for the pre- and post-slip transfer, and thus involve the plastic strain at the interface prior to the slip transfer \( \varepsilon_{ij}^{p,(pre)} \) and the one after the slip transfer \( \varepsilon_{ij}^{p,(post)} \) respectively. The overall plastic strain at the interface can be obtained by the summation of both plastic strains such as:
\[ \varepsilon_{ij}^{p} = \varepsilon_{ij}^{p,(pre)} + \varepsilon_{ij}^{p,(post)} \quad (2.32) \]

Substituting Equations (2.28), (2.29), (2.30) into Equation (2.26) for the bulk and Equation (2.31) into Equation (2.27) for the interface, and rearranging them in accordance with the energetic and the dissipative parts give the following expressions:
\[ \left( \sigma_{ij} - \rho \frac{\partial \psi}{\partial \varepsilon_{ij}^e} \right) \dot{\varepsilon}_{ij}^e + \left( \chi_{ij}^{en} - \rho \frac{\partial \psi}{\partial \varepsilon_{ij}^p} \right) \dot{\varepsilon}_{ij}^p + \left( S_{ijk}^{en} - \rho \frac{\partial \psi}{\partial \varepsilon_{ij,k}^p} \right) \dot{\varepsilon}_{ijk}^p \]
\[ + (\mathcal{A}_{en} - \rho s - \rho \frac{\partial \psi}{\partial T}) \dot{T} + (\mathcal{B}_l - \rho \frac{\partial \psi}{\partial T, i}) \dot{T}_l + \mathcal{X}_{ij}^{dis} \dot{\varepsilon}_{ij}^p \
\[ + S_{ij,k}^{dis} \dot{\varepsilon}_{ij,k}^p + A^{dis} \dot{T} - \frac{q_i}{T} \dot{T}_i \geq 0 \quad (2.33) \]
\[ \left( M_{ij}^{l,en} - \rho \frac{\partial \psi_{ij}^l}{\partial \varepsilon_{ij}^p} \right) \dot{\varepsilon}_{ij}^{p,l} + M_{ij}^{l,dis} \dot{\varepsilon}_{ij}^{p,l} \geq 0 \quad (2.34) \]

From the above equations with the assumption that the fifth term in Equation (2.33) is strictly energetic, one can retrieve the definition of the energetic part of the thermodynamic microstresses as follows:
\[ \sigma_{ij} = \rho \frac{\partial \psi}{\partial \varepsilon_{ij}^e}; \quad \chi_{ij}^{en} = \rho \frac{\partial \psi}{\partial \varepsilon_{ij}^p}; \quad S_{ijk}^{en} = \rho \frac{\partial \psi}{\partial \varepsilon_{ij,k}^p}; \]
\[ A^{en} = \rho \left( s + \frac{\partial \psi}{\partial T} \right); \quad B_l = \rho \frac{\partial \psi}{\partial T, i}; \]
\[ M_{ij}^{l,en} = \rho \frac{\partial \psi_{ij}^l}{\partial \varepsilon_{ij}^p} \quad (2.35) \]

Hence the residual respective dissipation is then obtained as:
\[ \mathcal{D} = \mathcal{X}_{ij}^{dis} \dot{\varepsilon}_{ij}^p + S_{ij,k}^{dis} \dot{\varepsilon}_{ij,k}^p + A^{dis} \dot{T} - \frac{q_i}{T} \dot{T}_i \geq 0 \quad (2.37) \]
\[ \mathcal{D}^l = M_{ij}^{l,dis} \dot{\varepsilon}_{ij}^{p,l} \geq 0 \quad (2.38) \]
where \( \mathcal{D} \) and \( \mathcal{D}^l \) are the dissipation densities per unit time for the bulk and the interface respectively. The definition of the dissipative thermodynamic microstresses can be obtained from the complementary part of the dissipation potentials \( \mathcal{D}(\dot{\varepsilon}_{ij}^p, \dot{\varepsilon}_{ij,k}^p, \dot{T}, \dot{T}_i) \) and \( \mathcal{D}^l(\dot{\varepsilon}_{ij}^{p,l}) \) such as
\[ \chi_{ij}^{dis} = \frac{\partial \mathcal{D}}{\partial \dot{\varepsilon}_{ij}^p}; \quad S_{ij,k}^{dis} = \frac{\partial \mathcal{D}}{\partial \dot{\varepsilon}_{ij,k}^p}; \quad A^{dis} = \frac{\partial \mathcal{D}}{\partial T}; \quad -\frac{q_i}{T} = \frac{\partial \mathcal{D}}{\partial T_i} \quad (2.39) \]
\[ M_{ij}^{l,dis} = \frac{\partial \mathcal{D}^l}{\partial \dot{\varepsilon}_{ij}^{p,l}} \quad (2.40) \]
One now proceeds to develop the constitutive laws for both the energetic and the dissipative parts which are achieved by employing the free energy and the dissipation potentials, which relate the stresses to their work-conjugate generalized stresses. The functional forms of the Helmholtz free energy and dissipation potential and the corresponding energetic and dissipative thermodynamic microstresses for the aforementioned two different cases of the model, i.e. the case with the dissipative higher order microstress quantities $S_{ijk}^{dis}$ and the one without $S_{ijk}^{dis}$, are developed in the remainder of Section 2.2.

2.2.5 Helmholtz free energy and energetic thermodynamic microstresses

Defining a specific form of the Helmholtz free energy function $\Psi$ is tremendously important since it constitutes the bases in deriving the constitutive equations, and it has to take not only the material type such as fcc metals, bcc metals, polymer, steel alloys, concrete, etc. but also the deformation condition such as rate independent/rate dependent and/or adiabatic/isothermal into consideration. The complexity of any model is directly determined by the form of the Helmholtz free energy and by the number of conjugate pair of variables. In the current work, the Helmholtz free energy function is put forward with three main counterparts, i.e. elastic, defect and thermal energy, as follows:

$$
\Psi = \left\{ \frac{1}{2\rho} \varepsilon^e_{ij} E_{ijkl} \varepsilon^e_{kl} - \frac{\alpha_t}{\rho} (T - T_r) \varepsilon^p_{ij} \delta_{ij} \right\}^{\psi^e_{(elastic)}} + \frac{1}{\rho} \left\{ \frac{h}{r + 1} \left( 1 - \left( \frac{T}{T_y} \right)^n \right) \varepsilon^{r+1}_p + \frac{G}{2} \varepsilon^p_{en} \varepsilon^p_{lm} \varepsilon^p_{lm,n} \right\}^{\psi^d_{(defect)}} + \left\{ -\frac{1}{2T_r} (T - T_r)^2 - \frac{1}{2\rho} \alpha T_r T_{ij} \right\}^{\psi^t_{(thermal)}}
$$

(2.41)

where $E_{ijkl}$ is the elastic modulus tensor, $\alpha_t$ is the coefficient of linear thermal expansion, $T_r$ is the reference temperature, $h$ is the hardening material constant corresponding to linear kinematic hardening, $r$ ($0 < r < 1$) is the isotropic hardening material constant, $\varepsilon_p = \sqrt{\varepsilon^p_{ij} \varepsilon^p_{ij}}$ is the accumulated plastic strain, $T_y$ and $n$ are the thermal material constants that need to be calibrated by comparing with the experimental data, $\ell_{en}$ is the energetic length scale that describes the feature of the short-range interaction of GNDs, $G$ is the shear modulus for isotropic linear elasticity, $c_e$ is the specific heat capacity at constant stress, and $\alpha$ is a material constant accounting for the interaction between energy carriers such as phonon-electron. The term $\left( 1 - \left( T / T_y \right)^n \right)$ in Equation (2.41) accounts for the thermal activation mechanism for overcoming the local obstacles to dislocation motion.

The first term of the defect energy $\psi^d_1$ characterizes the interaction between slip systems, i.e. the forest dislocations leading to isotropic hardening. This term is further assumed to be decomposed into the recoverable counterpart $\psi^d_{1,R}$ and non-recoverable counterpart $\psi^d_{1,NR}$. The
establishment of the plastic strain gradient independent stored energy of cold work with no additional material parameters is achievable with this decomposition.

The recoverable counterpart, $\Psi_{1}^{d,R}$, in the present work, accounts for the stored energy of cold work. When the elasto-plastic solid is cold-worked, most of the mechanical energy is converted into heat, but the remaining contributes to the stored energy of cold work through the creation and rearrangement of crystal defects such as dislocations, point defects, line defects and stacking faults (Rosakis et al., 2000). The ratio of the inelastic heating over the rate of the plastic work, commonly denoted by $\beta$, is determined by the specific form of the stored energy of cold work and the evolution laws governing plastic flow. In the early literature concerning this subject, it is typically assumed that $\beta$ is a constant. The reported values of $\beta$ ranges between zero and 20 percent (Belytschko et al., 1991; Kapoor and Nemat-Nasser, 1998; Needleman and Tvergaard, 1995) and these values are often justified by comparing with the experimental work of G. I. Taylor and co-workers (Farren and Taylor, 1925; Quinney and Taylor, 1937; Taylor and Quinney, 1934). However, it is known that $\beta$ is dependent on the history of the plastic deformation (Rosakis et al., 2000). Mason et al. (1994) investigated the functional dependence of $\beta$ on the strain and the strain rate in a range of metals via the fully dynamic Kolsky pressure bar tests and concluded that assuming $\beta$ to be a constant may result in inaccuracies in modeling the thermo-mechanical behaviour of materials. Thus, assuming a proper form of the free energy function is necessary to accurately account for the thermo-mechanical coupling and to model a complete thermo-plastic constitutive model.

In the present work, the plastic strain dependent free energy, $\Psi_{1}^{d,R}$, accounting for the stored energy of cold work is derived by assuming that the stored energy is related to the energy carried by dislocations. Mollica et al. (2001) investigated the inelastic behaviour of the metals subject to loading reversal by linking the hardening behaviour of the material to thermo-dynamical quantities such as the stored energy due to cold work and the rate of dissipation. In the work of Mollica et al. (2001), it is assumed that the stored energy depends on the density of the dislocation network that increases with monotonic plastic deformation until it is saturated at some point. This points out that the material stores this energy for a certain range of the accumulated plastic strain, after which the material will mainly dissipate the external work supply.

For the derivation of the stored energy of cold work, one assumes that the energetic microstress $\chi_{ij}^{en}$, given later by Equation (2.52), can be expressed by separation of variables as follows:

$$\chi_{ij}^{en}(\varepsilon_{ij}^{p}, T) = \Sigma(\varepsilon_{ij}^{p})\mathcal{T}(T)$$

(2.42)

with $\Sigma(\varepsilon_{ij}^{p}) = h\varepsilon_{ij}^{p}e^{r-1}$ and $\mathcal{T}(T) = (1 - (T/T_y)^n)$.

On the other hand, instead of using the plastic strain at the macroscale level to describe the plastic deformation, $\Sigma$ can be defined at the microscale level using the Taylor law, which gives a simple relation between the shear strength and the dislocation density, as follows:

$$\Sigma = \zeta Gb\sqrt{\rho_t}$$

(2.43)

where $\zeta$ is the statistical coefficient accounting for the deviation from regular spatial arrangements of the dislocation populations, $b$ is the magnitude of the Burgers vector, and $\rho_t$ is the equivalent total dislocation density and can be obtained by $(\Sigma/\zeta Gb)^2$ from Equation (2.43).

Here, it is assumed that the stored energy of cold work, the result of energy carried by each dislocation, results in an extra latent hardening which is recoverable and temperature independent. Thus, the recoverable energy of cold work can be put forward as follows:
\[
\psi_{1}^{d,R} = \mathbb{U}\rho_t
\] (2.44)

where \(\mathbb{U}\) is the elastic deformation energy of a dislocation and can be approximately given by

\[
\mathbb{U} = \frac{Gb^2}{4\pi} \ln \left( \frac{R}{R_0} \right)
\] (2.45)

where \(R\) is the cut-off radius (\(R \approx 10^3 b\)) and \(R_0\) is the internal radius (\(b < R_0 < 10 b\)) (Meyers and Chawla, 2009). By substituting \(\rho_t = (\Sigma / \zeta Gb)^2\) into Equation (2.45) along with Equation (2.42), one can obtain the stored energy of cold work as follows:

\[
\psi_{1}^{d,R} = \vartheta h^2 e_{p}^{2r}
\] (2.46)

where by comparing the aforementioned ranges for \(R, R_0\), and \(\zeta\) to the shear modulus \(G\), \(\vartheta\) can be expressed by

\[
\vartheta = \frac{1}{4\pi c^2 G} \ln \left( \frac{R}{R_0} \right) \approx \frac{1}{G}
\] (2.47)

The non-recoverable counterpart \(\psi_{1}^{d,NR}\) accounting for the energetically based hardening rule that mimics the dissipative behaviour by describing irreversible loading processes can then be derived as follows (Gurtin and Reddy, 2009):

\[
\psi_{1}^{d,NR} = \frac{h}{r + 1} \left( 1 - \left( \frac{T_r}{T_y} \right)^{n} \right) e_{p}^{r+1} - \vartheta h^2 e_{p}^{2r}
\] (2.48)

where \(\vartheta\) is a constant that depends on the material microstructure.

The second term of the defect energy \(\psi_{2}^{d}\) characterizes the short-range interactions between coupling dislocations moving on close slip planes and leads to the kinematic hardening. This defect energy \(\psi_{2}^{d}\) is recoverable in the sense that, by starting at any value of the accumulated plastic strain gradients, \(\psi_{2}^{d}\) returns to its original value as the accumulated plastic strain gradients return to their original value.

One can now obtain the energetic thermodynamic forces by using the definitions in Equation (2.35) along with the Helmholtz free energy given by Equation (2.41) as follows:

\[
\sigma_{ij} = E_{ijkl} e_{kl}^{p} - \alpha_{t}(T - T_r) \delta_{ij}
\] (2.49)

\[
\mathcal{A}^{en} = \rho \varepsilon - \alpha_{t}(T - T_r) \varepsilon_{ij}^{p} \delta_{ij} - \frac{c_{x}}{T_r} (T - T_r) - \frac{h e_{p}^{p+1} n}{r + 1} \left( \frac{T}{T_y} \right)^{n-1}
\] (2.50)

\[
B_i = -a T_i
\] (2.51)

\[
X_{ij}^{en} = h e_{ij}^{p} \left( 1 - \left( \frac{T}{T_y} \right)^{n} \right) e_{p}^{r-1}
\] (2.52)

\[
S_{ijk}^{en} = G \varepsilon_{ij}^{p} \varepsilon_{jk}^{p}
\] (2.53)

Here, according to the aforementioned decomposition of the first term of the defect energy into the recoverable and non-recoverable counterparts, \(X_{ij}^{en}\) can be further decomposed into recoverable \((X_{ij}^{en,R})\) and non-recoverable \((X_{ij}^{en,NR})\) counterparts as follows:

\[
X_{ij}^{en,R} = 2r \vartheta h^2 e_{ij}^{p} e_{p}^{2r-2}
\] (2.54)

\[
X_{ij}^{en,NR} = h e_{ij}^{p} \left( 1 - \left( \frac{T}{T_y} \right)^{n} \right) e_{p}^{r-1} - 2r \vartheta h^2 e_{ij}^{p} e_{p}^{2r-2}
\] (2.55)

From the aforementioned physical interpretations of \(\psi_{1}^{d,R}\) and \(\psi_{1}^{d,NR}\), \(X_{ij}^{en,R}\) and \(X_{ij}^{en,NR}\) can be defined as the terms describing the reversible loading due to the energy carried by
dislocations and the energetically based hardening rule that mimics dissipative behaviour by describing irreversible loading processes respectively.

Meanwhile, it is well known that the interface plays a role as the barrier to plastic slip in the early stages of plastically deforming phase, while it acts as a source of the dislocation nucleation in the later stages. The energetic condition in the area around the interface in affected by the long-range internal stress fields associated with constrained plastic flow which lead to the accumulated and pile-up of dislocations near the interface. Thus, the condition at the interface is determined by a surface energy that depends on the plastic strain state at the interface (Fredriksson and Gudmundson, 2005a).

The interfacial Helmholtz free energy per unit surface area of the interface in the present work, is put forward under the guidance of Fredriksson and Gudmundson (2005a) work such as

\[ \Psi^I = \frac{1}{2} G \ell_{en} \epsilon_{ij}^{l(pre)} \epsilon_{ij}^{p(pre)} \]  

(2.56)

where \( \ell_{en} \) is the interfacial recoverable length scale.

By substituting the interfacial Helmholtz free energy per unit surface given by Equation (2.56) into Equation (2.36), the interfacial recoverable microstresses \( \mathbb{M}_{ij}^{len} \) can be obtained as follows:

\[ \mathbb{M}_{ij}^{len} = G \ell_{en} \epsilon_{ij}^{p(pre)} \]  

(2.57)

As can be seen in Equation (2.57), \( \mathbb{M}_{ij}^{len} \) does not involve the plastic strain rate, which is related to the dislocation slip, and the temperature since the interfacial recoverable microstresses are activated by the recoverable stored energy.

It should be noted that the functional forms of the Helmholtz free energy for the bulk \( \Psi \) given by Equation (2.41), corresponding energetic thermodynamic microstresses given by Equation (2.49) ~ Equation (2.55), the functional form of the Helmholtz free energy for the interface \( \Psi^I \) given by Equation (2.56) and corresponding energetic thermodynamic microstresses given by Equation (2.57) are shared in both cases of the SGP model, i.e. the case with the dissipative higher order microstress quantities \( S_{ijkl}^{dis} \) and the one without \( S_{ijkl}^{dis} \).

2.2.6 Dissipation potential and dissipative thermodynamic microstresses

In this section, the dissipation potential functions for the aforementioned two cases of the SGP model are postulated respectively. The first case is derived from the dissipation potential dependent on the plastic strain gradient, which leads to the non-zero dissipative thermodynamic microstress \( S_{ijkl}^{dis} \neq 0 \), while the other case is derived from the dissipation potential independent on the plastic strain gradient, which leads to \( S_{ijkl}^{dis} = 0 \).

Coleman and Gurtin (1967) pointed out that the dissipation potential function is composed of two parts, the mechanical part which is dependent on the plastic strain and its gradient and the thermal counterpart which shows the purely thermal effect such as the heat conduction. In this sense, and in the context of Equation (2.37), the functional form of the dissipation potential, which is dependent on \( \dot{\epsilon}_{ij}^P \), for the former class can be put forward as:

---

3 It should be noted that it is possible to introduce another form of the surface energy if it is convex in \( \epsilon_{ij}^{pl} \).
\[
\mathcal{D} = \frac{\sigma_y}{2\mathcal{P}} \left( \left( \frac{\dot{\phi}}{\dot{\phi}_0} \right)^m \left( 1 - \left( \frac{T}{T_y} \right)^n \right) \varepsilon_{ij}^p \varepsilon_{ij}^p \right) + \varepsilon_{dis}^2 \left( \frac{\dot{\phi}}{\dot{\phi}_0} \right)^m \left( 1 - \left( \frac{T}{T_y} \right)^n \right) \varepsilon_{lm,k}^p \varepsilon_{lm,k}^p \right) - \frac{\dot{\sigma}}{2} \dot{T}^2 \tag{2.58}
\]

where \(\sigma_y\) is a material constant accounting for the yield strength, \(m\) is a non-negative material constant for the rate sensitivity parameter, in which the limit \(m \to 0\) corresponds to rate-independent material behaviour, \(\dot{\phi}_0\) is a constant for the reference flow rate, \(\varepsilon_{dis}\) is the dissipative length scale that corresponds to the dissipative effects in terms of the gradient of the plastic strain rate, \(\dot{\sigma}\) is the material constant accounting for the energy exchange between phonon and electron, and \(\kappa(T)\) is the thermal conductivity coefficient. The generalized dissipative effective plastic strain measure \(\dot{\phi}\) is defined as a function of the plastic strain rate, the gradient of the plastic strain rate and the dissipative length scale as follows:

\[
\dot{\phi} = \sqrt{\varepsilon_{ij}^p \varepsilon_{ij}^p + \varepsilon_{dis}^2 \varepsilon_{lm,k}^p \varepsilon_{lm,k}^p} \tag{2.59}
\]

It should be pointed out that the mechanical counterparts in Equation (2.58) only concern the initial yield stress depending on the accumulated dislocation density, introduced by Ohno and Okumura (2007), and does not involve the forest dislocation density, as it is considered by Gurtin and Ohno (2011), and hence addresses the interaction between the slip systems. In other words, the strengthening only depends on the accumulated dislocation density while the effect of the forest dislocation density on the yield stress is eliminated in the present theory in line with (Ohno and Okumura, 2007).

By using the dissipation potential given in Equation (2.58) along with Equation (2.39) and the assumption \(\kappa(T)/T = \kappa_0 = constant\), the dissipative thermodynamic forces for the former case (Case I) can be obtained as follows:

\[
\chi_{ij}^{\text{dis}} = \sigma_y \left( \frac{\dot{\phi}}{\dot{\phi}_0} \right)^m \left( 1 - \left( \frac{T}{T_y} \right)^n \right) \varepsilon_{ij}^p \tag{2.60}
\]

\[
\mathcal{S}_{ijk}^{\text{dis}} = \sigma_y \varepsilon_{dis}^2 \left( \frac{\dot{\phi}}{\dot{\phi}_0} \right)^m \left( 1 - \left( \frac{T}{T_y} \right)^n \right) \varepsilon_{ij,k}^p \tag{2.61}
\]

\[
\mathcal{A}_{\text{dis}} = -\dot{\sigma} \dot{T} \tag{2.62}
\]

\[
\mathcal{q}_d = -\kappa_0 T \dot{T} \tag{2.63}
\]

On the other hand, the functional form of the dissipation potential, which is independent of \(\varepsilon_{ij,k}^p\), for the latter case (Case II) can be postulated by setting \(\ell_{\text{dis}} = 0\) in Equation (2.58) as follows:

\[
\mathcal{D} = \frac{\sigma_y}{2} \left( \frac{\dot{\phi}_{\ell_{\text{dis}}=0}}{\dot{\phi}_0} \right)^m \left( 1 - \left( \frac{T}{T_y} \right)^n \right) \dot{\phi}_{\ell_{\text{dis}}=0} - \frac{\dot{\sigma}}{2} \dot{T}^2 - \frac{1}{2} \kappa(T) T_i T_j \geq 0 \tag{2.64}
\]

where \(\dot{\phi}_{\ell_{\text{dis}}=0}\) is given by \(\sqrt{\varepsilon_{ij}^p \varepsilon_{ij}^p}\) by setting \(\ell_{\text{dis}} = 0\) in Equation (2.59). By substituting Equation (2.64) into Equation (2.39), the dissipative thermodynamic forces for the latter case (Case II) can be obtained as follows:
\[ X_{ij}^{\text{dis}} = \sigma_y \left( \frac{\dot{p}_{ij \text{dis}}}{p_0} \right)^m \left( 1 - \left( \frac{T}{T_y} \right)^n \right) \frac{\dot{\varepsilon}_{ij}^p}{p_{ij \text{dis}}=0} \]  
(2.65)

\[ S_{ijk}^{\text{dis}} = 0 \]  
(2.66)

\[ A^{\text{dis}} = -\delta_i \dot{T} \]  
(2.67)

\[ q_i = -\kappa_0 T \dot{t}_i \]  
(2.68)

Meanwhile, Gurtin and Reddy (2009) pointed out that the classical isotropic hardening rule, which is dissipative in nature, may equally well be characterized via a defect energy since this energetically based hardening rule mimics the dissipative behaviour by describing loading processes that are irreversible. In this sense, as it was mentioned previously in this chapter, the energetic microstress \( X_{ij}^{\text{en}} \) is further decomposed into \( X_{ij}^{\text{en,NR}} \), that describes an irreversible loading process, and \( X_{ij}^{\text{en,R}} \) which describes a reversible loading process due to the energy carried by the dislocations. The present framework follows the theorem of Gurtin and Reddy (2009) in that the theory without a defect energy is equivalent to the theory with a defect energy by replacing the dissipation \( D \) by an effective dissipation \( D_{\text{eff}} \), which is defined as follows:

\[ D_{\text{eff}} = (X_{ij}^{\text{dis}} + X_{ij}^{\text{en,NR}})\dot{\varepsilon}_p^p + S_{ijk}^{\text{dis}} \dot{\varepsilon}_{ij,k} + A^{\text{dis}} \dot{\varepsilon}_k + q_i - \kappa_0 T \dot{t}_i \]  
(2.69)

where \( X_{ij}^{\text{en,NR}} \) may be viewed as the effectively dissipative microforce since it satisfies an effective dissipation inequality.

Meanwhile, there are two main mechanisms affecting the energy dissipation during the dislocation movement in the grain boundary area. The first mechanism is related to an energy change in the grain boundary region. The macroscopic accumulated plastic strain at the grain boundary can be connected to the microscopic deformation of the grain boundary through the quadratic mean of the deformation gradient. Thus, the energy change after the onset of slip transmission to the adjacent grain is able to be approximately determined by a quadratic function of the deformation gradient at the microscale and hence the interfacial plastic strain at the macroscale. The other mechanism introduces the energy involved in the deformation of the grain boundary. This energy is mainly due to the energy dissipation during the dislocation movement and can be taken as a linear function of the interfacial plastic strain.

The interfacial dissipation potential \( D^l \) in the current study is postulated by combing the above-mentioned mechanisms as follows:

\[ D^l = \frac{\dot{\varepsilon}_{\text{dis}}^l}{m^l + 1} \left( \sigma_y + h^l \varepsilon_p \varepsilon_p^{l \text{(post)}} \right) \left( 1 - \frac{T_i^l}{T_y^l} \right)^{n^l} \left( \frac{\varepsilon_p^{l \text{(post)}}}{p_0^l} \right) \frac{m^l}{\varepsilon_p^{l \text{(post)}}} \geq 0 \]  
(2.70)

where \( \dot{\varepsilon}_{\text{dis}}^l \) is the interfacial dissipative length scale, \( m^l \) and \( p_0^l \) are the viscous related material parameters, \( \sigma_y^l \) is a constant accounting for the interfacial yield stress at which the interface starts to deform plastically, \( h^l \) is an interfacial hardening parameter representing the slip transmission through the interface, \( T_i^l \) is the scale-independent interfacial thermal parameter at the onset of yield, \( n^l \) is the interfacial thermal parameter, and \( \varepsilon_p^{l \text{(post)}} = \sqrt{\dot{\varepsilon}_{ij}^{l \text{(post)}} \dot{\varepsilon}_{ij}^{l \text{(post)}}} \) and \( \dot{\varepsilon}_p^{l \text{(post)}} = \sqrt{\dot{\varepsilon}_{ij}^{l \text{(post)}} \dot{\varepsilon}_{ij}^{l \text{(post)}}} \) are defined respectively with the plastic strain at the interface after the slip transfer \( \varepsilon_p^{l \text{(post)}} \) and its rate \( \dot{\varepsilon}_{ij}^{l \text{(post)}} \). The rate-dependency and temperature-dependency of the
interfacial dissipation energy are clearly shown in Equation (2.70) through the terms \((\dot{\varepsilon}_p^{l(\text{post})} / \dot{\rho}_0)\) and \((1 - T_l / T_y)\)

The interfacial dissipative microstresses \(\mathbb{M}_{ij}^{l,\text{dis}}\) can be obtained by substituting Equation (2.70) into Equation (2.40) as follows:

\[
\mathbb{M}_{ij}^{l,\text{dis}} = \frac{\ell_{\text{dis}}}{m_l + 1} \left( \sigma_y + h_l \dot{\varepsilon}_p^{l(\text{post})} \right) \left( 1 - \left( \frac{T_l}{T_y} \right)^n \right) \left( \frac{\varepsilon_p^{l(\text{post})}}{\rho_0} \right) \frac{\dot{\varepsilon}_p^{l(\text{post})}}{\dot{\rho}_0} \tag{2.71}
\]

By substituting Equation (2.71) and Equation (2.57) into Equation (2.31), one can obtain the interfacial microtraction \(\mathbb{M}_{ij}^l\) as follows:

\[
\mathbb{M}_{ij}^l = G \dot{\varepsilon}_m^{l(p)} \varepsilon_{ij}^{l(p)} \left( \frac{\varepsilon_p^{l(\text{post})}}{\rho_0} \right) \frac{\dot{\varepsilon}_p^{l(\text{post})}}{\dot{\rho}_0} \tag{2.72}
\]

As can be seen in Equation (2.72), a free surface, i.e. microfree boundary condition, at the grain boundary can be described by setting \(\dot{\varepsilon}_m = \dot{\varepsilon}_{\text{dis}} = 0\) and it is also possible to describe a surface passivation, i.e. microclamped boundary condition, by setting \(\dot{\varepsilon}_m \to \infty\) and \(\dot{\varepsilon}_{\text{dis}} \to \infty\).

2.2.7 Flow rule

The flow rule in the present framework is established based on the nonlocal microforce balance, Equation (2.6), augmented by thermodynamically consistent constitutive relations for both energetic and dissipative microstresses. By substituting Equations (2.51), (2.53), (2.60) and (2.61) into Equation (2.6), one can obtain a second order partial differential form of the flow rule as follows:\(^4\)

\[
\tau_{ij} = \left( \left( \frac{\varepsilon_p^{l(p)}}{\rho_0} \right) \frac{\dot{\varepsilon}_p^{l(\text{post})}}{\dot{\rho}_0} \right) \varepsilon_{ij}^{l(p)} - \left( \frac{\sigma_y}{\rho_0} \right) \frac{\dot{\varepsilon}_p^{l(\text{post})}}{\dot{\rho}_0} \tag{2.73}
\]

where the under-braced term \(S_{ij,k,k}^{l}\) represents a backstress due to the energy stored in dislocations and results in the Bauschinger effect observed in the experiments (Liu et al., 2015; Nicola et al., 2006; Xiang et al., 2005; Xiang and Vlassak, 2006) and discrete dislocation plasticity (Nicola et al., 2006; Shishvyan et al., 2011; Shishvyan et al., 2010).

\(^4\) The flow rule, Equation (2.73), corresponds to the SGP model (Case I), in which the functional form of the dissipation potential is dependent on \(\dot{\varepsilon}_{ij,k,k}^{l(p)} (S_{ij,k,k}^{l} \neq 0)\). One can easily obtain the flow rule for the other case (Case II) of the SGP model, i.e. with \(S_{ij,k,k}^{l} = 0\), by setting \(\ell_{\text{dis}} = 0\).
2.2.8 Thermo-mechanical coupled heat equation

The evolution of the temperature field is governed by the law of conservation of energy (the first law of thermodynamics). The terms addressing heating as a result of the inelastic dissipation and thermo-mechanical coupling are involved for describing the evolution of the temperature field. The equation for the conservation of energy in the present work is put forward as follows:

\[ \sigma_{ij} \dot{e}_{ij}^p + \chi_{ij} \dot{e}_{ij}^p + \mathcal{S}_{ijk} \dot{e}_{ij,k} + \mathcal{A} \dot{T} + \mathcal{B}_l \dot{T}_j - \text{div} q_i + \rho \mathcal{H}_{\text{EXT}} - \rho \dot{\mathcal{E}} = 0 \]  \hspace{1cm} (2.74)

where \( \mathcal{H}_{\text{EXT}} \) is the specific heat from the external source.

By considering the effective dissipation potential given in Equation (2.69) along with the equations for the entropy production (the second law of thermodynamics) previously described in Equation (2.17), the relationship for the evolution of the entropy, which describes the irreversible process, can be derived as follows:

\[ \rho \dot{s} T = D_{\text{eff}} + \rho \mathcal{H}_{\text{EXT}} \]  \hspace{1cm} (2.75)

By using Equation (2.50) for solving the rate of the entropy \( \dot{s} \), the evolution of the temperature field can be obtained as follows:

\[
\begin{align*}
\rho c_0 \dot{T} &= \chi_{ij} \dot{e}_{ij}^p + \chi_{ij} \dot{e}_{ij}^p + \mathcal{S}_{ijk} \dot{e}_{ij,k} + \frac{\kappa(T)}{2T} T_{i,l} T_{i,l} + \alpha_{T} \dot{T}_{i,l,l} - \delta T_r \dot{T} \\
& - \alpha_{T} \dot{e}_{ij}^p \delta_{ij} T - \left\{ h e_{p}^{-1} \left( \frac{n}{T} \right)^{n-1} \dot{e}_{ij}^p + \frac{h e_{p}^{r+1}}{r+1} \left( \frac{n(n-1)}{T^2} \right)^{n-2} \dot{e}_{ij}^p \right\} T + \rho \mathcal{H}_{\text{EXT}} \hspace{1cm} (2.76)
\end{align*}
\]

where \( c_0 \) is the specific heat capacity at constant volume and given by \( c_0 = \text{constant} \equiv c_v T / T_r \). As shown in Equation (2.76), the following terms are depicted, ①: irreversible mechanical process, ②: generalized heat conduction, ③: thermo-elastic coupling, ④: thermo-plastic coupling, and ⑤: heat source, which are involved in the evolution of the temperature. The third-order mixed derivation term \( \alpha_{T} T_{i,l,l} \) in part ② introduces the microstructural interaction effect into the classical heat equation, in addition, the second-order time derivative term \( \delta T_r \dot{T} \) gives the thermal wave behaviour effect in heat propagation.

By substituting the constitutive equations of the energetic microstresses given by Equation (2.49) ~ Equation (2.53) and the dissipative microstresses given by Equation (2.60) ~ Equation (2.63) into Equation (2.76) and defining three additional terms \( t_{\text{eff}} = \kappa_0 / \rho c_v \), \( t_{\text{en}} = \alpha T_r / \kappa_0 \), and \( t_{\text{dis}} = \delta T_r / \rho c_v \), the evolution of temperature for the model, in which the functional form of the dissipation potential dependent on \( \dot{e}_{ij,k}^p \), i.e. \( \mathcal{S}_{ijk} \neq 0 \), can be obtained as follows:

28
\[
\begin{align*}
\frac{1}{\rho c_v (r + 1)} \left[ n(n - 1) \left( \frac{T}{T_y} \right)^{n} \right] \ddot{\epsilon}_p^{r+1} = & \frac{\dot{\epsilon}_p^{p}}{\rho c_v} \left[ \left( h \epsilon_p^{r-1} \left( 1 - \left( \frac{T}{T_y} \right)^{n} \right) - 2r \partial h^2 \epsilon_p^{2r-1} \right) \right. \\
& \left. - n h \epsilon_p^{r-1} \left( \frac{T}{T_y} \right)^{n} \epsilon_i^p + \sigma_y \left( \frac{\dot{p}}{\dot{p}_0} \right)^m \left( 1 - \left( \frac{T}{T_y} \right)^{n} \right) \tilde{\epsilon}_i^p \right] \\
& + \frac{1}{\rho c_v} \left[ \sigma_y \dot{\ell}_{d}^{d} \left( \frac{\dot{p}}{\dot{p}_0} \right)^m \left( 1 - \left( \frac{T}{T_y} \right)^{n} \right) \epsilon_i^p \epsilon_{ijk} \epsilon_i^p \epsilon_{ijk} - \alpha_t \epsilon_{ij} \delta_{ij} \dot{T} \\
& + \rho H_{\text{EXT}} \right] + [\dot{\epsilon}_{\text{en}} T_{il} + \dot{\epsilon}_{\text{eff}} T_{il}^{\text{en}} - \dot{\epsilon}_{\text{dis}} T_{il}]
\end{align*}
\]

In the absence of the mechanical terms, Equation (2.77) turns to the generalized heat equation including \( \dot{\epsilon}_{\text{en}} \) and \( \dot{\epsilon}_{\text{dis}} \). The evolution of temperature for the other case (Case II) of SGP model, i.e. with \( \ell_{\text{dis}} = 0 \) can be obtained by setting \( \ell_{\text{dis}} = 0 \) in Equation (2.77).

2.3 Finite element solution of the proposed strain gradient plasticity model

Ramaswamy and Aravas (1998b) investigated a finite element implementation of rate-independent gradient-type plasticity models in which spatial gradients of the plastic multiplier and state variables enter the gradient-dependent evolution equations for the state variables. The main issue of Ramaswamy and Aravas (1998b) was on the finite element implementation of the gradient-dependent model along with the interpretation of plastic loading in the discretized problems such as localization of plastic flow in plane strain tension and a mode-I plane strain crack.

In this chapter, a one-dimensional finite element model for the proposed SGP theory is developed to investigate the size dependent behaviour in the microscopic structures under macroscopically uniform uniaxial tensile stress. In a one-dimensional finite element implementation, the macroscopic partial differential equations for balance of linear momentum Equation (2.5) with the macroscopic boundary conditions, \( u_x = 0 \) and \( u_x = u^\dagger \) (prescribed), and the microscopic partial differential equations for nonlocal force balance Equation (2.6) with the microscopic boundary conditions, \( (\mathbf{M} - S)_{x=0} = 0 \) and \( (\mathbf{M} - S)_{x=L} = 0 \), yield the following expressions in a global weak form respectively\(^5\):

\[
\int_0^L (\sigma \dddot{u}_x) dx = 0
\]

\[
\int_0^L \left[ (\chi - \tau) \dddot{\epsilon}_p^p + S \dddot{\epsilon}_p^p \right] dx + M_{x=L} \dddot{\epsilon}_x^p - M_{x=0} \dddot{\epsilon}_x^p = 0
\]

\(^5\) The finite element solutions, in this work, depend only on the \( x \)-direction. A single crystal with the size of \( L \) bounded by two grain boundaries is analyzed (see Figure 2.7 for details in the latter part of this dissertation).
where the arbitrary virtual fields \( \tilde{u} \) and \( \tilde{\varepsilon}^p \) are assumed to be kinematically admissible weighting functions in the sense that \( \tilde{u}_{x=0} = \tilde{u}_{x=L} = 0 \).

The user-element subroutine UEL in the commercial finite element package ABAQUS/standard (2012) is developed in the present work in order to numerically solve the weak forms of the macroscopic and microscopic force balances, Equation (2.78) and Equation (2.79), respectively. In this finite element solution, the displacement field \( u \) and the plastic strain field \( \varepsilon^p \) are discretized independently and both of the fields are taken as fundamental unknown nodal degrees of freedom. In this regard, the displacement field and corresponding strain field \( \varepsilon \), and the plastic strain field and corresponding plastic strain gradient field \( \varepsilon^p_x \) can be obtained by using the interpolation as follows:

\[
\begin{align*}
    u(x) &= \sum_{\xi=1}^{n_u} N_{u,\xi}^{\xi} U_{u,\xi}^{\xi} \\
    \varepsilon(x) &= \frac{\partial u(x)}{\partial x} = \sum_{\xi=1}^{n_u} N_{u,\xi}^{\xi} u_{u,\xi}^{\xi} \\
    \varepsilon^p(x) &= \sum_{\xi=1}^{n_{\varepsilon}^p} N_{\varepsilon^p,\xi}^{\xi} \varepsilon_{\xi}^{\xi} \\
    \varepsilon^p_x(x) &= \frac{\partial \varepsilon^p(x)}{\partial x} = \sum_{\xi=1}^{n_{\varepsilon}^p} N_{\varepsilon^p,\xi}^{\xi} \varepsilon_x \xi^{\xi} 
\end{align*}
\]  

where \( N_{u,\xi}^{\xi} \) and \( N_{\varepsilon^p,\xi}^{\xi} \) are the shape functions, and \( U_{u,\xi}^{\xi} \) and \( \varepsilon_{\xi}^{\xi} \) are the nodal values of the displacements and the plastic strains at node \( \xi \) respectively. The terms \( n_u \) and \( n_{\varepsilon^p} \) represent the number of nodes per a single element for the displacement and the plastic strain respectively.

Substituting Equation (2.80) and Equation (2.81) into Equation (2.78) and Equation (2.79) give the nodal residuals for the displacement \( r_u \) and the plastic strain \( r_{\varepsilon^p} \) for each finite element \( el \) as follows:

\[
\begin{align*}
    (r_u)_\xi &= \int_{el} \left[ \sigma N_{u,\xi}^{\xi} \right] dx \\
    (r_{\varepsilon^p})_\xi &= \int_{el} \left[ (\mathcal{X} - \tau) N_{\varepsilon^p,\xi}^{\xi} + S N_{\varepsilon^p,\xi}^{\xi} \right] dx + \mathbb{M}^I N_{\varepsilon^p}^{\xi} 
\end{align*}
\]  

where the term \( \mathbb{M}^I N_{\varepsilon^p}^{\xi} \) is applied only for the nodes on the interface which is at \( x = 0 \) and \( x = L \) in the present work.

The global coupled system of equations, \( (r_u)_\xi = 0 \) and \( (r_{\varepsilon^p})_\xi = 0 \), are solved using ABAQUS/standard (2012) based on the Newton-Raphson iterative scheme. Occasionally, the modified Newton-Raphson method, referred to as quasi Newton-Raphson method, is employed in the case that the numerical solution suffers a divergence during the initial increment immediately after an abrupt change in loading. In quasi Newton-Raphson method, a specific correction factor, which is less than one, is multiplied by one portion of the stiffness matrix. By using this method,

\[6\] In the case of micro-clamped boundary condition, \( \varepsilon^p_{x=0} = \varepsilon^p_{x=L} = 0 \) is imposed at the grain boundaries to enforce the complete blockage of dislocations at the interface. In the case of micro-free boundary condition, on the other hand, the dislocations are free to move across the interface, which in turn, the proposed grain boundary flow rule is imposed.

\[7\] If a one-dimensional three-noded quadratic element is employed, \( n_u \) and \( n_{\varepsilon^p} \) are set up as three. On the other hand, these parameters are set up as two in the case that a one-dimensional two-noded linear element is used. It should be noted that \( n_u \) and \( n_{\varepsilon^p} \) do not necessarily have to be same as each other in the present finite element implementation, even though both the displacement field and the plastic strain fields are calculated by using the standard isoparametric shape functions.
a divergence problem can be overcome, however, convergence is expected to be slow because of the expensive computational cost. The Taylor expansion of the residuals with regard to the current nodal values can be expressed by assuming the nodal displacement and the plastic strain in iteration $\zeta$ as $\mathcal{U}_u^\zeta$ and $\mathcal{E}_{ep}^\zeta$ are respectively as follows:

\[
\begin{align*}
\left(r_u|_{u_u^\xi\mathcal{E}_{ep}^{\xi+1}}\right)_\mathcal{x} & = \left(r_u|_{u_u^\xi\mathcal{E}_{ep}^\xi}\right)_\mathcal{x} + \left(\frac{\partial r_u}{\partial \mathcal{U}_u^\xi}\right)|_{u_u^\xi} \Delta \mathcal{U}_u^\xi + \left(\frac{\partial r_u}{\partial \mathcal{E}_{ep}^\xi}\right)|_{\mathcal{E}_{ep}^\xi} \Delta \mathcal{E}_{ep}^\xi \\
& + \mathcal{O}\left(\left(\Delta \mathcal{U}_u^\xi\right)^2, \left(\Delta \mathcal{E}_{ep}^\xi\right)^2\right) \tag{2.84}
\end{align*}
\]

\[
\begin{align*}
\left(r_{ep}|_{u_u^\xi\mathcal{E}_{ep}^{\xi+1}}\right)_\mathcal{x} & = \left(r_{ep}|_{u_u^\xi\mathcal{E}_{ep}^\xi}\right)_\mathcal{x} + \left(\frac{\partial r_{ep}}{\partial \mathcal{U}_u^\xi}\right)|_{u_u^\xi} \Delta \mathcal{U}_u^\xi + \left(\frac{\partial r_{ep}}{\partial \mathcal{E}_{ep}^\xi}\right)|_{\mathcal{E}_{ep}^\xi} \Delta \mathcal{E}_{ep}^\xi \\
& + \mathcal{O}\left(\left(\Delta \mathcal{U}_u^\xi\right)^2, \left(\Delta \mathcal{E}_{ep}^\xi\right)^2\right) \tag{2.85}
\end{align*}
\]

where $\Delta \mathcal{U}_u^\xi = (\mathcal{U}_u^{\xi+1})_\mathcal{x} - (\mathcal{U}_u^\xi)_\mathcal{x}$, $\Delta \mathcal{E}_{ep}^\xi = (\mathcal{E}_{ep}^{\xi+1})_\mathcal{x} - (\mathcal{E}_{ep}^\xi)_\mathcal{x}$ and $\mathcal{O}\left(\left(\Delta \mathcal{U}_u^\xi\right)^2, \left(\Delta \mathcal{E}_{ep}^\xi\right)^2\right)$ is the big $O$ notation to represent the terms of higher order than the second degree. The residual is ordinarily calculated at the end of each time step, and the values of the nodal displacements and the plastic strains are updated during the iterations. The increments in nodal displacements and the plastic strains can be computed by solving the system of linear equations shown in Equation (2.86) with the Newton-Raphson iterative method:

\[
\begin{bmatrix}
K_{uu}^{el} & K_{uep}^{el} \\
K_{uep}^{el} & K_{ep}^{el}
\end{bmatrix}
\begin{bmatrix}
\Delta \mathcal{U}_u^\xi \\
\Delta \mathcal{E}_{ep}^\xi
\end{bmatrix}
= \begin{bmatrix}
\left(r_u|_{u_u^\xi\mathcal{E}_{ep}^\xi}\right)_\mathcal{x} \\
\left(r_{ep}|_{u_u^\xi\mathcal{E}_{ep}^\xi}\right)_\mathcal{x}
\end{bmatrix} \tag{2.86}
\]

where $K_{u}^{el}$ is the Jacobian (stiffness) matrix that needs to be defined in the user-subroutine for each element.

From Equations (2.84) and (2.85) along with the discretization for the displacements given by Equation (2.80) and the plastic strains given by Equation (2.81) at the end of a time step, and the functional forms of the energetic and dissipative higher order stresses defined in the previous section, the Jacobian matrix for the two cases of the proposed SGP theory can be obtained respectively as follows:

\[
\begin{align*}
K_{uu}^{el} & = -\frac{\partial r_u}{\partial \mathcal{U}_u^\xi}\bigg|_{u_u^\xi} = -\int_{el} \left(E \mathcal{N}_{u,x}^\xi \mathcal{N}_{u,x}^\xi\right) dx \\
K_{uep}^{el} & = -\frac{\partial r_u}{\partial \mathcal{E}_{ep}^\xi}\bigg|_{\mathcal{E}_{ep}^\xi} = \int_{el} \left(E \mathcal{N}_{e,p}^\xi \mathcal{N}_{u,x}^\xi\right) dx \\
K_{ep}^{el} & = -\frac{\partial r_{ep}}{\partial \mathcal{U}_u^\xi}\bigg|_{u_u^\xi} = \int_{el} \left(E \mathcal{N}_{u,x}^\xi \mathcal{N}_{e,p}^\xi\right) dx \\
K_{ep}^{el} & = -\frac{\partial r_{ep}}{\partial \mathcal{E}_{ep}^\xi}\bigg|_{\mathcal{E}_{ep}^\xi} = \int_{el} \left(E \mathcal{N}_{e,p}^\xi \mathcal{N}_{e,p}^\xi\right) dx
\end{align*} \tag{2.87-2.89}
\]
\[ (K^{el}_{e^p} e^p)_{S_{ij}^{dis} \neq 0} = \left( -\frac{\partial r_{e^p}}{\partial \varepsilon_{e^p}^\xi} \right)_{S_{ij}^{dis} \neq 0} \]

\[
= \int_{et} \left\{ E + \left( rh(e^p) r + \frac{\sigma_y(\dot{\phi})^{m-1}}{\Delta t(\dot{\phi_0})^m} \right) \left( 1 - \left( \frac{T}{T_y} \right)^n \right) \right\} N^\xi_{e^p} N^\xi_{e^p} \]

\[
+ \left\{ \left( G \ell_{en}^2 + \frac{\sigma_y(\dot{\phi})^{m-1}}{\Delta t(\dot{\phi_0})^m} \right) \left( 1 - \left( \frac{T}{T_y} \right)^n \right) \right\} N^\xi_{e^p x} N^\xi_{e^p x} \] for bulk \]

\[
\frac{\Delta t}{\Delta t} \int_{et} \left\{ E + \left( rh(e^p) r + \frac{\sigma_y(\dot{\phi})^{m-1}}{\Delta t(\dot{\phi_0})^m} \right) \left( 1 - \left( \frac{T}{T_y} \right)^n \right) \right\} N^\xi_{e^p} N^\xi_{e^p} \]

\[
+ \left\{ \left( G \ell_{en}^2 \left( 1 - \left( \frac{T}{T_y} \right)^n \right) \right) \right\} N^\xi_{e^p x} N^\xi_{e^p x} \] for bulk \]

\[
\frac{\Delta t}{\Delta t} \int_{et} \left\{ E + \left( rh(e^p) r + \frac{\sigma_y(\dot{\phi})^{m-1}}{\Delta t(\dot{\phi_0})^m} \right) \left( 1 - \left( \frac{T}{T_y} \right)^n \right) \right\} N^\xi_{e^p} N^\xi_{e^p} \]

\[
+ \left\{ \left( G \ell_{en}^2 \left( 1 - \left( \frac{T}{T_y} \right)^n \right) \right) \right\} N^\xi_{e^p x} N^\xi_{e^p x} \]

and

\[
(K^{el}_{e^p} e^p)_{S_{ij}^{dis} = 0} = \left( -\frac{\partial r_{e^p}}{\partial \varepsilon_{e^p}^\xi} \right)_{S_{ij}^{dis} = 0} \]

\[
= \int_{et} \left\{ E + \left( rh(e^p) r + \frac{\sigma_y(\dot{\phi})^{m-1}}{\Delta t(\dot{\phi_0})^m} \right) \left( 1 - \left( \frac{T}{T_y} \right)^n \right) \right\} N^\xi_{e^p} N^\xi_{e^p} \]

\[
+ \left\{ \left( G \ell_{en}^2 \left( 1 - \left( \frac{T}{T_y} \right)^n \right) \right) \right\} N^\xi_{e^p x} N^\xi_{e^p x} \] for bulk \]

\[
\frac{\Delta t}{\Delta t} \int_{et} \left\{ E + \left( rh(e^p) r + \frac{\sigma_y(\dot{\phi})^{m-1}}{\Delta t(\dot{\phi_0})^m} \right) \left( 1 - \left( \frac{T}{T_y} \right)^n \right) \right\} N^\xi_{e^p} N^\xi_{e^p} \]

\[
+ \left\{ \left( G \ell_{en}^2 \left( 1 - \left( \frac{T}{T_y} \right)^n \right) \right) \right\} N^\xi_{e^p x} N^\xi_{e^p x} \] for bulk \]

\[
\frac{\Delta t}{\Delta t} \int_{et} \left\{ E + \left( rh(e^p) r + \frac{\sigma_y(\dot{\phi})^{m-1}}{\Delta t(\dot{\phi_0})^m} \right) \left( 1 - \left( \frac{T}{T_y} \right)^n \right) \right\} N^\xi_{e^p} N^\xi_{e^p} \]

\[
+ \left\{ \left( G \ell_{en}^2 \left( 1 - \left( \frac{T}{T_y} \right)^n \right) \right) \right\} N^\xi_{e^p x} N^\xi_{e^p x} \] for interface \]

where \( \Delta t \) is a time step and the interfacial terms in \((K^{el}_{e^p} e^p)_{S_{ij}^{dis} \neq 0}\) and \((K^{el}_{e^p} e^p)_{S_{ij}^{dis} = 0}\) are applied only for the nodes on the interface which is at \( x = 0 \) and \( x = L \) in the present work.

2.4 Finite element implementation of the proposed strain gradient plasticity model

2.4.1 Experimental validation of the proposed strain gradient plasticity model

In this section, the proposed SGP model and corresponding finite element code are validated by comparing with the experimental results from three sets of size effect experiments. The material parameters for the proposed SGP model used in this chapter are also calibrated in this section by using the experimental data. In addition, the comparison between the proposed SGP model and Voyiadjis and Faghihi (2014) is carried out to show the increase in accuracy of the proposed model. To the best of the authors’ knowledge, no experimental studies investigating the
effect of the abrupt surface passivation have been performed. This is the reason that Fleck et al. (2014, 2015) emphasized the necessity of the experimental study in order to judge the physical acceptance of the stress jump. In this section, three experimental sets on the size effect of the thin films are taken into account as an alternative. To examine the applicability of the proposed finite element implementation to the various kinds of materials, it is considered in the present work that each set of three experiments involves the three different materials, viz. aluminum (Al), copper (Cu) and nickel (Ni). The first one, which was performed by Haque and Saif (2003), is the uniaxial tension tests of the freestanding Al thin films with the various nanoscale thicknesses and the second one, which was performed by Xiang and Vlassak (2006), is the biaxial bulge tests to show the size effect in electroplated Cu thin films with the various microscale thickness. The experimental work of Han et al. (2008), which is the micro-tensile test on the Ni thin films at elevated temperature, is selected for the third experimental validation of the proposed SGP model.

2.4.1.1 Size-dependent phenomena in Al thin films: the uniaxial tensile test

Table 2.1. The general and calibrated material parameters used for the validation of the proposed strain gradient plasticity model.

<table>
<thead>
<tr>
<th>General</th>
<th>Copper</th>
<th>Aluminum</th>
<th>Nickel</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$ (GPa)</td>
<td>Elastic modulus for isotropic linear elasticity</td>
<td>110</td>
<td>70</td>
</tr>
<tr>
<td>$G$ (GPa)</td>
<td>Shear modulus for isotropic linear elasticity</td>
<td>48</td>
<td>27</td>
</tr>
<tr>
<td>$\rho$ (g · cm$^{-3}$)</td>
<td>Density</td>
<td>8.960</td>
<td>2.702</td>
</tr>
<tr>
<td>$c_\varepsilon$ (J/g · °K)</td>
<td>Specific heat capacity at constant stress</td>
<td>0.385</td>
<td>0.910</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Calibrated</th>
<th>Copper</th>
<th>Aluminum</th>
<th>Nickel</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_y$ (MPa)</td>
<td>Yield stress</td>
<td>195</td>
<td>700</td>
</tr>
<tr>
<td>$h$ (MPa)</td>
<td>Hardening material parameter</td>
<td>600</td>
<td>1,700</td>
</tr>
<tr>
<td>$\phi_0$ (s$^{-1}$)</td>
<td>Reference effective plastic strain rate</td>
<td>0.04</td>
<td>0.04</td>
</tr>
<tr>
<td>$r$</td>
<td>Nonlinear hardening material parameter</td>
<td>0.6</td>
<td>0.2</td>
</tr>
<tr>
<td>$m$</td>
<td>Non-negative rate sensitivity parameter</td>
<td>0.05</td>
<td>0.05</td>
</tr>
<tr>
<td>$T_y$ (°K)</td>
<td>Thermal material parameter</td>
<td>1,358</td>
<td>933</td>
</tr>
<tr>
<td>$n$</td>
<td>Temperature sensitivity parameter</td>
<td>0.3</td>
<td>0.3</td>
</tr>
<tr>
<td>$t_{en}$ (µm)</td>
<td>Energetic length scale</td>
<td>1.5 (1.0 µm)</td>
<td>0.9 (100 nm)</td>
</tr>
<tr>
<td>$t_{dis}$ (µm)</td>
<td>Dissipative length scale</td>
<td>2.5 (1.0 µm)</td>
<td>8.0 (100 nm)</td>
</tr>
</tbody>
</table>

Haque and Saif (2003) developed Micro-Electro Mechanical Systems (MEMS) based testing techniques for uniaxial tensile testing of nanoscale freestanding Al thin films to explore the effect of strain gradient in 100 nm, 150 nm and 485 nm thick specimens with average grain size of 50 nm, 65 nm and 212 nm respectively. The specimens with 99.99 % pure sputter-deposited freestanding Al thin films are 10 µm wide and 275 µm long. All experiments are carried out in-situ in SEM and the stress and strain resolutions for the tests are set 5 MPa and 0.03 % respectively. In particular, the comparison between the proposed SGP model and Voyiadjis and Faghihi (2014) is carried out to show the increase in accuracy of the proposed model. The
calibrated material parameters as well as the general material parameters for the Al are presented in Table 2.1 and the numerical results from both the proposed SGP model and Voyiadjis and Faghihi (2014) are shown in Figure 2.2 in conjunction with the experimental data of Haque and Saif (2003). As it is clearly shown in this figure, the size effect: Smaller is Stronger is observed on the stress-strain curves of the Al thin films. Furthermore, the calculated results of the proposed SGP model display a tendency to be more coincident to the experimental data than those of Voyiadjis and Faghihi (2014).

Figure 2.2. The validation of the proposed strain gradient plasticity model by comparing the numerical results from the proposed model with those from Voyiadjis and Faghihi (2014) and the experimental measurements from Haque and Saif (2003) on the stress-strain response of the sputter-deposited Al thin films.

2.4.1.2 Size-dependent phenomena in Cu thin films: the biaxial bulge test

![Schematic representation of the plane strain bulge test technique proposed by Xiang and Vlassak (2006).](image)

Figure 2.3. Schematic representation of the plane strain bulge test technique proposed by Xiang and Vlassak (2006).

Xiang and Vlassak (2006) investigated the size effect with a variety of film thicknesses on the plastic behaviour of the freestanding electroplated Cu thin films by performing the plane strain bulge test. In this plane strain bulge test, the rectangular freestanding membranes surrounded by a rigid silicon (Si) frame are deformed in plane strain by applying a uniform pressure to one side of
the membrane as shown in Figure 2.3. The displacement and pressure resolutions for this bulge tests system are 0.3 \( \mu m \) and 0.1 \( kPa \) respectively. The stress-strain response of either a single material membrane or a stack of multiple membranes adhered on a rigid Si frame can be obtained by using the following two simple equations:

\[
\sigma = \frac{P(d^2 + \Delta^2)}{2t\Delta} \quad (2.92)
\]

\[
\varepsilon = \varepsilon_r + \frac{(d^2 + \Delta^2)}{2d\Delta} \arcsin\left(\frac{2d\Delta}{d^2 + \Delta^2}\right) - 1 \quad (2.93)
\]

where \( P \) is the applied stress, \( \Delta \) is the corresponding film deflection, \( t \) is the film thickness, \( 2d \) is the film window width and \( \varepsilon_r \) is a residual strain in the film. As can be seen in the work of Xiang and Vlassak (2006), the stress-strain curves of the Cu thin films with a passivation layer on both surfaces clearly show the size effect due to the presence of a boundary layer with high dislocation density near the film-passivation layer interfaces. In this sense, the bulge test of electroplated Cu thin films with both surfaces passivated by 20 \( nm \) of titanium (Ti) is considered here for the experimental validation of the proposed SGP model. In order to describe the passivation effect on the proposed SGP model, the micro-clamped condition, which causes the dislocations to be completely blocked at the grain boundary, is imposed at both surfaces of the Cu thin films. Meanwhile, the experiments are performed with the various thicknesses of the Cu thin films of 1.0 \( \mu m \), 1.9 \( \mu m \) and 4.2 \( \mu m \). The average grain sizes in all cases are given by 1.5 \( \pm 0.05 \mu m \), 1.51 \( \pm 0.04 \mu m \) and 1.5 \( \pm 0.05 \mu m \) respectively, which mean almost equal each to each. The calibrated and general material parameters for the copper are presented in Table 2.1 and the comparison between the experimental measurements from the bulge tests and the calculated results from the proposed SGP model is shown in Figure 2.4. As it is clearly shown in this figure, the size effect according to the variation of the Cu thin film thicknesses is well observed in both
the proposed SGP model and the experimental work of Xiang and Vlassak (2006). Moreover, the numerical results from the proposed model are in good agreement with the experimental measurements.

2.4.1.3 Temperature effect on Ni thin films: the micro-tensile test

![Figure 2.5](image1.png)

**Figure 2.5.** The specimen dimensions for the experimental validation of the proposed model (Han et al., 2008).

![Figure 2.6](image2.png)

**Figure 2.6.** The validation of the proposed strain gradient plasticity model by comparing the numerical results from the proposed model with those from Voyiadjis and Faghihi (2014) and the experimental measurements from Han et al. (2008) on the stress-strain response of Ni thin films.

Han et al. (2008) developed the microscale tensile testing system, which is composed of a high temperature furnace, a micro motor actuator and the Digital Image Correlation (DIC) system, for evaluating the mechanical properties of the Ni thin films at high temperatures. Dog bone shaped specimens used in their experiments were made by Micro-electro mechanical system (MEMS) processes and the primary dimensions of the specimen are shown in Figure 2.5.

The calibrated material parameters as well as the general parameters for Ni are presented in Table 2.1. The results of microscale tensile tests at four different temperatures, i.e. 25 °C, 75 °C, 145 °C and 218 °C, and corresponding numerical results from the proposed model are shown in Figure 2.6. As shown in this figure, it is clear from both the experimental and numerical results that the Young’s modulus is not affected by variations in temperature while the yield and tensile strength decrease as the specimen temperature increases. In addition, Figure 2.6 clearly shows that
the Bauschinger effect is not affected very much by variations in the specimen temperature. Meanwhile, the calculated results of the proposed model compare better to the experimental data than those of Voyiadjis and Faghihi (2014) (Figure 2.6).

2.4.2 Stretch-Passivation problem

![One-dimensional model for a single grain with two grain boundaries.](image)

Figure 2.7. One-dimensional model for a single grain with two grain boundaries.

In the previous section, two cases of the proposed SGP theory are presented in order to investigate the size effect in small-scale metallic volumes based on a thermo-mechanical version of the second thermodynamics law and a system of microscopic force balances. Based on the proposed theoretical formulations, the numerical solutions for the stretch-passivation problem with the two cases of the proposed SGP theory are presented in this section. The proposed frameworks represent the nonlocal flow rules in the form of partial differential equations when the microscopic force balances are integrated with the thermodynamically consistent constitutive equations. To interpret and analyze the physical phenomena characterized by the proposed frameworks is very complicated, in this sense, a one-dimensional theory and a corresponding numerical solution are developed for this work.

An initially uniform single grain with the size of $L$ is used with two grain boundaries as shown in Figure 2.7. The grain is assumed to be infinitely long along the $x$-direction and initially homogeneous, therefore, the solution depends only on the $x$-direction. In the one-dimensional stretch-passivation problem, the grain is deformed into the plastic regime by uniaxial tensile stretch with no constraint on plastic flow at the grain boundaries. Then, at a certain point, the plastic flow is constrained by blocking off the dislocations from passing out of the grain boundary, which leads the further plastic strain not to occur at the grain boundary.

2.4.3 Numerical results

In this section, an extensive numerical work is carried out based on the validated code in order to compare the results from the aforementioned two cases of the proposed SGP model and to analyze the characteristics of the stress jump phenomenon. This section is largely composed of four subparts. In the first part, the occurrence of the stress jump phenomenon under the stretch-surface passivation condition is introduced in conjunction with three experiments used in Section 0. The second part is focused on indicating that the results are contrary to each other for the two cases of the proposed SGP model. An extensive parametric study is conducted in terms of the various material parameters and the evolution of the free energy involving the stored energy of cold work and the dissipation potentials during the plastic deformation are discussed in the third part. In the last part, the two-dimensional simulation is also given to examine the gradient and
grain boundary effect, the mesh sensitivity of the two-dimensional model and the stress jump phenomenon.

2.4.3.1 Introduction of a finite stress jump due to infinitesimal changes in the plastic strain increment

In this section, the finite element implementation validated in Section 0 by the comparison with the experimental works of Han et al. (2008); Haque and Saif (2003); Xiang and Vlassak (2006) and the corresponding material parameters presented in Table 2.1 are used again for introducing the finite stress jump phenomenon due to infinitesimal changes in the plastic strain induced by an abrupt surface passivation.

![Figure 2.8](image)

Figure 2.8. A finite stress jump due to infinitesimal changes in the plastic strain. The numerical implementation of the SGP model with the dissipative potential dependent on $\dot{\varepsilon}_{ij,k}$, i.e. $\mathcal{S}_{ij,k}^{\text{dis}} \neq 0$, is carried out based on the experiments of Haque and Saif (2003) with the various thicknesses of the Al thin films of 100 nm, 150 nm and 485 nm.

The numerical results on the stress-strain behaviours of Al and Cu thin films for the SGP model with the corresponding dissipative microstress quantities are presented in Figure 2.8 and Figure 2.9 respectively. In both simulations, a significant stress jump is observed at the onset of passivation. In particular, it is shown that the very first slopes immediately after the passivation increase as the film thicknesses decrease, viz. the dissipative length scales increase, in both simulations. Thus, the stress jump phenomenon is revealed to be highly correlated with the dissipative higher order microstress quantities $\mathcal{S}_{ij,k}^{\text{dis}}$. 

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Figure 2.9. A finite stress jump due to infinitesimal changes in the plastic strain. The numerical implementation of the SGP model with the dissipative potential dependent on $\dot{\varepsilon}_{ij,k}^p$, i.e. $\mathcal{S}_{ij,k}^{\text{dis}} \neq 0$, is carried out based on the experiments of Xiang and Vlassak (2006) with the various thicknesses of the Cu thin films of 1.0 $\mu$m, 1.9 $\mu$m and 4.2 $\mu$m.

Figure 2.10. A finite stress jump due to infinitesimal changes in the plastic strain. The numerical implementation of the SGP model with the dissipative potential dependent on $\dot{\varepsilon}_{ij,k}^p$, i.e. $\mathcal{S}_{ij,k}^{\text{dis}} \neq 0$, is carried out based on the experiments of Han et al. (2008) at the various temperatures of the Ni thin films of 25 $^\circ$C, 75 $^\circ$C, 145 $^\circ$C and 218 $^\circ$C. The circles on the curve indicate the passivation point.

Figure 2.10 shows the numerical results on the stress-strain behaviours of Ni thin films for the SGP model with the dissipative microstress quantities. As shown in this figure, the magnitudes of the stress jump are less than expected in all cases since the dissipative length scale $\ell_{\text{dis}}$ is set
0.1 which is much smaller than the energetic length scale $\ell_{en} = 1.0$. Nevertheless, the very first slopes immediately after the passivation are calculated as $E_{25^\circ C} = 58.0 \text{ GPa}$, $E_{75^\circ C} = 59.2 \text{ GPa}$, $E_{145^\circ C} = 72.6 \text{ GPa}$ and $E_{218^\circ C} = 105.0 \text{ GPa}$ respectively, and this shows the responses immediately after the passivation get gradually closer to the elastic response $E = 115 \text{ GPa}$ as the temperature increases.

2.4.3.2 Comparison of the two cases of the SGP model in terms of a stress jump

The numerical implementations to specify whether or not the stress jump phenomenon occurs under the stretch-surface passivation have been hitherto conducted within the framework of the SGP model with $S_{ijkl}^{\text{dis}} \neq 0$. Hereafter, the numerical simulations are given more focus on the direct comparison of the material response on the stress-strain curves between the two cases of the SGP models. The material parameters used for these implementations are presented in Table 2.2.

<table>
<thead>
<tr>
<th>For grain (bulk)</th>
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<tbody>
<tr>
<td>$E$</td>
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<tr>
<td>$\sigma_y$</td>
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<tr>
<td>$h$</td>
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<tr>
<td>$\rho_0$</td>
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<td>$T_0$</td>
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<td>$n$</td>
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<tr>
<td>$\rho$</td>
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<tr>
<td>$c_e$</td>
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<table>
<thead>
<tr>
<th>For grain boundary (interface)</th>
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<tbody>
<tr>
<td>$\sigma_y^I$</td>
</tr>
<tr>
<td>$h^I$</td>
</tr>
<tr>
<td>$\rho_0^I$</td>
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<tr>
<td>$n^I$</td>
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<tr>
<td>$m^I$</td>
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<tr>
<td>$T_y^I$</td>
</tr>
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</table>

Figure 2.11 clearly shows this point by comparing the results from the two cases. The behaviour of the SGP model with $S_{ijkl}^{\text{dis}} \neq 0$ is in stark contrast with that of the SGP case with $S_{ijkl}^{\text{dis}} = 0$ after the passivation point. A significant stress jump with the slope $E_{\text{passivation}}$ similar
to the modulus of elasticity $E$ is shown in the SGP case with $S_{ij}^{dis} \neq 0$. On the other hand, no elastic stress jump is observed in the SGP case with $S_{ij}^{dis} = 0$. This result is exactly in agreement with the prediction in Fleck et al. (2014, 2015). In the case that the dissipative potential is independent of $\dot{\varepsilon}_{ij,k}^P$, the contribution from the plastic strain gradients are entirely energetic as can be seen in Section 2.2.6. Both the increase in the yield strength in the early stages of passivation and subsequent hardening due to the effects of the plastic strain gradient are observed along with the increase of the energetic length scale as shown in Figure 2.11.

2.4.3.3 Parametric study

The comparison of the results from the SGP model case with the dissipative potential dependent on $\dot{\varepsilon}_{ij,k}^P$ is shown in Figure 2.12 with various dissipative length scales, i.e. $\ell_{dis} = 0.1$, 0.3, 0.5, 1.0, 1.5 and 2.0. As can be seen in this figure, the magnitude of the stress jump significantly increases as the dissipative length scale increases, on the other hand, the stress jump phenomenon disappears as the dissipative length scale tends to zero. This is because the dissipative higher order microstress quantities $S_{ij}^{dis}$, which is the main cause of the stress jump, vanishes when the dissipative length scale $\ell_{dis}$ is equal to zero. It is worthy noticing that the very first behaviour immediately after the passivation indicates a substantial difference with varying dissipative length scales. As the dissipative length scales increase from 0.1 to 2.0, the corresponding slopes of the very first response $E$ also increase from 13.3 GPa to 198.4 GPa. The main reason of this phenomenon in terms of the dissipative length scale is also because the dissipative higher order microstress quantities $S_{ij}^{dis}$ sharply increases with increasing $\ell_{dis}$.

![Figure 2.11](image-url)

Figure 2.11. Comparison of the results from the two models (the SGP model with the dissipative potential dependent on $\dot{\varepsilon}_{ij,k}^P$ (i.e. $S_{ij}^{dis} \neq 0$) and the SGP model with the dissipative potential independent on $\dot{\varepsilon}_{ij,k}^P$ (i.e. $S_{ij}^{dis} = 0$)). The results for the latter model are computed with three different values of energetic length scales $\ell_{en} = 0.1, 0.2$ and 0.3.
Figure 2.12. Comparison of the results from the SGP model with the dissipative potential dependent on $\varepsilon_{ij,k}^P$ (i.e. $S_{ij,k}^{dis} \neq 0$) with various dissipative length scales ($\ell_{dis} = 0.1, 0.3, 0.5, 1.0, 1.5$ and $2.0$).

The comparison of the results from the case of the SGP model with the dissipative potential dependent on $\varepsilon_{ij,k}^P$ is shown in Figure 2.13 for various passivation points. The energetic and dissipative length scales are set identical in all cases. The magnitudes of the stress jump with the magnitudes of $\varepsilon = 0.2 \%, 0.3 \%, 0.4 \%, 0.5 \%$ and $0.6 \%$ are obtained as $13.8 \ M P a$, $16.2 \ M P a$, $18.6 \ M P a$, $21.1 \ M P a$ and $23.5 \ M P a$ respectively, and the values normalized by the value of the magnitude $\varepsilon = 0.2 \ %$ are calculated as $1.00$, $1.17$, $1.30$, $1.40$ and $1.48$ respectively as shown in Figure 2.13. Thus, it is worth noticing that the stress jump phenomenon is highly correlated with the dissipative higher order microstress quantities $S_{ij,k}^{dis}$. In addition, the very first responses immediately after the passivation also make a substantial difference with varying passivation points. The slopes of the very first responses for the magnitudes of $\varepsilon = 0.2 \ %$, $0.3 \ %$, $0.4 \ %$, $0.5 \ %$ and $0.6 \ %$ are calculated as $64.8 \ G P a$, $87.1 \ G P a$, $109.7 \ G P a$, $132.5 \ G P a$ and $155.5 \ G P a$ respectively.

The effects of various parameters on the mechanical behaviour of the stretch-surface passivation problem are investigated by using a one-dimensional finite element code developed for this work. The numerical results reported in this parametric studies are obtained by using the values of the material parameters in Table 2.2 unless it is differently mentioned.

The stress-strain graphs for various values of the hardening material parameter $h$ are shown in Figure 2.14 with two different cases of the SGP theory, which are the case with the dissipative higher order microstress quantities $S_{ij,k}^{dis}$ and the case without $S_{ij,k}^{dis}$. The numerical simulations are carried out with $h = 100 \ M P a$, $200 \ M P a$, $300 \ M P a$, $400 \ M P a$ and $500 \ M P a$, respectively. For the SGP model with $S_{ij,k}^{dis} \neq 0$, the slopes of the very first response immediately after the passivation are obtained as $E_h = 109.7 \ G P a$ in all simulations, and the corresponding magnitudes
of the stress jump for each simulation are respectively obtained as \( \sigma'_{h=100\,MPa} = 18.6\,MPa \), \( \sigma'_{h=200\,MPa} = 18.6\,MPa \), \( \sigma'_{h=300\,MPa} = 18.7\,MPa \), \( \sigma'_{h=400\,MPa} = 18.7\,MPa \) and \( \sigma'_{h=500\,MPa} = 18.7\,MPa \). There is little difference between all the simulations. For the SGP model with \( S_{ijk}^{\text{dis}} = 0 \), no stress jump phenomena are observed in all simulations.

Figure 2.13. Comparison of the results from the SGP model with the dissipative potential dependent on \( \dot{\varepsilon}_{ij,k} \) (i.e. \( S_{ijk}^{\text{dis}} \neq 0 \)) for various passivation points (\( \varepsilon = 0.2\% \), 0.3\%, 0.4\%, 0.5\% and 0.6 \% with identical energetic and dissipative length scales).

Figure 2.14. Comparison of the results from two SGP models (the model with the dissipative potential dependent on \( \dot{\varepsilon}_{ij,k} \) (i.e. \( S_{ijk}^{\text{dis}} \neq 0 \)) and the one with the dissipative potential independent on \( \dot{\varepsilon}_{ij,k} \) (i.e. \( S_{ijk}^{\text{dis}} = 0 \))) with the effects of the hardening material parameter \( \dot{\varepsilon}_{ij,k} \). The numerical simulations are carried out with \( h = 100\,MPa, 200\,MPa, 300\,MPa, 400\,MPa \) and 500\,MPa.
The effects of the non-negative rate sensitivity parameter \( m \) on the stress-strain behaviour for the two cases of the SGP model are represented in Figure 2.15. It is clearly shown in this figure that by increasing the rate sensitivity parameter, the stress jump phenomena are significantly manifested in the case of the SGP model with \( S_{ijk}^{\text{dis}} \neq 0 \) in terms of both the slope of the very first response immediately after the passivation and the corresponding magnitude of the stress jump. In the case of the SGP model with \( S_{ijk}^{\text{dis}} = 0 \), on the other hand, the material behaviour is not affected a lot by the rate sensitivity parameter \( m \). In the SGP model with \( S_{ijk}^{\text{dis}} \neq 0 \), the slopes of the very first response immediately after the passivation (\( E_m \)) and the corresponding magnitudes of the stress jump (\( \sigma'_m \)) are obtained as \( E_{m=0.2} = 96.7 \text{ GPa} \), \( E_{m=0.25} = 103.0 \text{ GPa} \), \( E_{m=0.3} = 109.7 \text{ GPa} \), \( E_{m=0.35} = 116.5 \text{ GPa} \) and \( \sigma'_{m=0.2} = 14.8 \text{ MPa} \), \( \sigma'_{m=0.25} = 16.7 \text{ MPa} \), \( \sigma'_{m=0.3} = 18.6 \text{ MPa} \), \( \sigma'_{m=0.35} = 20.6 \text{ MPa} \) respectively. Thus, it is clearly shown that both the slope of the very first response immediately after the passivation and the corresponding magnitude of the stress jump increase as the non-negative rate sensitivity parameter \( m \) increases.

![Figure 2.15. Comparison of the results from two SGP models (the model with the dissipative potential dependent on \( \dot{\varepsilon}_{ij}^p \) (i.e. \( S_{ijk}^{\text{dis}} \neq 0 \)) and the one with the dissipative potential independent of \( \dot{\varepsilon}_{ij}^p \) (i.e. \( S_{ijk}^{\text{dis}} = 0 \)) with the effects of the non-negative rate sensitivity parameter \( m \). The numerical simulations are carried out with \( m = 0.2, 0.25, 0.3 \) and 0.35.](image)

The effects of the temperature sensitivity parameter \( n \) on the stress-strain behaviour for the two cases of the SGP model are represented in Figure 2.16. It is clearly shown in this figure that the yield stress significantly increases as the temperature sensitivity parameter \( n \) increases, while the strain hardening is not influenced a lot by this parameter. This is because the temperature affects the strain hardening mechanism through the dislocation forest barriers while the backstress, i.e. energetic gradient hardening, is almost independent of the temperature. Meanwhile, the temperature sensitivity parameter \( n \) significantly affects the stress-strain response in the case of the SGP model with \( S_{ijk}^{\text{dis}} \neq 0 \). In this case, the slopes of the very first response immediately after the passivation are obtained as \( E_{n=0.4} = 112.5 \text{ GPa} \), \( E_{n=0.6} = 109.7 \text{ GPa} \), \( E_{n=0.8} = 107.8 \text{ GPa} \).
and $E_{n=1.0} = 106.6 \, GPa$, and the corresponding magnitudes of the stress jump are obtained as

$\sigma'_n=0.4 = 16.6 \, MPa$, $\sigma'_n=0.6 = 18.6 \, MPa$, $\sigma'_n=0.8 = 19.7 \, MPa$ and $\sigma'_n=1.0 = 20.4 \, MPa$ respectively. Thus, in contrast with the rate sensitivity parameter $m$, the slope of the very first response immediately after the passivation decreases while the corresponding magnitude of the stress jump increases as the temperature sensitivity parameter $n$ increases.

The effects of the thermal material parameter $T_y$ on the stress-strain behaviour with the two cases of the SGP model are represented in Figure 2.17. Similar to the temperature sensitivity parameter $n$, the yield stress significantly increases as the thermal material parameter $T_y$ increases, while the strain hardening is not influenced a lot by this parameter. In the case of the SGP model with $S_{ijk}^{\text{dis}} \neq 0$, the slopes of the very first response immediately after the passivation ($E_{T_y}$) and the corresponding magnitudes of the stress jump ($\sigma'_y$) are obtained as $E_{T_y=500 \, °K} = 111.9 \, GPa$, $E_{T_y=1000 \, °K} = 109.7 \, GPa$, $E_{T_y=1500 \, °K} = 108.7 \, GPa$, $E_{T_y=2000 \, °K} = 108.1 \, GPa$ and $\sigma'_y=500 \, °K = 17.1 \, MPa$, $\sigma'_y=1000 \, °K = 18.6 \, MPa$, $\sigma'_y=1500 \, °K = 19.2 \, MPa$, $\sigma'_y=2000 \, °K = 19.6 \, MPa$ respectively. These results from the simulations with various thermal material parameter $T_y$ are very similar to those with the temperature sensitivity parameter $n$, in the sense that the slope of the very first response immediately after the passivation decreases while the corresponding magnitude of the stress jump increases as the temperature sensitivity parameter $n$ increases.

Figure 2.16. Comparison of the results from two SGP models (the model with the dissipative potential dependent on $\dot{\varepsilon}_{ijkl}^p$ (i.e. $S_{ijk}^{\text{dis}} \neq 0$) and the one with the dissipative potential independent on $\dot{\varepsilon}_{ijkl}^p$ (i.e. $S_{ijk}^{\text{dis}} = 0$)) with the effects of the temperature sensitivity parameter $n$. The numerical simulations are carried out with $n = 0.4, 0.6, 0.8$ and 1.0.

The effects of the interfacial temperature sensitivity parameter $n'$ on the stress-strain behaviour for the two cases of the SGP model are presented in Figure 2.18. It is clearly shown in this figure that increasing interfacial temperature sensitivity parameter makes the grain boundary (interface) harder and results in less variation of the stress jump in both cases of the SGP model with $S_{ijk}^{\text{dis}} \neq 0$ and $S_{ijk}^{\text{dis}} = 0$. In the case of the SGP model with $S_{ijk}^{\text{dis}} \neq 0$, the slopes of the very
first response immediately after the passivation are obtained as 
\( E_{n^t=0.1} = 109.7 \, \text{GPa} \), 
\( E_{n^t=0.2} = 80.4 \, \text{GPa} \), 
\( E_{n^t=0.3} = 70.3 \, \text{GPa} \) and 
\( E_{n^t=0.5} = 62.1 \, \text{GPa} \), and the corresponding magnitudes of 
the stress jump are obtained as 
\( \sigma'_{n^t=0.1} = 18.6 \, \text{MPa} \), 
\( \sigma'_{n^t=0.2} = 17.6 \, \text{MPa} \), 
\( \sigma'_{n^t=0.3} = 17.1 \, \text{MPa} \) and 
\( \sigma'_{n^t=0.5} = 16.4 \, \text{MPa} \) respectively. From these results, it is easily observed that the slope of the 
very first response after the passivation and the 
corresponding magnitude of the stress jump 
increase as the interfacial temperature sensitivity parameter \( n^I \) decreases. In addition, the 
variations along with the different cases are shown 
to be more drastic by decreasing the interfacial 
temperature sensitivity parameter \( n^I \). Similarly, for 
the case of the SGP model with \( S^\text{dis}_{ijkl} \neq 0 \), and 
also by decreasing the interfacial temperature sensitivity parameter makes the variation more 
radiically changing as shown in Figure 2.18.

![Figure 2.17. Comparison of the results from the two SGP models (the model with the dissipative potential dependent on \( \varepsilon^P_{ijkl} \) (i.e. \( S^\text{dis}_{ijkl} \neq 0 \)) and the one with the dissipative potential independent on \( \varepsilon^P_{ijkl} \) (i.e. \( S^\text{dis}_{ijkl} = 0 \)) with the effects of the thermal material parameter \( T^I_y \). The numerical simulations are carried out with \( T^I_y = 500 \, \text{°K}, 1000 \, \text{°K}, 1500 \, \text{°K} \) and \( 2000 \, \text{°K} \).](image)

The effects of the interfacial thermal material parameter \( T^I_y \) on the stress-strain behaviour 
for the two cases of the SGP model are represented in Figure 2.19. As can be seen in this figure, 
the overall characteristic from the simulation results with various \( T^I_y \) is similar to those with 
various \( n^I \) in the sense that increasing \( T^I_y \) makes the grain boundary (interface) harder and results 
in less variation of the stress jump in both cases of the SGP model with \( S^\text{dis}_{ijkl} \neq 0 \) and \( S^\text{dis}_{ijkl} = 0 \). In 
the case of the SGP model with \( S^\text{dis}_{ijkl} \neq 0 \), the slopes of the very first response immediately after 
the passivation are obtained as 
\( E_{T^I_y=600 \, \text{°K}} = 114.0 \, \text{GPa} \), 
\( E_{T^I_y=700 \, \text{°K}} = 109.7 \, \text{GPa} \), \( E_{T^I_y=1000 \, \text{°K}} = 101.7 \, \text{GPa} \) and 
\( E_{T^I_y=1300 \, \text{°K}} = 97.1 \, \text{GPa} \), and the corresponding magnitudes of the stress jump are 
obtained as 
\( \sigma'_{T^I_y=600 \, \text{°K}} = 18.7 \, \text{MPa} \) , 
\( \sigma'_{T^I_y=700 \, \text{°K}} = 18.6 \, \text{MPa} \) , 
\( \sigma'_{T^I_y=1000 \, \text{°K}} = 18.4 \, \text{MPa} \) and 
\( \sigma'_{T^I_y=1300 \, \text{°K}} = 18.3 \, \text{MPa} \) respectively.
Figure 2.18. Comparison of the results from two SGP models (the model with the dissipative potential dependent on $\varepsilon_{ij,k}^P$ (i.e. $S_{ij,k}^{\text{diss}} \neq 0$) and the one with the dissipative potential independent on $\varepsilon_{ij,k}^P$ (i.e. $S_{ij,k}^{\text{diss}} = 0$)) with the effects of the interfacial temperature sensitivity parameter $n^I$. The numerical simulations are carried out with $n^I = 0.1, 0.2, 0.3$ and 0.5.

Figure 2.19. Comparison of the results from the two SGP models (the model with the dissipative potential dependent on $\varepsilon_{ij,k}^P$ (i.e. $S_{ij,k}^{\text{diss}} \neq 0$) and the one with the dissipative potential independent on $\varepsilon_{ij,k}^P$ (i.e. $S_{ij,k}^{\text{diss}} = 0$)) with the effects of the interfacial thermal material parameter $T_{y}^{I}$. The numerical simulations are carried out with $T_{y}^{I} = 600 \, ^{\circ}K, 700 \, ^{\circ}K, 1000 \, ^{\circ}K$ and $1300 \, ^{\circ}K$.

2.4.3.4 The evolution of the free energy and dissipation potentials

Based on the calibrated model parameters of Ni (Table 2.1), the evolution of the various
potentials during the plastic deformation are investigated with four different temperatures, i.e. 25 °C, 75 °C, 145 °C and 218 °C, in this section. Figure 2.20 shows (a) the variation of the plastic strain dependent free energies ($\Psi_1^d$, $\Psi_1^{d,R}$ and $\Psi_1^{d, NR}$), (b) plastic strain dependent dissipation rate $\mathcal{D}_1$ (i.e. plastic strain dependent term in Equation (2.58)), (c) plastic strain gradient dependent free energy ($\Psi_2^d$) and dissipation rate $\mathcal{D}_2$ (i.e. plastic strain gradient dependent term in Equation (2.58)), and (d) amount of stored energy ($\Psi_1^d + \Psi_2^d$) and dissipated energy ($\mathcal{D} = \int (\mathcal{D}_1 + \mathcal{D}_2) dt$).

As can be seen in Figure 2.20 (a), both free energies $\Psi_1^d$ and $\Psi_1^{d, NR}$ decrease as the temperature increases. The stored energy of cold work $\Psi_1^{d, R}$ is also presented in this figure. One can observe that $\Psi_1^d$ and $\Psi_1^{d, NR}$ has a strong temperature dependency while the stored energy of cold work has no variation with varying temperatures. In addition, the stored energy of cold work tends to saturate after some critical point since the stored energy of cold work is proportional to the dislocation density that remains constant after the aforementioned critical point. Meanwhile, it is shown in Figure 2.20 (b) and (c) that rates of dissipation, $\mathcal{D}_1$ and $\mathcal{D}_2$, are dependent on the temperature such that both $\mathcal{D}_1$ and $\mathcal{D}_2$ increase with decreasing temperatures while $\Psi_2^d$ shows no temperature dependency. The amount of stored and dissipated energies are shown in Figure 2.20 (d). As it is shown in this figure, the amount of stored energy is larger than the dissipated energy and both decrease as the temperature increases.

Figure 2.20. The evolution of free energy and dissipation potentials based on the calibrated model parameters (Han et al., 2008): (a) plastic strain dependent free energy, (b) plastic strain dependent dissipation rate, (c) plastic strain gradient dependent free energy and dissipation rate (The primary $y$-axis on the LHS: $\mathcal{D}_2$, the secondary $y$-axis on the RHS: $\Psi_2^d$), and (d) amount of stored and dissipated energies.

(fig. cont’d.)
2.4.3.5 The evolution of the free energy and dissipation potentials

In this subsection, the one-dimensional finite element implementation is extended to the two-dimensional one. The simple tension problem of the square plate is solved to study the strain gradient effects, the mesh sensitivity of the model with the three cases according to the number of elements (100, 400 and 1600 elements), and the stress jump phenomena under the abrupt surface passivation. Each edge of the plate has a length of \( \omega \) and the material parameters in Table 2.2 are used again for these simulations.

Figure 2.21 (a) and (b) show the stress-strain behaviour of the plate with the various energetic length scales \( (\ell_{en}/\omega = 0.0, 0.1, 0.3, 0.5, 0.7 \text{ and } 1.0 \text{ with } \ell_{dis}/\omega = 0.0) \) and dissipative length scales \( (\ell_{dis}/\omega = 0.0, 0.1, 0.2, 0.3, 0.4 \text{ and } 0.5 \text{ with } \ell_{en}/\omega = 0.0) \) respectively. In common with the one-dimensional simulations, the numerical results show the energetic hardening as the energetic length scale increases as well as the dissipative strengthening as the dissipative length scale increases.

Figure 2.21 (c) shows the grain boundary effect of the square plate. It is well known that the grain boundary blocks the dislocation movement, which in turn, leads to the strengthening of the material. The energetic and dissipative length scales reported in these simulations are set zero and the micro-clamped condition is imposed at the grain boundary, which is indicated by the bold line in the figure. The strengthening caused by increasing the grain boundary area is well observed as expected. For the simulations presented in Figure 2.21 (a), (b) and (c), \( 20 \times 20 \) elements are used.

The mesh sensitivity of the two-dimensional numerical model is examined in terms of the energetic and dissipative length scales with \( 10 \times 10, 20 \times 20 \) and \( 40 \times 40 \) mesh elements in Figure 2.21 (d) and (e) respectively. Figure 2.21 (d) shows the stress-strain behaviour of the plate with the various energetic length scales \( (\ell_{en}/\omega = 0.1, 0.5 \text{ and } 1.0 \text{ with } \ell_{dis}/\omega = 0) \) compared to those in the absence of the gradient effects \( (\ell_{en}/\omega = \ell_{dis}/\omega = 0) \). The numerical results without the gradient terms significantly show the mesh sensitivity as expected, while for all non-zero values of \( \ell_{en}/\omega \), the numerical solutions show the mesh-independent behaviour. In addition, Figure 2.21 (d) also shows the energetic hardening as the energetic length scale increases. The mesh-independent behaviour is also observed with varying dissipative length scales \( (\ell_{dis}/\omega = 0.1, 0.2 \text{ and } 0.3 \text{ with } \ell_{en}/\omega = 0) \) in Figure 2.21 (e) as with the case for the energetic length scale. The dissipative strengthening is also observed in this figure.

Lastly, the stress jump phenomenon hitherto extensively studied in the one-dimensional finite element implementation is also examined for the two-dimensional simulation. \( 20 \times 20 \) elements with \( \ell_{en}/\omega = 0.0 \) and \( \ell_{dis}/\omega = 0.2 \) are used for this simulation. Figure 2.21 (f) show the material behaviours of the unpassivated plate, the passivated plate and the plate abruptly passivated at some point. As can be seen in this figure, the stress jump is significantly observed by the numerical results, which are identical to the one-dimensional case.
Figure 2.21. The stress-strain behaviour of the square plate: (a) the energetic hardening, (b) the dissipative strengthening, (c) the grain boundary effect, (d) the mesh sensitivity with varying $\ell_{en}$, (e) the mesh sensitivity with varying $\ell_{dis}$ and (f) the stress jump phenomenon.
fig. cont’d.
In this chapter, a phenomenological thermodynamic-based higher order gradient plasticity theory for a single grain is proposed and applied to the stretch-surface passivation problem for investigating the material behaviour under the non-proportional loading condition. The thermodynamic potentials such as the Helmholtz free energy and the dissipation potential are established based on the concepts of the dislocation interaction mechanism and the thermal activation energy. The microstructural interface (grain boundary) effect between two grains is also incorporated into the formulation, such that the developed grain boundary flow rule is able to account for the energy storage at the grain boundary caused by the dislocation pile up as well as the energy dissipation through the grain boundary caused by the dislocation transfer. The thermodynamic conjugate forces are divided into two components \( (\mathcal{X}_{ij} = \mathcal{X}_{ij}^{en} + \mathcal{X}_{ij}^{dis}, S_{ijk} = S_{ijk}^{en} + S_{ijk}^{dis}) \), which are the energetic and dissipative counterparts. The formulation is tested for two cases in the presence of the dissipative higher order microstress quantities \( S_{ijk}^{dis} \). In the first case, the dissipation potential is dependent on the gradients of the plastic strain rate \( \dot{\varepsilon}_{ijk}^p \), as a result, \( S_{ijk}^{dis} \) does not have a value of zero in this formulation. In the second case the dissipation potential is independent of \( \dot{\varepsilon}_{ijk}^p \), which in turn, \( S_{ijk}^{dis} \) does not exist. It is noticed by Fleck et al. (2014, 2015) that \( S_{ijk}^{dis} \) always give rise to the stress jump phenomenon, which causes a controversial dispute in the field of SGP theory with respect to whether it is physically acceptable or not, under the non-proportional loading condition.

In the present work, new formulations for the two cases of the SGP theory with and without the dissipative higher order microstress quantities \( S_{ijk}^{dis} \) are theoretically proposed with the new forms of the free energy and the dissipation potentials for eliminating an elastic loading gap and corresponding finite element solution for the stretch-surface passivation problem is developed in order to investigate and compare the responses from two cases under the non-proportional loading condition by using the commercial finite element package ABAQUS/standard (2012) via the user-subroutine UEL. In the developed code, the displacement field and the plastic strain field are
discretized independently from each other, in other words, the plastic strain field is employed as an additional nodal degree of freedom in addition to the displacement field.

Prior to exploring the effect of the dissipative higher order microstress quantities \( S^{\text{dis}}_{ijkl} \) on the stress-strain behaviour for the two cases of the SGP theory with and without \( S^{\text{dis}}_{ijkl} \), the proposed model and corresponding finite element code are validated by comparing with three sets of small-scale experiments. The material parameters for the proposed SGP model are also calibrated in this chapter by using the experimental data. Particularly, each set of three experiments involving Al, Cu and Ni are selected respectively to examine the applicability of the proposed finite element implementation to the various kinds of materials. The first experiment, which was performed by Haque and Saif (2003), is the uniaxial tensile testing of nanoscale freestanding Al thin films to explore the effect of strain gradient in 100 nm, 150 nm and 485 nm thick specimens with average grain size of 50 nm, 65 nm and 212 nm respectively. In particular, the comparison between the proposed SGP model and Voyiadjis and Faghihi (2014) model is carried out to show the increase in accuracy of the proposed model. The results clearly show the size effect on the stress-strain curves of the Al thin films, in addition, the calculated results of the proposed SGP model display a tendency to be more coincident to the experimental data than those of Voyiadjis and Faghihi (2014). For the second experimental validation, the experimental work of Xiang and Vlassak (2006) on the size effect in electroplated Cu thin films with the various microscale thickness is selected since the effect of passivation on the stress-strain behaviour of the Cu thin film is also considered in their work. In order to describe the passivation effect on the proposed SGP model, the micro-clamped condition, which causes the dislocations to be completely blocked at the grain boundary, is imposed at both surfaces of the Cu thin films. The stress-strain curves from the numerical results of the proposed SGP model are in good agreement with the experimental measurements. The size effect according to the variation of the film thicknesses is also well observed from the results. For the third experimental validation, the micro-tensile test on the temperature effect on Ni thin films by Han et al. (2008) is employed since, in the nano- or micro-systems, the effect of the higher order gradient on temperature also needs to be considered for the fast transient behaviour. From both the experimental and numerical results, it is shown that the Young’s modulus is not affected by the variations in temperature while the yield and tensile strength decrease as the specimen temperature increases. The calculated results of the proposed model compare better to the experimental data than those of Voyiadjis and Faghihi (2014).

The numerical simulation part is largely composed of four subparts. The main purpose of the first part is to examine the occurrence of the stress jump phenomenon under the stretch-surface passivation condition in conjunction with the aforementioned three experiments. In all simulations, a stress jump is clearly observed at the onset of passivation. The second part is carried out in order to clearly show the results to be contrary to each other from the two cases of the SGP model. The conclusion in this part is drawn such that a significant stress jump with the slope \( E^{\text{passivation}} \) similar to the modulus of elasticity \( E \) is shown in the case of the SGP model with \( S^{\text{dis}}_{ijkl} \neq 0 \), on the other hand, no elastic stress jump is observed in the case of the SGP model with \( S^{\text{dis}}_{ijkl} = 0 \). This result is exactly in agreement with the prediction in Fleck et al. (2014, 2015).

An extensive parametric study is presented in the third part of this work in terms of the effects of the dissipative length scale \( \ell^{\text{dis}} \), the onset point of passivation, the hardening material parameter \( h \), the non-negative rate sensitivity parameter \( m \), the temperature sensitivity parameter \( n \), the thermal material parameter \( T^i \), the interfacial temperature sensitivity parameter \( n^I \), and the interfacial thermal material parameter \( T^I \) on the stress-strain response for the two SGP cases.
respectively. There are a number of conclusions worth mentioning here namely: (1) the magnitude of the stress jump significantly increases as the dissipative length scale increases, on the other hand, the stress jump phenomena disappear as the dissipative length scale comes closer to zero, (2) the slopes of the very first response $E$ immediately after the passivation also increase as the dissipative length scales increase, (3) the stress jump phenomenon is highly correlated with the dissipative higher order microstress quantities $S_{ijk}^{\text{dis}}$, in addition, the very first responses immediately after the passivation also make a substantial difference with varying passivation points, (4) the hardening material parameter $h$ does not affect the stress jump significantly in the case of the SGP model with $S_{ijk}^{\text{dis}} \neq 0$, (5) both the slope of the very first response immediately after the passivation and the corresponding magnitude of the stress jump substantially increase as the non-negative rate sensitivity parameter $m$ increases in the case of the SGP model with $S_{ijk}^{\text{dis}} \neq 0$, (6) as the temperature-related parameters for the bulk such as the temperature sensitivity parameter $n$ and the thermal material parameter $T_y$ increase, the slope of the very first response immediately after the passivation decreases and the corresponding magnitude of the stress jump increases in the case of the SGP model with $S_{ijk}^{\text{dis}} \neq 0$, (7) the slope of the very first response after the passivation, the corresponding magnitude of the stress jump increase and the variations along with the cases are shown more drastically by decreasing the temperature-related parameters for the interface, such as the interfacial temperature sensitivity parameter $n^I$ and the interfacial thermal material parameter $T_y^I$ in the case of the SGP model with $S_{ijk}^{\text{dis}} \neq 0$, and finally (8) no stress jump is observed in all cases with $S_{ijk}^{\text{dis}} = 0$.

Meanwhile, the plastic strain dependent free energy accounting for the stored energy of cold work is derived in this chapter by assuming that the stored energy is related to the energy carried by dislocations. Accordingly, the variation of free energies and dissipation potentials during the plastic deformation are investigated with four different temperatures, i.e. 25 °C, 75 °C, 145 °C and 218 °C. From the numerical results, it is shown that the stored energy of cold work has no temperature dependency, in addition, the stored energy of cold work tends to saturate after some critical point since the stored energy of cold work is proportional to the dislocation density that remains constant after the aforementioned critical point.

Lastly, the two-dimensional tension problem of the square plate is solved to examine the mesh sensitivity of the model. The effects of the strain gradient and grain boundary are also studied. As expected, a strong mesh-dependence stress-strain behaviour is observed in the case of no gradient effects, while the numerical results with the gradient effects show the mesh-independent behaviour. The energetic hardening, the dissipative strengthening, the grain boundary strengthening and the stress jump phenomena are well observed in common with the results from the one-dimensional simulation.
3 THERMODYNAMICALLY CONSISTENT STRAIN GRADIENT PLASTICITY MODELS AND APPLICATIONS FOR SMALL DEFORMATIONS: SIZE EFFECTS

3.1 Introduction

The conventional continuum plasticity model is characteristically size-independent and is not capable of capturing the size effects, in particular, when the material is subjected to the nonhomogeneous (heterogeneous) plastic deformation under the fast transient time and its size ranges from a few hundreds of nanometers to a few tens of micrometers. The evidence of such a behaviour is found in many micro-mechanical experimental observations such as nano/micro-indentation hardness (Almasri and Voyiadjis, 2010; Kim and Park, 1996; Lim et al., 2017; Park et al., 1996; Voyiadjis et al., 2010a; Voyiadjis and Peters, 2010; Voyiadjis and Zhang, 2015; Zhang and Voyiadjis, 2016), nano/micro-pillars (Hwang et al., 1995), torsion of micron-dimensioned metal wires (Fleck and Hutchinson, 1997; Kim et al., 1994), bending of micro-scale single and polycrystalline thin films (Venkatraman et al., 1994), thin beams under micron-dimensioned tension/bending (Huang et al., 2006; Parilla et al., 1993), flow strength of nano-crystalline metals (Bergeman et al., 2006) and microscale reverse extrusion of copper (Zhang et al., 2018).

It is commonly accepted that the interaction between the statistically stored dislocations (SSDs) and the geometrically necessary dislocations (GNDs) gives rise to the size effect observed in micro/nano-scale metallic volumes. The SSDs are stored by random trapping each other and increase with the plastic strain, whereas the GNDs are stored to preserve the compatibility of diverse material components and increase with the gradient of the plastic strain. As the size of material specimen decreases, the GNDs increase the resistance to deformation by acting as the blockages to the SSDs (Fleck et al., 1994). This mechanism is called glide-control because the existence of GNDs, caused by non-uniform deformation or the prescribed boundary conditions, restrains the slip of dislocation glide (Muhlhaus and Aifantis, 1991; Nicola et al., 2006; Xiang and Vlassak, 2006). Another mechanism for the size effect is the dislocation starvation caused by the insufficient amount of dislocations that arises from the small volumes (Bergeman et al., 2006; Giacomazzi et al., 2004; Yaghoobi and Voyiadjis, 2016).

Numerous theoretical and numerical works have been carried out to explore the aforementioned phenomena based on the gradient-enhanced nonlocal plasticity theory (Fleck and Hutchinson, 1997; Gudmundson, 2004; Gurtin and Anand, 2009; Hutchinson, 2012; Ivanitsky and Kadakov, 1983; Lele and Anand, 2008; Song and Voyiadjis, 2018a; Voyiadjis and Song, 2017) since the pioneering investigations of Aifantis (Aifantis, 1984, 1987) which incorporate the gradient term in the conventional flow rule. McDowell (2010) reviewed the trends in plasticity research for metals over the 25 years prior to the publication year (2010) in terms of the multiscale kinematics, the effect of material length scale, the role of grain boundaries, and so forth.

Hutchinson (2012) classified the strain gradient version of J2 flow theories into two classes: Incremental theory developed by Fleck and Hutchinson and non-incremental theory developed by Gudmundson, Gurtin, and Anand (c.f. see Fleck et al. (2014, 2015); Gudmundson (2004); Gurtin and Anand (2005a, 2009); Hutchinson (2012) for details). Fleck and co-workers (Fleck et al., 2014, 2015) then pointed out that the specific phenomenon, which exhibits a significant stress jump due to infinitesimal variation in the direction of plastic strain that may occur

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8 Reprinted with permission from Song and Voyiadjis (2018a)
under the non-proportional loading, arise in the non-incremental theory and also discussed its physical acceptance in their work. Fleck and co-workers (Fleck et al., 2014, 2015) have shown this phenomenon with two plane strain problems, stretch-bending problem and stretch-surface passivation problem, for non-proportional loading condition. In their work, it is noted that the dissipative higher order microforces always cause the significant stress gap or jump under the non-proportional loading conditions. Recently, Voyiadjis and Song (2017) examined the stress jump phenomenon with the stretch-surface passivation problem using the one-dimensional finite element implementation, and an extensive parametric study is also performed in order to investigate the characteristics of the stress jump phenomenon.

Another important issue in the strain gradient plasticity (SGP) theory is the thermal effect. In the nano/micro systems, the effect of temperature gradient needs to be considered for the fast transient time. If the mean free path of phonons is approximately the medium size, heat transfer is partly ballistic rather than purely diffusive. This is caused by the small depth of the zone influenced by heat or small size of the structure and the non-equilibrium transition of thermodynamic circumstances related to reducing the response time (Tzou and Zhang, 1995). Moreover, when the response time in nano/micro-scale materials decreases to the thermalization time range, it results in the non-equilibrium conversion of thermodynamic states between phonons and electrons (Brorson et al., 1990; Tzou and Zhang, 1995). The conventional heat equation is not capable of capturing the effect of electron-phonon interaction in this time frame, thus, the microscopic generalized heat equation has to be employed to interpret these phenomena.

Voyiadjis and co-workers (Voyiadjis and Deliktas, 2009a, b; Voyiadjis and Faghihi, 2012; Voyiadjis et al., 2014; Voyiadjis and Song, 2017; Voyiadjis et al., 2017) have developed the thermodynamically consistent and coupled thermo-mechanical SGP models to study the characteristics of nano/micro-scale metallic materials. All those works, however, have been limited to one-dimensional finite element implementation. As it is well known, there is bound to be a fundamental difference between one-dimensional finite element implementation and two-dimensional one. For example, in one-dimensional case, some special complications, e.g. the resonance between the physical scale and mesh scale, cannot be considered during the simulation. It should be noted that there is no difference between the different dimensions from the variational point of view, however, the difference exists in the description of the finite dimensional approximation spaces. The finite element implementation in multi-dimension is based on the same principle of the one in the one-dimension, thus the piecewise-polynomial functions of low degree with many terms are considered for accuracy. In the two-dimensional model, it is significantly more complicated since the polynomial functions have more variables, and the open sets are much more varied than in the one-dimensional model. In terms of the dimensional extension, there is the simple modification from one-dimensional finite element implementation for the strain gradient plasticity model to the two-dimensional one in Voyiadjis and Song (2017). However, in that work, the effects of temperature and its gradient were not considered, but just addressed the effect of the mechanical component of the thermodynamic microforces in terms of the stress jump phenomenon. Recently, in Song and Voyiadjis (2018a), the two-dimensional finite element implementation of the coupled thermo-mechanical strain gradient plasticity model is performed. In that work, two null boundary conditions, i.e. microscopically free and hard boundary conditions, are considered at the grain boundary to describe the dislocation movement and the plastic flow at the grain boundary areas.

It is well known that the free surface may act as the source for the defect development and its propagation towards the grain inside, whereas the grain boundaries block this dislocation
movement, consequently give rise to the strain gradients to accommodate the geometrically necessary dislocations (Hirth and Lothe, 1982). In addition, the grain boundaries can be the source of dislocation through the transmission of plastic slip to the neighboring grains (Clark et al., 1992). Besides these physical remarks, from the mathematical viewpoint, the nonstandard boundary conditions are necessary at the external boundary of a region for the well-posed governing equations in the implementation of higher order strain gradient plasticity models. Therefore, careful modeling of the grain boundary is important in the continued development of higher order strain gradient plasticity models.

The experimental observations on slip transmission motivate one to assume that the effect of surface/interfacial energy and the global nonlocal energy residual should be non-vanishing. Examples can be found from the in-situ TEM direct observations, e.g., Lee et al. (1989), or using the geometrically necessary dislocation (GND) concept in the description of observations in bicrystallines, e.g., Sun et al. (2000) and nanoindentation tests close to the grain boundary, e.g., Soer et al. (2005). This results in a new type of boundary condition, in the context of strain gradient plasticity incorporating the interfacial energy, accounting for the surface resistance to the slip transfer due to the grain boundary misalignment. See e.g., Aifantis and Willis (2005); Cermelli and Gurtin (2002); Fredriksson and Gudmundson (2007a); Gudmundson (2004); Gurtin (2008).

Also, in this chapter, two-dimensional numerical simulation in the context of the small deformation framework is developed incorporating the temperature and rate dependent flow rules for the grain interior and grain boundary, and the proposed model is validated by comparing against two sets of small-scale experiments showing the size effects. The reason for choosing these two experiments is that these experiments were also used in Voyiadjis and Song (2017) for validating the one-dimensional model, so it will be possible to compare the numerical results and validated material properties directly. The simple shear problem is solved based on the validated model in order to examine the size effect in the small-scale metallic materials. The square plate problem with the various grain boundary conditions is also solved to investigate the grain boundary effect in conjunction with the length scales.

3.1.1 Kinematics

In this chapter, tensors are denoted by the subscripts $i, j, k, l, m, n$. The superscripts $e, p, int, ext, en, dis$ and etc. imply specific quantities such as elastic state, plastic state, internal, external, energetic, dissipative and etc. respectively. Also, the superimposed dot represents derivative with respect to time, and the indices after a comma represent the partial derivatives.

In the conventional continuum plastic theory of the isotropic solids for the small deformation assumption, the displacement gradient $u_{i,j}$ is decomposed into elastic $u_{i,j}^e$ and plastic counterparts $u_{i,j}^p$ as follows:

$$u_{i,j} = u_{i,j}^e + u_{i,j}^p \quad \text{where} \quad u_{k,k}^p = 0 \quad (3.1)$$

where the elastic distortion $u_{i,j}^e$ and the plastic distortion $u_{i,j}^p$ indicate the recoverable stretching and rotation, and the evolution of dislocations in the material structure respectively.

For the small deformation framework in the conventional theory, the strain tensor $\varepsilon_{ij}$ is also decomposed into the elastic and plastic elements as follows:

$$\varepsilon_{ij} = \varepsilon_{ij}^e + \varepsilon_{ij}^p = \frac{1}{2}(u_{i,j}^e + u_{j,i}^e) + \frac{1}{2}(u_{i,j}^p + u_{j,i}^p) \quad (3.2)$$
Here, the plastic strain is assumed to be deviatoric, \( \varepsilon_{kk}^p = 0 \), since the material volume is not changed by the dislocation glide-induced plastic deformation (Gurtin and Anand, 2009). The plastic rotation is then given as follows:

\[
W_{ij}^p = \frac{1}{2} \left( u_i^p - u_j^p \right)
\]  

(3.3)

In the conventional isotropic plasticity theory, since the plastic rotations (the rotation of material relative to the lattice) may be absorbed by their elastic counterparts without any influence on the field equations, they are fundamentally irrelevant to the theory. In this sense, the plasticity irrotational assumption is principally adopted in this chapter as indicated in Equation (3.4) (see Gurtin et al. (2010)).

\[
W_{ij}^p = 0
\]  

(3.4)

Accordingly, \( u^p_{i,j} = \varepsilon^p_{i,j} \).

Meanwhile, the direction of plastic flow \( N_{ij} \) is given by

\[
N_{ij} = \frac{\varepsilon_{ij}^p}{\| \varepsilon_{ij}^p \|} = \frac{\dot{\varepsilon}_{ij}^p}{\dot{\varepsilon}^p} \Rightarrow \dot{\varepsilon}_{ij}^p = \dot{\varepsilon}^p N_{ij}
\]  

(3.5)

with the accumulated plastic strain rate \( \dot{\varepsilon}^p \) given by

\[
\dot{\varepsilon}^p = \| \dot{\varepsilon}_{ij}^p \| = \sqrt{\dot{\varepsilon}_{ij}^p \dot{\varepsilon}_{ij}^p}
\]  

(3.6)

Correspondingly, the accumulated plastic strain \( e^p \) can be obtained by

\[
e^p = \int_0^t \dot{\varepsilon}^p dt
\]  

(3.7)

3.2 Theoretical formulation of the proposed model

3.2.1 Principle of virtual power: grain interior

Recently, the thermodynamically consistent SGP theories have been developed by Voyiadjis and his co-workers to account for the characteristics of small-scale metallic material behaviour based on the principle of virtual power (Voyiadjis and Song, 2017; Voyiadjis et al., 2017).

The internal power \( p^{int} \) is presented with a combination of three energy contributions, i.e. the macro-, micro- and thermal-energy contributions, in the arbitrary region \( \Omega_0 \) as follows:

\[
p^{int} = \int_{\Omega_0} \left( \sigma_{ij} \dot{\varepsilon}_{ij}^{p_{\text{Macro}}} + x \dot{e}^p + Q_i \dot{e}_{i}^{p_{\text{Micro}}} + \mathcal{A} \dot{T} + \mathcal{B}_i \dot{T}_i \right) dV
\]  

(3.8)

where \( x \) and \( Q_i \) are the thermodynamic microforces conjugate respectively to \( \dot{e}^p \) and \( \dot{e}_{i}^{p_{\text{Macro}}} \), and \( \sigma_{ij} \) is the Cauchy stress tensor. It is assumed in this chapter that extra contributions to the internal power exist from the temperature. \( \mathcal{A} \) and \( \mathcal{B}_i \) are the micromorphic scalar and vector generalized stress-like variables conjugate to the temperature rate \( \dot{T} \) and the first gradient of the temperature rate \( \dot{T}_i \) respectively. These terms are introduced in a micromorphic fashion to lead the additional thermal balance equations considering the nonlocal thermal effects (Liu et al., 2017). Therefore, the purely mechanical part of the internal power is complemented by the thermal contributions that represent the thermal part of the power of work, which is the convectively performed power. Note that only the first gradient of temperature rate is considered, for the sake of simplicity. Meanwhile,
one can refer to Faghihi and Voyiadjis (2014) to see the model in the absence of the temperature-related terms $\mathcal{A}$ and $\mathcal{B}_i$.

The internal power $\mathcal{P}^{\text{int}}$ for $\Omega_0$ is equated with the external power $\mathcal{P}^{\text{ext}}$ expended by the macro and microtractions ($t_i$, $m$) on the external surface $\partial \Omega_0$ and the body forces acting within $\Omega_0$ as shown below:

$$\mathcal{P}^{\text{ext}} = \int_{\Omega_0} \frac{\mathcal{B}_i \dot{u}_i}{\text{Macro}} dV + \int_{\partial \Omega_0} \left( t_i \dot{u}_i + m \dot{\mathcal{E}}^p + a \mathcal{A} \right) dS$$

(3.9)

where $\mathcal{B}_i$ is the generalized external body force conjugate to the macroscopic velocity $\dot{u}_i$. Furthermore, it is assumed for the external power to have the term of $\mathcal{A}$, conjugate to $\mathcal{T}$ for the thermal effect.

By using the equation, $\mathcal{P}^{\text{int}} = \mathcal{P}^{\text{ext}}$, in conjunction with the divergence theorem and factoring out the common terms, the balance equations for the macroscopic linear momentum, nonlocal microforce and generalized stresses $\mathcal{A}$ and $\mathcal{B}_i$ for volume $\Omega_0$ can be obtained respectively as follows (see Appendix A for detailed derivations):

$$\sigma_{ij,i} + \delta_i = 0 \quad (3.10)$$

$$\bar{\sigma}_{ij} = (x - Q_{kk}) N_{ij} \quad (3.11)$$

$$\mathcal{B}_{il} - \mathcal{A} = 0 \quad (3.12)$$

where $\bar{\sigma}_{ij}$ is the deviatoric part of $\sigma_{ij}$ with the Kronecker delta $\delta_{ij}$ ($\bar{\sigma}_{ij} = \sigma_{ij} - \sigma_{kk} \delta_{ij}/3$).

On $\partial \Omega_0$, the balance equations for the local surface traction and the nonlocal microtraction are expressed with the outward unit normal vector to $\partial \Omega_0$, $n_i$, respectively as

$$t_i = \sigma_{ij} n_i \quad (3.13)$$

$$m = Q_{ij} n_i \quad (3.14)$$

$$a = \mathcal{B}_{il} n_i \quad (3.15)$$

The first law of thermodynamics is considered here to derive the thermodynamically consistent formulation to account for the thermo-viscoplastic small-scale behaviour of the metallic volumes during the fast transient time. The adiabatic viscoplastic deformation for metals is affected by the initial temperature, the loading rate, and the temperature evolution caused by the transition from plastic work to heat. The enhanced gradient theory is employed for the mechanical part of the formulation, whereas the micromorphic model is employed for the thermal part as follows (see the work of Forest and Amestoy (2008)):

$$\rho \dot{\mathcal{E}} = \sigma_{ij} \dot{\varepsilon}_{ij}^p + x \dot{\mathcal{E}}^p + \mathcal{A} \mathcal{T} + \mathcal{B}_i \mathcal{T}_i - q_{li} + \rho \mathcal{H}^{\text{ext}}$$

(3.16)

where $\rho$ is the mass density, $\mathcal{E}$ is the specific internal energy, $q_i$ is the thermal flux vector, and $\mathcal{H}^{\text{ext}}$ is the specific heat from the external source.

The second law of thermodynamics introduces a physical base to account for the GNDs distribution in the body. The following entropy production inequality can be obtained based on the basic statement of this law, that the free energy must increase at a rate less than the one at which the work is carried out, with the specific entropy $s$ and the micromorphic approach by Forest (2009):

$$-\rho \dot{\mathcal{E}} + \rho \dot{s} \mathcal{T} + \sigma_{ij} \dot{\varepsilon}_{ij}^p + x \dot{\mathcal{E}}^p + \mathcal{Q}_{ij} \dot{\varepsilon}_{ij}^p + \mathcal{A} \dot{\mathcal{T}} + \mathcal{B}_i \dot{\mathcal{T}}_i - q_{li} \frac{\mathcal{T}_i}{\mathcal{T}} \geq 0$$

(3.17)

The entropy production vector is assumed in this chapter to be equal to the thermal flux vector divided by the temperature, as given in Coleman and Noll (1963).
3.2.2 Energetic and dissipative thermodynamic microforces: grain interior

The Helmholtz free energy $\Psi$ (per unit volume) is obtained with the entropy $s$, internal energy $E$ and temperature $T$ describing a current state of the material as follows:

$$\Psi = E - Ts$$

By using Equations (3.17) and (3.18), the Clausius-Duhem inequality is derived as follows:

$$\sigma_{ij} \dot{e}_{ij} + x \dot{e}^p + Q_i \dot{e}_i^p + A \dot{T} + B_i \dot{j}_i - \rho \dot{\Psi} - \rho s \dot{T} - q_i \frac{J_i}{J} \geq 0$$

(3.19)

For deriving the constitutive equations within a small-scale framework, an attempt to address the effect of the non-uniform microdefect distribution with the temperature is carried out in the present work with the functional form of the Helmholtz free energy given as:

$$\Psi = \Psi(e_{ij}^e, e_i^p, T, J_i)$$

(3.20)

In the process of developing the constitutive equations, the plastic dissipation work must be non-negative. By taking the time derivative of the Helmholtz free energy, $\dot{\Psi}$ is expressed as follows:

$$\dot{\Psi} = \frac{\partial \Psi}{\partial e_{ij}^e} \dot{e}_{ij} + \frac{\partial \Psi}{\partial e_i^p} \dot{e}_i^p + \frac{\partial \Psi}{\partial T} \dot{T} + \frac{\partial \Psi}{\partial J_i} \dot{J}_i$$

(3.21)

Substituting Equation (3.21) into Equation (3.19) and factoring the common terms out gives the inequality as follows:

$$\left(\sigma_{ij} - \rho \frac{\partial \Psi}{\partial e_{ij}^e}\right) \dot{e}_{ij} + \left(x - \rho \frac{\partial \Psi}{\partial e_i^p}\right) \dot{e}_i^p + \left(Q_i - \rho \frac{\partial \Psi}{\partial e_i^p}\right) \dot{e}_i^p + \left(A - \rho s - \rho \frac{\partial \Psi}{\partial T}\right) \dot{T} + \left(B_i - \rho \frac{\partial \Psi}{\partial J_i}\right) \dot{j}_i - q_i \frac{J_i}{J} \geq 0$$

(3.22)

Meanwhile, the thermodynamic conjugate microforces $x$, $Q_i$ and $A$ are assumed to be decomposed into the energetic and the dissipative elements as follows:

$$x = x^{en} + x^{dis}$$

(3.23)

$$Q_i = Q_i^{en} + Q_i^{dis}$$

(3.24)

$$A = A^{en} + A^{dis}$$

(3.25)

Substituting Equations (3.23), (3.24) and (3.25) into Equation (3.22) and rearranging them in accordance with the energetic and the dissipative parts results in the following expression:

$$\left(\sigma_{ij} - \rho \frac{\partial \Psi}{\partial e_{ij}^e}\right) \dot{e}_{ij} + \left(x^{en} - \rho \frac{\partial \Psi}{\partial e_i^p}\right) \dot{e}_i^p + \left(Q_i^{en} - \rho \frac{\partial \Psi}{\partial e_i^p}\right) \dot{e}_i^p$$

$$+ \left(A^{en} - \rho s - \rho \frac{\partial \Psi}{\partial T}\right) \dot{T} + \left(B_i - \rho \frac{\partial \Psi}{\partial J_i}\right) \dot{j}_i + x^{dis} \dot{e}_i^p$$

$$+ Q_i^{dis} \dot{e}_i^p + A^{dis} \dot{j}_i - q_i \frac{J_i}{J} \geq 0$$

(3.26)

By assuming that the fifth term in Equation (3.26) is strictly energetic, the energetic components of the thermodynamic microforces are defined as follows:

$$\sigma_{ij} = \rho \frac{\partial \Psi}{\partial e_{ij}^e}$$

(3.27)

$$x^{en} = \rho \frac{\partial \Psi}{\partial e_i^p}$$

(3.28)
\[ Q_i^{en} = \rho \frac{\partial \Psi}{\partial \varepsilon_i^p} \]  

\[ A_i^{en} = \rho \left( s + \frac{\partial \Psi}{\partial \dot{\varepsilon}_i^p} \right) \]  

\[ B_i = \rho \frac{\partial \Psi}{\partial \dot{T}_{i,j}} \]  

The dissipation density per unit time \( \mathcal{D} \) is then obtained as:

\[ \mathcal{D} = x^{dis} \dot{\varepsilon}^p + Q_i^{dis} \dot{\varepsilon}_i^p + A^{dis} \dot{T} - \frac{q_i}{T} T_{i,j} \geq 0 \]  

The dissipative counterparts of the thermodynamic microforces are obtained from the dissipation potential \( \mathcal{D}(\dot{\varepsilon}^p, \dot{\varepsilon}_i^p, \dot{T}, T_{i,j}) \) as follows:

\[ x^{dis} = \frac{\partial \mathcal{D}}{\partial \dot{\varepsilon}^p} \]  

\[ Q_i^{dis} = \frac{\partial \mathcal{D}}{\partial \dot{\varepsilon}_i^p} \]  

\[ A^{dis} = \frac{\partial \mathcal{D}}{\partial \dot{T}} \]  

\[ - \frac{q_i}{T} = \frac{\partial \mathcal{D}}{\partial \dot{T}_{i,j}} \]  

It is necessary to define the proper formulation of Helmholtz free energy \( \Psi \) because it establishes the basis for the derivation of the constitutive relations. It has to take not only the material type such as fcc metals, bcc metals, polymer, steel alloys, concrete, etc. but also the deformation condition such as rate dependence of the material into consideration. In the current work, the Helmholtz free energy function is put forward with three main counterparts, i.e. elastic energy \( \Psi^e \), defect energy \( \Psi^d \) and thermal energy \( \Psi^{th} \), as follows (Voyiadjis and Song, 2017; Voyiadjis et al., 2017):

\[ \Psi(e_{ij}, e^p, e_i^p, T, T_{i,j}) = \Psi^e(e_{ij}, T) + \Psi^d(e^p, e_i^p, T) + \Psi^{th}(T, T_{i,j}) \]  

with

\[ \Psi^e(e_{ij}, T) = \frac{1}{2\rho} e_{ij} E_{ijkl} e_{kl}^e - \frac{a^{th}}{\rho} (T - T_r) e_{ij}^p \delta_{ij} \]  

\[ \Psi^d(e^p, e_i^p, T) = \frac{\mathcal{H}_0}{\rho (r + 1)} \left[ 1 - \left( \frac{T}{T_r} \right)^n \right] (e^p)^{r+1} \]  

\[ + \frac{\sigma_0}{\rho (\vartheta + 1)} \left( \ell_{en} (e_i^p e_i^p) \right)^{\frac{\vartheta + 1}{2}} \]  

\[ \Psi^{th}(T, T_{i,j}) = - \frac{1}{2 \rho} (T - T_r)^2 - \frac{1}{2 \rho} \sigma \dot{T}_{i,j} \]  

where \( a^{th} \) is the thermal expansion coefficient, \( E_{ijkl} \) is the elastic modulus tensor, \( \mathcal{H}_0 \) is the standard isotropic hardening parameter, \( r (0 < r < 1) \) is the isotropic hardening material parameter, \( T_r \) and \( n \) are the thermal material parameters, \( \sigma_0 > 0 \) is the stress-dimensioned scaling parameter to explain the initial slip resistance, \( \ell_{en} \) is the energetic material length scale describing the feature of the short-range interaction of the GNDs, \( \sigma \) is the material constant for the isotropic
heat conduction which accounts for the interaction of the energy carriers, \( \theta \) is the parameter for governing the nonlinearity of the gradient dependent defect energy, \( T_r > 0 \) is the reference temperature, and \( c_e \) is the specific heat capacity at the constant stress. In this chapter, \( T_y \) is determined by the calibration with experimental data.

The second term of the defect energy \( \Psi^d_2 \) is postulated as a function of \( e^p_i \), and the condition \( \theta > 0 \) ensures the convexity of \( \Psi^d_2(\theta) \). In particular, by setting \( \theta = 1 \), the function \( \Psi^d_2 \) turns to the quadratic formula (see Bardella (2006); Gurtin (2004)), while the \( L_2 \)-norm of \( e^p_i \) is used in Garroni et al. (2010) and Ohno and Okumura (2007) by setting \( \theta = 0 \). It is worth mentioning that \( \Psi^d_2 \) is independent of the temperature since it indicates the energy carried by the dislocations, thus it is energetic in nature (Lele and Anand, 2008).

Since the central objective of the present work is to account for thermal variation, thermal terms are included in the free energy. The elastic and defect parts of the Helmholtz free energy functions, \( \Psi^e \) and \( \Psi^d \), are locally convex with respect to strain-related terms at all points of the body in the equilibrium state. However, \( \Psi^e \) is a concave function of the temperature (Lubarda, 2008). The second order variation of \( \Psi \) is related to the second order variation of \( E \) by using Equation (3.18) and taking the virtual variations of temperature and entropy states into account such as \( \frac{\partial^2 \Psi}{\partial T^2} (\delta T)^2 = -\frac{\partial^2 E}{\partial s^2} (\delta s)^2 \). Thus, \( E \) is convex with respect to entropy \( s \), and \( \Psi \) is concave with respect to temperature since \( \frac{\partial^2 E}{\partial s^2} (\delta s)^2 > 0 \rightarrow \frac{\partial^2 \Psi}{\partial T^2} (\delta T)^2 < 0 \). In addition, it can be assumed that entropy increases monotonically with respect to temperature, thus \( \frac{\partial s}{\partial T} = -\frac{\partial^2 \Psi}{\partial T^2} \) (Callen, 1985).

One can now obtain the energetic thermodynamic forces by using the definitions in Equations (3.27)-(3.31) in conjunction with Equations (3.37)-(3.40) as follows:

\[
\sigma_{ij} = E_{ijkl}e^e_{kl} - \alpha^{th}(T - T_r)\delta_{ij} \tag{3.41}
\]

\[
x^{en} = H_0 \left[ 1 - \left( \frac{T}{T_y} \right)^n \right] (e^p)^r \tag{3.42}
\]

\[
Q^e_i = \sigma_0 e^e_i [e^e_j e^e_j]^{\frac{\theta-1}{2}} e^p_i \tag{3.43}
\]

\[
A^{en} = \rho s - \alpha^{th}(T - T_r) e^e_i \delta_{ij} - \frac{c_e}{T_r} (T - T_r) - \frac{H_0 (e^p)^{r+1}}{r+1} \left( \frac{T}{T_y} \right)^{n-1} \tag{3.44}
\]

\[
B_i = -\alpha T_i \tag{3.45}
\]

It is assumed here that the dissipation potential function is composed of two parts, the mechanical part which is dependent on the plastic strain and plastic strain gradient, and the thermal counterpart which shows the purely thermal effect such as the heat conduction. In this sense, and in the context of Equation (3.32), the functional form of the dissipation potential, which is dependent on \( e^p_i \), can be put forward as:

\[
D = \mathcal{D}^p(e^p, e^p, \dot{e}^p, T) + \mathcal{D}^\theta(\dot{e}^p_i, T) + \mathcal{D}^{th}(\dot{T}, T_i) \tag{3.46}
\]

where \( \mathcal{D}^p \) and \( \mathcal{D}^\theta \) are the mechanical parts and \( \mathcal{D}^{th} \) accounts for the purely thermal effect. The functional forms of each part are given as follows:

\[\text{footnote 9: The short-range interaction of the coupling dislocations shifting on the adjacent slip planes, so-called GNDs core energy, is characterized by the defect energy } \Psi^d_2. \Psi^d_2 \text{ may be assumed to be a function of the GNDs density. It is assumed in this work that the plastic strain gradient is viewed as a macroscopic measure of GNDs.}\]

63
\[ D^p(e^p, \varepsilon^p, \dot{e}^p, \mathcal{T}) = \sigma_0 \sqrt{\mathcal{H}^2(e^p) + \xi^2 \left( \frac{\mu}{\sigma_0} \right)^2 b \varepsilon^p \left[ 1 - \left( \frac{\mathcal{T}}{\tau_y} \right)^n \right]^n \left( \frac{\dot{e}^p}{\dot{\varphi}_1} \right)^m_1 \dot{e}^p } \quad (3.47) \]

\[ D^q(\dot{e}^p, \mathcal{T}) = \sigma_0 \left[ 1 - \left( \frac{\mathcal{T}}{\tau_y} \right)^n \right]^n \left( \frac{\dot{\varphi}_2}{\dot{\varphi}_1} \right)^{m_2} \dot{\varphi} \quad (3.48) \]

\[ D^{th}(\dot{\mathcal{T}}, \mathcal{T}_i) = -\frac{\zeta}{2} \dot{\mathcal{T}}^2 - \frac{1}{2} \frac{\mathcal{K}(\mathcal{T})}{\mathcal{L}} \mathcal{T}_i \mathcal{T}_j \quad (3.49) \]

where \( \xi \) and \( b \) are the numerical parameter and magnitude of the Burgers vector, which are characteristically given as \( 0.2 \leq \xi \leq 0.5 \) and \( b \approx 0.3 \) nm for metals respectively. The parameter \( \mu \) is the shear modulus, \( \dot{\varphi}_1 \) and \( \dot{\varphi}_2 \) are the non-negative reference rates, \( m_1 \) and \( m_2 \) are the non-negative strain rate sensitivity parameters, \( \zeta \) is the material constant characterizing the energy exchange between phonon and electron, and \( \mathcal{K}(\mathcal{T}) \) is the thermal conductivity coefficient. The dimensionless function \((\dot{e}^p/\dot{\varphi}_1)^{m_1}\) in Equation (3.47) leads to different physical effects from the term \((\dot{\varphi}_2/\dot{\varphi}_1)^{m_2}\) in Equation (3.48), in spite of the similar forms (see Lele and Anand (2008) for more details).

The parameter \( \dot{\varphi} \) is a scalar measuring the plastic strain rate gradient, which is defined by

\[ \dot{\varphi} \equiv \ell_{dis} \| \dot{e}^p \| = \ell_{dis} \sqrt{\dot{e}^p, i \dot{e}^p, i} \quad (3.50) \]

where \( \ell_{dis} \) is the dissipative length scale.

The dimensionless function \( \mathcal{H}(e^p) \) is related to the strain hardening/softening behaviour with \( \mathcal{H}(0) = 1 \). In the current work, the following form of mixed-hardening function is adopted (Voce, 1955).

\[ \mathcal{H}(e^p) = 1 + (\chi - 1)[1 - \exp(-\omega e^p)] + \frac{\mathcal{H}_0}{\sigma_0} e^p \quad (3.51) \]

where \( \chi \) and \( \omega \) are the material parameters. The strain hardening, strain softening and strain hardening/softening can be modeled based on the particular choices for these parameters.

The Nye dislocation density tensor \( \alpha_{ij} \), which indicates the i-component of the resultant Burgers vector related to GNDs of line vector \( j \), is exploited here to account for the effects of plastic strain gradient (Arsenlis and Parks, 1999; Fleck and Hutchinson, 1997). Non-vanishing \( \alpha_{ij} \) indicates that the GNDs exist, and the net Burgers vector \( \mathcal{B}_i \) can be obtained by using the Stokes’ theorem as follows:

\[ \mathcal{B}_i = \oint_C u^p_{i,k} dx_k = \int_S \epsilon_{jkl} u^p_{i,tk} n_j dS \quad (3.52) \]

where \( \epsilon_{jkl} \) is the permutation tensor and \( n_j \) is the unit vector normal to the surface \( S \) whose boundary is the curve \( C \). Under the assumption that the plastic flow is irrotational, the Nye dislocation density tensor \( \alpha_{ij} \) is given by

\[ \alpha_{ij} = \epsilon_{ikl} u^p_{j,tk} = \epsilon_{ikl} \epsilon^p_{jkl} \quad (3.53) \]

in which, in the work of Gurtin (2004), \( \alpha_{ij} \) is indicated as the Burgers tensor.

With neglecting the interaction between different slip systems, the total accumulation of GNDs is calculated as follows:

\[ \varepsilon^p \equiv \| \alpha_{ij} \| = b \rho_G \quad (3.54) \]

where \( \varepsilon^p \) is a scalar measure of an effective plastic strain gradient, and \( \rho_G \) is the total GNDs density. In order to present the microstructural hardening induced by GNDs, another length scale parameter, designated as the N-G length scale parameter, is defined here:
\[ \ell_{N-G} \equiv \xi^2 \left( \frac{\mu}{\sigma_0} \right)^2 b \]  

(3.55)

where the N-G length scale parameter was first introduced by Nix and Gao (1998). With the definition of \( \ell_{N-G} \), Equation (3.47) can be expressed by

\[
D^p(e^p, \varepsilon^p, \dot{\varepsilon}^p, T) = \sigma_0 \sqrt{\mathcal{H}^2(e^p) + \ell_{N-G} \varepsilon^p} \left[ 1 - \left( \frac{T}{T_y} \right)^n \right] \left( \frac{\dot{\varepsilon}^p}{\dot{\varepsilon}^p_1} \right)^m \dot{\varepsilon}^p
\]

(3.56)

In the special case \( \ell_{N-G} = 0 \) and \( \mathcal{H}(e^p) = 1 \), Equation (3.56) reduces to \( D^p = \sigma_0 \left( 1 - \left( \frac{T}{T_y} \right)^n \right) (\dot{\varepsilon}^p / \dot{\varepsilon}^p_1)^m \dot{\varepsilon}^p \), a form in Voyiadjis and Song (2017).

Using the dissipative potential given in Equations (3.47)-(3.49) and (3.56) along with Equations (3.33)-(3.36) and considering \( \mathcal{K}(T) / T = \mathcal{K}_0 = \text{constant} \), the constitutive relations for the dissipative microforces are obtained as follows:

\[
x^{\text{dis}} = \sigma_0 \sqrt{\mathcal{H}^2(e^p) + \ell_{N-G} \varepsilon^p} \left[ 1 - \left( \frac{T}{T_y} \right)^n \right] \left( \frac{\dot{\varepsilon}^p}{\dot{\varepsilon}^p_1} \right)^m \dot{\varepsilon}^p
\]

(3.57)

\[
Q_i^{\text{dis}} = \sigma_0 e_i^{\text{dis}} (m_2 + 1) \left[ 1 - \left( \frac{T}{T_y} \right)^n \right] \left( \frac{\dot{\varepsilon}^p}{\dot{\varepsilon}^p_1} \right)^m \dot{\varepsilon}_i^p
\]

(3.58)

\[
\mathcal{A}^{\text{dis}} = -c \tilde{f}^i
\]

(3.59)

\[
\dot{q}_i / T = \mathcal{K}_0 \mathcal{J}_k
\]

(3.60)

3.2.3 Flow rule: grain interior

The flow rule in the present framework is established based on the nonlocal microforce balance, given in Equation (3.11), and strengthened by thermodynamically consistent constitutive relations for both energetic and dissipative microforces. By considering the backstress, the microforce equilibrium can be expressed as follows:

\[
\bar{\sigma}_{ij} - \frac{(-Q_{en}^n N_{ij}}{B_{\text{backstress}}} = (x - Q_{k,k}^{\text{dis}}) N_{ij}
\]

(3.61)

By substituting Equations (3.42), (3.43), (3.57) and (3.58) into Equation (3.61), one can obtain a second order partial differential flow rule as follows:

\[
\bar{\sigma}_{ij} - \left[ -\sigma_0 e_{en} \left\{ e_{en} \left( e_i^p e_j^p \right)^{\frac{n-1}{2}} \right\} \dot{\varepsilon}_{kk} \right] N_{ij}
\]

\[
= \left[ \mathcal{H}_0 \left[ 1 - \left( \frac{T}{T_y} \right)^n \right] \left( e^p \right)^n \right]
\]

\[
+ \sigma_0 \sqrt{\mathcal{H}^2(e^p) + \ell_{N-G} \varepsilon^p} \left[ 1 - \left( \frac{T}{T_y} \right)^n \right] \left( \frac{\dot{\varepsilon}^p}{\dot{\varepsilon}^p_1} \right)^m \dot{\varepsilon}^p
\]

\[
- \sigma_0 e^{\text{dis}} (m_2 + 1) \left[ 1 - \left( \frac{T}{T_y} \right)^n \right] \left( \frac{\dot{\varepsilon}^p}{\dot{\varepsilon}^p_1} \right)^m \dot{\varepsilon}_k^p
\]

\[
N_{ij}
\]

(3.62)

It is required to accompany the initial conditions for \( e^p \) and \( \varepsilon^p \) in the flow rule. A standard initial condition, for the behaviour starting at time \( t = 0 \) from a virgin state, is assumed here such that

\[
e^p_{t=0} = \varepsilon^p_{t=0} = 0
\]

(3.63)
3.2.4 Thermodynamic derivations of the heat evolution equation

Heat flow is controlled by the first law of thermodynamics, i.e. the energy conservation law, given in Equation (3.16). The temperature field is governed by the heat flow generated through the inelastic dissipation and thermo-mechanical coupling effect. By considering the law of energy conservation given in Equation (3.16) along with the dissipation potential given in Equations (3.32) and (3.46)-(3.49) in conjunction with the equations for the energetic and dissipative components of the thermodynamics microforces given respectively by Equations (3.27)-(3.31) and Equations (3.33)-(3.36), the relationship for the evolution of the entropy, which describes the irreversible process, can be derived as follows:

$$\rho \dot{s} = \dot{D} + \rho \dot{H}^{\text{ext}} \quad (3.64)$$

By using Equation (3.44) for solving the rate of the entropy $\dot{s}$ and assuming the specific heat capacity at the constant volume $c_0$ as $c_0 = \text{constant} \approx c E T / T_r$, the temperature evolution can be obtained as follows:

$$\rho c_0 \dot{T} = x^{\text{dis}} \dot{p}^p + Q^{\text{dis}}_i \dot{e}_i^p - \left( \alpha \left( T - T_r \right) \dot{e}_i^e \delta_{ij} T \right)$$

$$- \left( \dot{p} T \right)_{\text{plastic-thermal coupling}} + \frac{k_0}{2} J_i J_i + \rho \dot{H}^{\text{ext}}$$

(3.65)

where

$$\dot{p} = H_0 (e^p)^r \left( \frac{T}{T_y} \right) \left( \frac{T}{T_y} \right)^{n-1}$$

$$+ n \left( n + 1 \right) \left( \frac{T}{T_y} \right) \left( \frac{T}{T_y} \right)^{n-1} \dot{T}$$

(3.66)

It should be noted that the heat conduction term can be generalized to the microscale heat equation by considering the effects of the temperature gradient on the stored energy and the temperature on the energy dissipation individually in terms of the two extra material intrinsic time scale parameters (Voyiadjis and Faghihi, 2012). By substituting the constitutive equations of the dissipative microforces into Equation (3.65) and assuming that the external heat source is absent, the temperature evolution is consequently obtained as

$$\left[ 1 + n H_0 (e^p)^{r+1} \left( \frac{T}{T_y} \right)^n \right] \dot{T} = \frac{1}{\rho c_0} \left[ \sigma_0 \sqrt{\dot{H}^2 (e^p)} + \ell_N \dot{e}_p^p \left\{ 1 - \left( \frac{T}{T_y} \right)^n \right\} \frac{\dot{e}_p^p}{\phi_1} \right]$$

$$- H_0 (e^p)^r \left( \frac{T}{T_y} \right)^n \dot{e}_p^p$$

$$+ \sigma_0 \ell^2 \left( m_2 + 1 \right) \left\{ 1 - \left( \frac{T}{T_y} \right)^n \right\} \left( \frac{\dot{p}}{\dot{p}_2} \right)^{m_2} \frac{\dot{e}_p^p}{\dot{p}}$$

$$- \alpha \left( T - T_r \right) \dot{e}_i^e \delta_{ij} T + \tau_{\text{eff}} J_{il}$$

(3.67)

where the additional term $\tau_{\text{eff}}$ is defined as $\tau_{\text{eff}} = k_0 / 2 \rho c_0$.

3.2.5 Principle of virtual power: grain boundary
One of the main goals in this study is to develop the thermodynamically consistent gradient-enhanced plasticity model for the grain boundary, which should be also consistent with the one for the grain interior. Hereafter, the superscript GB and the expression GB will be used to denote the specific variables at the grain boundary.

Two grain $G_1$ and $G_2$ separated by the grain boundary are taken into account in this chapter and the displacement field is assumed to be continuous, i.e. $u_i^{G_1} = u_i^{G_2}$, across the grain boundary. The internal part of the principle of virtual power for the grain boundary is assumed to depend on the GB accumulated plastic strain rates $\dot{\varepsilon}^{pGB}_{G_1}$ at $S^{GB}_{G_1}$ and $\dot{\varepsilon}^{pGB}_{G_2}$ at $S^{GB}_{G_2}$ in the arbitrary surface $S^{GB}$ of the grain boundary as follows:

$$P_{\text{intGB}} = \int_{S^{GB}} \left( M^{GBG_1}_i \dot{\varepsilon}^{pGBG_1}_i + M^{GBG_2}_i \dot{\varepsilon}^{pGBG_2}_i \right) dS^{GB}$$

(3.68)

where the GB microscopic moment tractions $M^{GBG_1}_i$ and $M^{GBG_2}_i$ are assumed to expend power over $\dot{\varepsilon}^{pGBG_1}$ and $\dot{\varepsilon}^{pGBG_2}$ respectively. In addition, the GB external power $P_{\text{extGB}}$ is expended by the macrotractions $\sigma_{ij}^{G_1}(-n_j^G)$ and $\sigma_{ij}^{G_2}(n_j^G)$ conjugate to the macroscopic velocity $\dot{u}_i$, and the microtractions $Q_k^{G_1}(-n_k^G)$ and $Q_k^{G_2}(n_k^G)$ that are conjugate to $\dot{\varepsilon}^{pGBG_1}$ and $\dot{\varepsilon}^{pGBG_2}$ respectively as follows:

$$P_{\text{extGB}} = \int_{S^{GB}} \left\{ \left( \sigma_{ij}^{G_1} n_j^G - \sigma_{ij}^{G_2} n_j^G \right) \dot{u}_i + Q_k^{G_1} n_k^G \dot{\varepsilon}^{pGBG_1} - Q_k^{G_2} n_k^G \dot{\varepsilon}^{pGBG_2} \right\} dS^{GB}$$

(3.69)

where $n^G$ is the unit outward normal vector of the grain boundary surface. From $P_{\text{intGB}} = P_{\text{extGB}}$, the macro- and microforce balances for the grain boundary are obtained as follows:

$$\left( \sigma_{ij}^{G_1} - \sigma_{ij}^{G_2} \right) n_j^G; \quad M^{GBG_1}_i + Q_k^{G_1} n_k^G = 0; \quad M^{GBG_2}_i - Q_k^{G_2} n_k^G = 0$$

(3.70)

The first and second laws of thermodynamics are considered to construct the thermodynamically consistent gradient- and temperature-enhanced framework for the grain boundary as follows:

$$\dot{\varepsilon}^{GB} = M^G \dot{\varepsilon}^{pGB} + q_l^G n_l^G$$

(3.71)

$$\dot{\varepsilon}^{GB} \dot{J}^{GB} - q_l^G n_l^G \geq 0$$

(3.72)

where $\dot{\varepsilon}^{GB}$ is the GB surface energy density, $q_l^G$ is the GB heat flux vector and $\dot{\varepsilon}^{GB}$ is the surface density of the entropy of the grain boundary.

3.2.6 Energetic and dissipative thermodynamic microforces: grain boundary

By using the time derivative of the equation, $\Psi^{GB} = \dot{\varepsilon}^{GB} - J^{GB} \dot{\varepsilon}^{GB}$, and substituting it into Equations (3.71) and (3.72), the following Clausius-Duhem inequality for the grain boundary is obtained.

$$M^G \dot{\varepsilon}^{pGB} - \dot{\Psi}^{GB} - \dot{\varepsilon}^{GB} \dot{J}^{GB} \geq 0$$

(3.73)

One assumes the isothermal condition for the grain boundary ($J^{GB} = 0$) and the Helmholtz free energy for the grain boundary is given by $\Psi^{GB} = \Psi^{GB}(\dot{\varepsilon}^{pGB})$. Substituting the time derivative of $\Psi^{GB}$ into Equation (3.73) gives the following inequality.

$$M^G \dot{\varepsilon}^{pGB} - \rho \left( \frac{\partial \Psi^{GB}}{\partial \dot{\varepsilon}^{pGB}} \right) \dot{\varepsilon}^{pGB} \geq 0$$

(3.74)
The GB thermodynamic microforce quantity $\mathbb{M}^{GB}$ is further assumed to be decomposed into the energy and dissipative components such as $\mathbb{M}^{GB} = \mathbb{M}^{GB, en} + \mathbb{M}^{GB, dis}$. The components $\mathbb{M}^{GB, en}$ and $\mathbb{M}^{GB, dis}$ indicate the mechanisms for the pre- and post-slip transfer, and thus involve the plastic strain at the grain boundary prior to the slip transfer $e^{p,GB(pre)}$ and the one after the slip transfer $e^{p,GB(post)}$ respectively ($e^{p,GB} = e^{p,GB(pre)} + e^{p,GB(post)}$). From Equation (3.74) one obtains,

$$
\left(\mathbb{M}^{GB, en} - \rho \frac{\partial \Psi^{GB}}{\partial e^{p,GB}}\right) \dot{e}^{p,GB} + \mathbb{M}^{GB, dis} \dot{e}^{p,GB} \geq 0
$$

(3.75)

The GB energetic microforce can be obtained as:

$$
\mathbb{M}^{GB, en} = \rho \frac{\partial \Psi^{GB}}{\partial e^{p,GB}}
$$

(3.76)

Hence the GB dissipative microforce can then be obtained as:

$$
\mathbb{M}^{GB, dis} = \frac{\partial \mathcal{D}^{GB}}{\partial \dot{e}^{p,GB}}
$$

(3.77)

where $\mathcal{D}^{GB}$ is the non-negative dissipation density per unit time for the grain boundary, given by $\mathcal{D}^{GB} = \mathbb{M}^{GB, dis} \dot{e}^{p,GB} \geq 0$. This non-negative plastic dissipation condition can be satisfied when the GB plastic dissipation potential is a convex function of the GB accumulated plastic strain rate.

In this chapter, it is assumed by following Fredriksson and Gudmundson (2007a) that the GB Helmholtz free energy per unit surface has the form of the general power law as follows:

$$
\Psi^{GB}(e^{p,GB}) = \frac{1}{2} G \ell_{en}^{GB} \left( e^{p,GB(pre)} \right)^2
$$

(3.78)

where $G$ is the shear modulus in the case of isotropic linear elasticity, $\ell_{en}^{GB}$ is the GB energetic length scale. By substituting Equation (3.78) into Equation (3.76), the GB energetic microforce quantity can be obtained as follows:

$$
\mathbb{M}^{GB, en} = G \ell_{en}^{GB} e^{p,GB(pre)}
$$

(3.79)

Note that $\mathbb{M}^{GB, en}$ is independent of the plastic strain rate and temperature since this variable comes from the recoverable stored energy.

Meanwhile, two major factors might be identified affecting the energy dissipation when the dislocations move in the grain boundary area (Aifantis and Willis, 2005). When dislocations encounter a grain boundary, they pile up there. Slip can transmit to the adjacent grain only when the stress field ahead of the pileup is high enough. Direct observation of the process using transmission electron microscopy (TEM) also shows that the main mechanisms for the aforementioned slip transmission are the dislocation absorption and re-emission for the low angle boundaries (Soer et al., 2005) and the dislocation nucleation in the adjacent grain for the high angle boundaries (Ohmura et al., 2004) respectively. As soon as deformation initiates in the adjacent grain, the grain boundary begins to deform and the plastic strain on the grain boundary increases. The energy associated with the deformation of the grain boundary in this case is taken to be mainly due to the energy dissipation as dislocations move in the grain boundary region. In addition to considering the resistance force to dislocation motion being temperature and rate dependent, this energy dissipation can be taken as a linear function of GB plastic strain.

Moreover, change in the grain boundary area can also affect the energy dissipation. The macroscopic accumulated plastic strain at the grain boundary, $e^{p,GB}$, can be related to the microscopically deformation of the grain boundary through the root-mean-square of the gradient of this deformation. In addition, the energy change after the grain boundary has yielded, i.e. onset
of slip transmission, can be approximated by a quadratic function of the aforementioned displacement gradient at microscale and hence the GB plastic strain at macroscale.

Combining both aforementioned mechanisms, i.e. change in the grain boundary area and deformation of the grain boundary due to the dislocation movement, involved in the energy dissipation due to the plastic strain transfer across the grain boundary, one can postulate the following generalized expression for the GB dissipation potential:

\[
D_{GB} = \frac{\ell_{GB \_dis}^2}{m_{GB} + 1} \left( \sigma_{0 \_GB}^2 + \mathcal{H}_{0 \_GB} e^{p_{GB \_post}} \right) \left( 1 - \frac{T_{GB}}{T_y} \right)^{n_{GB}} \left( \frac{\dot{e}_{p_{GB \_post}}}{\varphi_{GB}} \right)^{m_{GB}} \geq 0
\]  

(3.80)

where \( \ell_{GB \_dis} \) is the GB dissipative length scale, \( m_{GB} \) and \( \varphi_{GB} \) are the viscous related material parameters, \( \sigma_{0 \_GB} \) is a constant accounting for the GB yield stress, \( \mathcal{H}_{0 \_GB} \) is the GB hardening parameter, \( T_y \) is the scale-independent GB thermal parameter at the onset of yield, and \( n_{GB} \) is the GB thermal parameter. The temperature- and rate-dependency of the GB energy are shown respectively in the terms \( \left( 1 - \frac{T_{GB}}{T_y} \right)^{n_{GB}} \) and \( \left( \frac{\dot{e}_{p_{GB \_post}}}{\varphi_{GB}} \right)^{m_{GB}} \).

By using Equations (3.77) and (3.80), the GB dissipative microforce \( \mathbb{M}_{GB \_dis} \) can be obtained as

\[
\mathbb{M}_{GB \_dis} = \ell_{GB \_dis}^2 \left( \sigma_{0 \_GB} + \mathcal{H}_{0 \_GB} e^{p_{GB \_post}} \right) \left( 1 - \frac{T_{GB}}{T_y} \right)^{n_{GB}} \left( \frac{\dot{e}_{p_{GB \_post}}}{\varphi_{GB}} \right)^{m_{GB}}
\]  

(3.81)

Therefore, the GB thermodynamic microforce \( \mathbb{M}_{GB} \) can be obtained as

\[
\mathbb{M}_{GB} = G \ell_{en}^2 e^{p_{GB \_pre}} + \ell_{dis}^2 \left( \sigma_{0 \_GB} + \mathcal{H}_{0 \_GB} e^{p_{GB \_post}} \right) \left( 1 - \frac{T_{GB}}{T_y} \right)^{n_{GB}} \left( \frac{\dot{e}_{p_{GB \_post}}}{\varphi_{GB}} \right)^{m_{GB}}
\]  

(3.82)

3.2.7 Flow rule: grain boundary

The flow rule for the grain boundary can be derived by substituting Equation (3.82) into the microforce balances for the grain boundary, Equation (3.70), such as:

for \( S_{GB \_1} \),

\[
\sigma_0 \ell_{en}^2 \left[ \ell_{en}^2 \left( e_{k \_p} \right) \right]^{\theta - 1} e_{k \_p} + \sigma_0 \ell_{dis}^2 (m_2 + 1) \left[ 1 - \left( \frac{T_y}{T_y} \right)^{n_{GB}} \right] \left( \frac{\varphi}{\varphi_2} \right)^{m_2} \dot{e}_{p_{GB \_post}}^2 \left( \frac{\varphi}{\varphi_2} \right)^{m_{GB}}
\]  

(3.83)

for \( S_{GB \_2} \),
\[
\begin{align*}
\sigma_0 \ell^2 \left[ \ell^2 \left( \ell^2 \left( e^p_{k} e^P_{k} \right) \right) \right]^{\frac{q-1}{2}} e^p_i + \sigma_0 \ell^2 \ell^2 (m_2 + 1) \left[ 1 - \left( \frac{\mathcal{T}}{\mathcal{T}^*} \right)^n \right] \left( \frac{\dot{p}}{\mathcal{P}} \right)^{m_2} \phi^p_i \left[ n_k \right]^{\text{GB}} \\
- G \ell^2 \ell^2 \left( e^p \mathcal{S} \right) \left( \sigma^G_0 + \mathcal{S}^G \right) \left( 1 - \frac{\mathcal{T}^G}{\mathcal{T}^G} \right) \left( \frac{\dot{p}^G}{\mathcal{P}^G} \right)^m \left[ n_k \right]^{\text{GB}}
\end{align*}
\] (3.84)

where the second term in LHS of both equations represent the backstress. Note that, in general case, the grain boundary model parameters are not identical on each side, however in this chapter, the same values are assumed to be considered for simplification.

Considering the GB flow rules as the boundary conditions of the grain interior flow rule, Equation (3.62), results in a yield condition accounting for the temperature and rate dependent barrier effect of grain boundaries on the plastic slip and consequently the influence on the GNDs evolution in the grain interior.

3.3 Finite element formulation of the proposed SGP model

A two-dimensional finite element model for the proposed SGP model is developed to account for the size dependent response for microscopic structures. The boundary value problem consists of solving the flow rules for the grain interior/boundary given in Section 3.2.3 and Section 3.2.7 in conjunction with the constitutive equations given in Section 3.2.2 and Section 3.2.6 subjected to the prescribed displacement conditions \( u_i^t \) on part of the boundary \( \partial \Omega_0 \) and traction free condition on the remaining boundary part of the body. The microscopic and macroscopic force balances can then be described in the global weak form after utilizing the principle of virtual power and applying the corresponding boundary conditions, i.e. arbitrary virtual displacement fields \( \delta u = 0 \) on \( \partial \Omega_0 \) and arbitrary virtual plastic strain fields \( \delta e^p = 0 \) on \( \partial \Omega_0' \) as follows:

\[
\int_{\Omega_0} \left( \sigma_{ij} \delta u_{i,j} \right) dV = 0 \tag{3.85}
\]

\[
\int_{\Omega_0} \left[ (x - \bar{\sigma}) \delta e^p + Q_i \delta e^p_i \right] dV = 0 \tag{3.86}
\]

where \( \bar{\sigma} \) is the resolved shear stress defined by

\[
\bar{\sigma} = \sigma_{ij} N_{ij} = \bar{\sigma}_{ij} N_{ij} \tag{3.87}
\]

The UEL subroutine in the finite element software ABAQUS/standard (2012) is built in this chapter for numerically solving the global weak forms of macroscopic and microscopic force balances, Equation (3.85) and Equation (3.86), respectively. In this finite element formulation, the plastic strain field \( e^p \) as well as the displacement field \( u_i \) are discretized independently and both of the fields are taken as fundamental unknown nodal degrees of freedom. In this regard, the displacement and corresponding strain field \( \varepsilon_{ij} \), and the plastic strain and corresponding plastic strain gradient field \( e_{ij}^p \) are obtained by using the interpolation as follows:

\[
\sum_{n=1}^{n_u} u_i^\eta N_{ui}^\eta \tag{3.88}
\]

70
\[ \varepsilon_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) = \frac{1}{2} \sum_{\eta=1}^{n_u} \left( U_{u_i}^\eta \frac{\partial N_u^\eta}{\partial x_j} + U_{u_j}^\eta \frac{\partial N_u^\eta}{\partial x_i} \right) \]  

(3.89)

\[ e^p = \sum_{\eta=1}^{n_{ep}} \varepsilon_{ep}^\eta N_{ep}^\eta \]  

(3.90)

\[ e_{ij}^p = \frac{\partial e^p}{\partial x_j} = \sum_{\eta=1}^{n_{ep}} \varepsilon_{ep}^\eta \frac{\partial N_{ep}^\eta}{\partial x_j} \]  

(3.91)

where \( N_u^\eta \) and \( N_{ep}^\eta \) denote the interpolation functions, and \( U_{u_i}^\eta \) and \( \varepsilon_{ep}^\eta \) denote the nodal values of the plastic strains and displacements at node \( \eta \) respectively. The terms \( n_u \) and \( n_{ep} \) represent the number of nodes per single element for displacement and plastic strain respectively. Since a two-dimensional quadratic 9-node element is used in this chapter, \( n_u \) and \( n_{ep} \) are set up as nine. It should be noted that \( n_u \) and \( n_{ep} \) do not necessarily have to be the same as each other in the present finite element implementation, even though both the displacement and plastic strain fields are calculated by using the standard isoparametric interpolation functions.

The body is approximated using finite elements, \( \Omega = \bigcup \Omega_{el} \). By substituting Equations (3.88)-(3.91) into Equations (3.85) and (3.86), the nodal residuals for the displacement \( R_{ul} \) and the plastic strain \( R_{ep} \) for each element \( \Omega_{el} \) can be obtained as

\[ \left( R_{ul} \right)_\eta = - \int_{\Omega_{el}} \left( \sigma_{ij} \frac{\partial N_u^\eta}{\partial x_j} \right) dV \]  

(3.92)

\[ \left( R_{ep} \right)_\eta = - \int_{\Omega_{el}} \left[ (x - \bar{\sigma})N_{ep}^\eta + Q_l \frac{\partial N_{ep}^\eta}{\partial x_l} \right] dV \]  

(3.93)

The system of linear equations, \( \left( R_{ul} \right)_\eta = 0 \) and \( \left( R_{ep} \right)_\eta = 0 \), are solved using ABAQUS/standard (2012) based on the Newton-Raphson iterative method. Occasionally, the modified Newton-Raphson method, referred to as quasi Newton-Raphson method, is employed in the case that the numerical solution suffers a divergence during the initial increment immediately after an abrupt change in loading. In the quasi Newton-Raphson method, a specific correction factor, which is less than one, is multiplied by one portion of the stiffness matrix. By using this method, a divergence problem can be overcome, however, convergence is expected to be slow because of the expensive computational cost. The Taylor expansion of the residuals with regard to the current nodal values can be expressed by assuming the nodal displacement and the plastic strain in iteration \( \zeta \) as \( U_{ul}^{\zeta} \) and \( \varepsilon_{ep}^{\zeta} \) are respectively as follows:

\[ \left( R_{ul} \right)_{ul}^{\zeta+1} e_{ul}^{\zeta+1} \]  

\[ = \left( R_{ul} \right)_{ul}^{\zeta} e_{ul}^{\zeta} + \left( \frac{\partial R_{ul}}{\partial u_i^\eta} \right) \Delta U_{ul}^\eta + \left( \frac{\partial R_{ul}}{\partial \varepsilon_{ep}^\eta} \right) \Delta \varepsilon_{ep}^\eta \]  

(3.94)
\[
\left( \mathbb{R}_{ep} \right|_{u_i^{\xi+1}, \varepsilon_{ep}^{\xi+1}} \eta = \left( \mathbb{R}_{ep} \right|_{u_i^{\xi}, \varepsilon_{ep}^{\xi}} \eta + \left( \frac{\partial \mathbb{R}_{ep}}{\partial U_{uk}} \right) \Delta U_{uk}^{\eta} + \left( \frac{\partial \mathbb{R}_{ep}}{\partial \varepsilon_{ep}^{\xi}} \right) \Delta \varepsilon_{ep}^{\eta} \right) (3.95) \\
+ \mathcal{O} \left( (\Delta U_{uk}^{\eta})^2, (\Delta \varepsilon_{ep}^{\eta})^2 \right) \\
\]
where \( \Delta U_{ui} = (u_i^{\xi+1})_\eta - (u_i^{\xi})_\eta \), \( \Delta \varepsilon_{ep} = (\varepsilon_{ep}^{\xi+1})_\eta - (\varepsilon_{ep}^{\xi})_\eta \) and \( \mathcal{O} \) is the big O notation to represent the terms of higher order than the second degree. These residuals are repetitively calculated at every time step, and the calculated numerical results are updated during the whole iterations. The increments in the nodal displacement and plastic strains can be obtained by computing the system of linear equations shown in Equation (3.96):

\[
\begin{bmatrix}
K_{u_iuk}^{\Omega_{el}} & K_{u_i ep}^{\Omega_{el}} \\
K_{e_p uk}^{\Omega_{el}} & K_{e_p ep}^{\Omega_{el}}
\end{bmatrix}
\begin{bmatrix}
\Delta U_{uk}^{\eta} \\
\Delta \varepsilon_{ep}^{\eta}
\end{bmatrix}
= 
\begin{bmatrix}
\mathbb{R}_{u_i} \left|_{u_i^{\xi}, \varepsilon_{ep}^{\xi}} \right. \eta \\
\mathbb{R}_{e_p} \left|_{u_i^{\xi}, \varepsilon_{ep}^{\xi}} \right. \eta
\end{bmatrix}
\]
(3.96)

where \( \mathbf{K}_{\Omega_{el}} \) is the Jacobian (stiffness) matrix.

From the functional forms of the thermodynamic microforces defined in Section 3.2.2 and Section 3.2.6 and Equations (3.94) and (3.95) along with the Equations (3.88)-(3.91) at the end of each time step, each component of the Jacobian matrix can be obtained respectively as follows:

\[
K_{u_iuk}^{\Omega_{el}} = - \left( \frac{\partial \mathbb{R}_{u_i}}{\partial U_{uk}} \right) \left|_{U_{uk}^{\xi}} \right. = \int_{\Omega_{el}} \left( E_{ijkl} \frac{\partial N_u^\eta}{\partial x_j} \frac{\partial N_u^\eta}{\partial x_l} \right) dV
(3.97)
\]

\[
K_{u_i e_p}^{\Omega_{el}} = - \left( \frac{\partial \mathbb{R}_{u_i}}{\partial \varepsilon_{ep}^{\xi}} \right) \left|_{\varepsilon_{ep}^{\xi}} \right. = \int_{\Omega_{el}} \left( E_{ijkl} \frac{\partial N_u^\eta}{\partial x_j} \frac{\partial N_{e_p}^\eta}{\partial x_k} \right) dV
(3.98)
\]

\[
K_{e_p uk}^{\Omega_{el}} = - \left( \frac{\partial \mathbb{R}_{e_p}}{\partial U_{uk}} \right) \left|_{U_{uk}^{\xi}} \right. = \int_{\Omega_{el}} \left( E_{ijkl} \frac{\partial N_{e_p}^\eta}{\partial x_j} \frac{\partial N_{e_p}^\eta}{\partial x_k} \right) dV
(3.99)
\]
\( K_{\Omega\ell} = - \frac{\partial \mathcal{R}_{\ell}}{\partial \mathcal{E}_{\eta}} \bigg|_{\ell} \)

\[
= \int_{\Omega_{\ell}} \left[ \left( r^2 \mathcal{H}_0 (e^p)^r + \mathcal{H}_0 \left( \frac{\dot{e}^p}{\dot{p}_1} \right)^m_1 \right) + \sigma_0 \sqrt{\mathcal{H}^2 (e^p) + \ell_{N-G} e^p} \frac{m_1 \dot{e}^p m_1^-1}{\dot{p}_1^m \Delta t} \right] \left[ 1 - \left( \frac{T}{T_y} \right)^n \right] \mathcal{N}_{\ell} \mathcal{N}_{\ell_p} \\
+ \sigma_0 \dot{\ell}_{\ell}^2 \left( \ell_{\ell}^m - 1 \right) \left[ 1 - \left( \frac{T}{T_y} \right)^n \right] \mathcal{N}_{\ell} \mathcal{N}_{\ell_p} \\
+ \sigma_0 \dot{\ell}_{\ell}^4 \left( \ell_{\ell}^m + 1 \right) \left[ 1 - \left( \frac{T}{T_y} \right)^n \right] \mathcal{N}_{\ell} \mathcal{N}_{\ell_p} \\
- \left[ G \dot{\ell}_{\ell} \right] \mathcal{N}_{\ell} \mathcal{N}_{\ell_p} \\
+ \dot{\ell}_{\ell}^2 \frac{\sigma_0 + \mathcal{H}_0 e^{p^{GB}(post)}}{(\Delta t \dot{p}^{GB}) m^{GB}} \left[ 1 - \left( \frac{T}{T_y^{GB}} \right)^{n^{GB}} \mathcal{N}_{\ell} \mathcal{N}_{\ell_p} \right] \\
- \frac{\ell_{\ell}^{GB} \dot{p}^{GB}(post) m^{GB} - 1}{\dot{p}_1^m} \mathcal{N}_{\ell} \mathcal{N}_{\ell_p}
\]

(3.100)

where \( \Delta t \) is a time step. The grain boundary terms in Equation (3.100) is only applied for nodes on the grain boundary area.

3.4 Validation of the proposed SGP model

In this section, the proposed SGP theory and corresponding finite element implementation are validated through the comparison against the experimental measurements from two sets of size effect tests: Aluminum thin films experiments by Haque and Saif (2003) and Nickel thin films experiments by Han et al. (2008). The material parameters for two different metals, Aluminum and Nickel, are also calibrated by using the experimental data. The parameters \( \sigma_0 \) and \( \mathcal{H}_0 \) are determined by extrapolating the experimental data, and the material length scales are determined based on the suggestion by Anand et al. (2005). In their work, an initial assumption for the material length scales are suggested by matching the numerical results from the proposed flow rule to the yield strength and backstress experimental measurements under the assumption of \( \ell_{\ell} = 0 \) and \( \ell_{\ell} = 0 \) at each case respectively. The rest of the material parameters come from the literature (Han et al., 2008; Haque and Saif, 2003; Voyiadjis and Song, 2017). The grain boundary flow rule is not considered in Sections 3.5, 3.6 and 3.7.

Haque and Saif (2003) developed the Micro-Electro Mechanical Systems (MEMS) based testing skill for the nanoscale Aluminum (Al) thin films under the uniaxial tensile loading to
investigate the strain gradient effect in 100 nm, 150 nm, 200 nm and 485 nm thick specimens, which have the average grain sizes of 50 nm, 65 nm, 80 nm and 212 nm respectively. The specimens with 99.99 % pure sputter-deposited freestanding Al thin films are 10 μm wide and 275 μm long. All experiments are carried out in-situ in SEM and the strain and stress resolutions for the tests are set as 0.03 % and 5 MPa respectively. The general and calibrated material parameters are shown in Table 3.1. Figure 3.1 displays the direct comparison between the proposed model and the experimental observations. As clearly shown in this figure, the size effect: Smaller is Stronger is observed on the stress-strain curves, furthermore, the numerical results from the proposed SGP model and the experimental data correspond closely with each other.

Table 3.1. The general and calibrated material parameters used for the validation of the proposed strain gradient plasticity model.

<table>
<thead>
<tr>
<th>General</th>
<th>Aluminum</th>
<th>Nickel</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$ (GPa)</td>
<td>Elastcity modulus for isotropic linear elasticity</td>
<td>70</td>
</tr>
<tr>
<td>$ν$</td>
<td>Poisson’s ratio</td>
<td>0.30</td>
</tr>
<tr>
<td>$μ$ (GPa)</td>
<td>Shear modulus for isotropic linear elasticity</td>
<td>27</td>
</tr>
<tr>
<td>$ρ$ ($g⋅cm^{-3}$)</td>
<td>Density</td>
<td>2.702</td>
</tr>
<tr>
<td>$c_v$ ($J/g⋅°K$)</td>
<td>Specific heat capacity at constant stress</td>
<td>0.910</td>
</tr>
<tr>
<td>$α^{th}$ (μm/m⋅°K)</td>
<td>Thermal expansion coefficient</td>
<td>24.0</td>
</tr>
<tr>
<td>$\dot{ρ}_1, \dot{ρ}_2$ (s^{-1})</td>
<td>Reference plastic strain rate</td>
<td>0.04</td>
</tr>
<tr>
<td>$r$</td>
<td>Nonlinear hardening material constant</td>
<td>0.6</td>
</tr>
<tr>
<td>$m_1$</td>
<td>Non-negative strain rate sensitivity parameter</td>
<td>0.05</td>
</tr>
<tr>
<td>$m_2$</td>
<td>Non-negative strain rate sensitivity parameter</td>
<td>0.2</td>
</tr>
<tr>
<td>$T_y$ (°K)</td>
<td>Thermal material parameter</td>
<td>933</td>
</tr>
<tr>
<td>$n$</td>
<td>Temperature sensitivity parameter</td>
<td>0.3</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Calibrated</th>
<th>Aluminum</th>
<th>Nickel</th>
</tr>
</thead>
<tbody>
<tr>
<td>$σ_0$ (MPa)</td>
<td>Stress-dimensioned scaling constant</td>
<td>1,000</td>
</tr>
<tr>
<td>$H_0$ (MPa)</td>
<td>Isotropic hardening parameter</td>
<td>1,000</td>
</tr>
<tr>
<td>$ℓ_{en}$ (μm)</td>
<td>Energetic length scale</td>
<td>1.2</td>
</tr>
<tr>
<td>$ℓ_{dis}$ (μm)</td>
<td>Dissipative length scale</td>
<td>0.7</td>
</tr>
<tr>
<td>$ℓ_{N-G}$ (μm)</td>
<td>N-G length scale</td>
<td>1.0</td>
</tr>
</tbody>
</table>
Figure 3.1. The validation of the proposed SGP model by comparing the numerical results from the proposed model with the experimental measurements from Haque and Saif (2003) on the stress-strain response of the sputter-deposited Al thin films.

Figure 3.2. The schematic illustration of the dog bone specimen and its main dimensions (Han et al., 2008).

The microscale tensile experiment skill for evaluating the mechanical and thermal properties of the Nickel (Ni) thin films at high temperatures is developed by Han et al. (2008). The dog bone shaped specimens used in their experiments were made by Micro-electro mechanical system (MEMS) processes and the primary dimensions of the specimen are given in Figure 3.2. The general and calibrated material parameters for Ni are presented in Table 3.1. The experimental measurements at four different temperatures, i.e. 25 °C, 75 °C, 145 °C and 218 °C, and corresponding numerical values from the proposed model are presented in Figure 3.3. As shown in this figure, it is obvious from both the numerical and experimental results that the Young’s modulus is not affected by variations in temperature while the yield strength decreases as the specimen temperature increases, in addition, Figure 3.3 clearly shows that the Bauschinger effect is not affected very much by variations in the specimen temperature. All these observations are not much different from those observed in one-dimensional finite element simulations (Voyiadjis and Song, 2017).
Figure 3.3. The validation of the proposed SGP model by comparing the numerical results from the proposed model with the experimental measurements from Han et al. (2008) on the stress-strain response of the Ni thin films.

3.5 Microfree grain boundary

The characteristics of the proposed SGP theory under the microfree boundary condition at the grain boundary is addressed in this section by solving the shear problem of a rectangular plate with varying material parameters.

By following Gurtin (2003), the simple class of microscopically free boundary condition on a prescribed subsurface is employed from Equation (3.14) as follows:

\[ m = \mathcal{Q}_i n_i = 0 \]  

(3.101)

The schematic illustration of the problem, the initial conditions, and the macroscopic and microscopic boundary conditions are shown in Figure 3.4. The parameter \( u^\dagger(t) \) represents the prescribed displacement. The stress-strain behaviour and the distributions of the temperature and accumulated plastic strain across the plate in \( x_2 \)-direction are investigated for the various material length scales (\( \ell_{en}, \ell_{dis} \) and \( \ell_{N-G} \)), the hardening parameter \( H_0 \) and the temperature-related parameters (\( n \) and \( T_y \)). The material parameters in Table 3.2 are used for this section unless stated otherwise.
Figure 3.4. The schematic illustration of the simple shear problem including the macroscopic and microscopic boundary conditions, and initial conditions.

Table 3.2. The material parameters used in Section 3.5 and Section 3.6.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>General</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$ (GPa)</td>
<td>Elastic modulus for isotropic linear elasticity</td>
<td>110</td>
</tr>
<tr>
<td>$\nu$</td>
<td>Poisson’s ratio</td>
<td>0.33</td>
</tr>
<tr>
<td>$\mu$ (GPa)</td>
<td>Shear modulus for isotropic linear elasticity</td>
<td>48</td>
</tr>
<tr>
<td>$\rho$ ($g \cdot cm^{-3}$)</td>
<td>Density</td>
<td>8.960</td>
</tr>
<tr>
<td>$c_e$ ($J / g \cdot ^\circ K$)</td>
<td>Specific heat capacity at constant stress</td>
<td>0.385</td>
</tr>
<tr>
<td>$\alpha^{th}$ ($\mu m / m \cdot ^\circ K$)</td>
<td>Thermal expansion coefficient</td>
<td>24.0</td>
</tr>
<tr>
<td>$\dot{\rho}_1, \dot{\rho}_2$ ($s^{-1}$)</td>
<td>Reference plastic strain rate</td>
<td>0.04</td>
</tr>
<tr>
<td>$r$</td>
<td>Nonlinear hardening material constant</td>
<td>0.6</td>
</tr>
<tr>
<td>$m_1$</td>
<td>Non-negative strain rate sensitivity parameter</td>
<td>0.05</td>
</tr>
<tr>
<td>$m_2$</td>
<td>Non-negative strain rate sensitivity parameter</td>
<td>0.2</td>
</tr>
<tr>
<td>$T_y$ ($^\circ K$)</td>
<td>Thermal material parameter</td>
<td>1,358</td>
</tr>
<tr>
<td>$n$</td>
<td>Temperature sensitivity parameter</td>
<td>0.3</td>
</tr>
<tr>
<td>$\sigma_0$ (MPa)</td>
<td>Stress-dimensioned scaling constant</td>
<td>1,000</td>
</tr>
<tr>
<td>$\mathcal{H}_0$ (MPa)</td>
<td>Isotropic hardening parameter</td>
<td>1,000</td>
</tr>
</tbody>
</table>

3.5.1 Energetic gradient hardening

For exploring the characteristics of the energetic gradient hardening only, the dissipative gradient and GNDs gradient terms are assumed to vanish by imposing $\ell_{dis} = \ell_{N-G} = 0$. The stress-strain behaviours and the distributions of $e^P$ and $T$ along the height of the plate for $\ell_{en}/L = 0, 0.1, 0.2, 0.3, 0.5, 0.7$ and $1.0$ with $\mathcal{H}_0 = 0$ MPa are shown in Figure 3.5. For the case of $\ell_{en}/L = 0$, the stress-strain curve does not show hardening as expected, and the distribution of $e^P$ is uniform. As $\ell_{en}/L$ increases, the rates of the hardening increase as shown in Figure 3.5. (a) and
the distributions of $e^p$ and $\mathcal{T}$ become more parabolic. When the dissipative length scale $\ell_{\text{dis}}$ is absent, the heat generation is governed by the amount of $e^p$, therefore the distribution of $\mathcal{T}$ is identical to the one of $e^p$ as observed in Figure 3.5. (b) and (c). Due to the microhard boundary condition, the temperature does not rise at the boundary, and the maximum temperature is observed at the center of the plate.

Figure 3.5. The effects of the energetic gradient hardening with the energetic length scale only ($\ell_{\text{dis}} = \ell_{N-G} = 0$): (a) the stress-strain response, (b) the temperature distribution, and (c) the accumulated plastic strain distribution.

(fig. cont’d.)
3.5.2 Dissipative gradient strengthening

Figure 3.6. The effects of the dissipative gradient strengthening with the dissipative length scale only ($\ell_{en} = \ell_{N-G} = 0$): (a) the stress-strain response, (b) the temperature distribution, and (c) the accumulated plastic strain distribution.

(fig. cont’d.)
It is now assumed that the energetic and GNDs hardening disappear by setting $\ell_{en} = \ell_{N-G} = 0$. The isotropic hardening parameter is also set as $\mathcal{H_0} = 0 \, MPa$. The stress-strain curves and the distributions of $e^p$ and $T$ across the height of the plate for $\ell_{dis}/L = 0, 0.05, 0.1, 0.2, 0.3, 0.5$ and $0.7$ are shown in Figure 3.6. As $\ell_{dis}/L$ increases, it is shown in Figure 3.6. (a) that the initial yield strength increases without strain hardening. The non-monotonic behaviour of $e^p$ with $\ell_{dis}/L$ is elucidated by plotting the maximal values of $e^p$ at the center of the plate for varying $\ell_{dis}/L$ as shown in Figure 3.6. (c). This numerical results are in line with the works of Bardella (2006) and Fleck and Hutchinson (2001). The drastic change shown in the accumulated plastic strain distribution according to varying $\ell_{dis}/L$ prominently affect the temperature distribution. According to Equation (3.67), both the plastic strain and its gradient are involved in the evolution
of $\mathcal{T}$. As observed from Figure 3.6 (b), the large amounts of plastic strain gradient raise the temperature at the boundary, on the other hand, the temperature at the center of the plate is primarily influenced by plastic strain.

3.5.3 GNDs hardening

![Graph showing stress-strain response and temperature distribution](image)

**Figure 3.7.** The effects of the GNDs hardening with the N-G length scale only ($\ell_{en} = \ell_{dis} = 0$): (a) the stress-strain response, (b) the temperature distribution, and (c) the accumulated plastic strain distribution.

(fig. cont’d.)
It is now assumed that the energetic and dissipative gradient terms disappear by setting \( \ell_{\text{en}} = \ell_{\text{dis}} = 0 \). The stress-strain curves and the distributions of \( e^p \) and \( T \) across the height of the plate for \( \ell_{N-G}/L = 0, 0.1, 0.2, 0.5, 1.0, 1.5 \) and \( 2.0 \) with \( H_0 = 0 \, MPa \) are shown in Figure 3.7. As \( \ell_{N-G}/L \) increases, the rates of the strain hardening increase more significantly, while no initial yield strength is observed. Similar to the energetic gradient hardening case, in the absence of \( \ell_{\text{dis}} \), the distribution of temperature is identical to the one of plastic strain.

3.5.4 Temperature-related parametric study

The effects are now investigated of the two material parameters, \( n \), and \( T_y \), on the stress-strain behaviour, the distributions of the temperature and accumulated plastic strain, and the temperature evolution in conjunction with \( \ell_{\text{en}}/L = 1.0, \ell_{\text{dis}}/L = 0.5 \) and \( \ell_{N-G}/L = 1.0 \).

Figure 3.8 and Figure 3.9 show the effect of the material parameters \( n \) and \( T_y \) applying the temperature-dependent behaviour of the present model on the stress-strain curve, the distributions of the temperature and accumulated plastic strain distribution, and the evolution of the temperature at the midpoint of the plate. As shown in these figures, the effects of the two parameters on the thermal and mechanical material response are similar to each other due to the fact that two parameters affect the temperature-related term \( \left( 1 - \left( T/T_y \right)^n \right) \) in the flow rule, which explains the thermal activation mechanism for overcoming the local barriers to the dislocation movement, in a similar way. In this chapter, the normal parameter is employed as a normalizing constant that should be calibrated by using the experimental data.

It is clearly observed in Figure 3.8. (a) and Figure 3.9. (a) that, as \( n \) and \( T_y \) increase, the strain hardening and the initial yield strength also increase. The effect, nevertheless, is more prominent in initial yield strength, because strain hardening mechanism is affected by temperature through the dislocation forest barriers, on the other hand, the backstress does not depend on the temperature. For both \( n \) and \( T_y \), it is shown in Figure 3.8. (b) and (c), and Figure 3.9. (b) and (c) that the accumulated plastic strains at the boundary (\( 0 < x_2/L < 0.2 \) and \( 0.8 < x_2/L < 1 \) are
almost identical with respect to the different values of $n$ and $T_y$, on the other hand, the most significant differences in the temperature profiles occur at the same range for both parameters. In contrast to this, the most substantial differences in the accumulated plastic strain profiles according to the values of $n$ and $T_y$ occur in the middle ($0.2 < x_2/L < 0.8$) of the plate, on the other hand, the temperature profiles at this part do not show considerable difference.

Figure 3.8. The effects of the thermal material parameter $n$ with $\ell_{en}/L = 1.0$, $\ell_{dis}/L = 0.5$ and $\ell_{N-G}/L = 1.0$: (a) the stress-strain response, (b) the temperature distribution, and (c) the accumulated plastic strain distribution.

(fig. cont’d.)
Figure 3.9. The effects of the thermal material parameter $T_y$ with $\ell_{en}/L = 1.0$, $\ell_{dis}/L = 0.5$ and $\ell_{N-G}/L = 1.0$: (a) the stress-strain response, (b) the temperature distribution, and (c) the accumulated plastic strain distribution.

(fig. cont’d.)
3.6 Microhard grain boundary

In this section, a microhard boundary condition, which describes that the dislocation movements are blocked completely at the grain boundary, is assumed to hold on the grain boundary as follows:

$$e^p = 0$$  \hspace{1cm} (3.102)

The square plate with an edge of \( W \) is solved to investigate the effect of this grain boundary condition. The top edge of the plate is subject to a prescribed condition in terms of the displacement \( (u_1^{\text{top}}(x_1, W, t) = u_1^*(t), u_2^{\text{top}}(x_1, W, t) = 0) \), while the bottom edge is fixed \( (u_1^{\text{bot}}(x_1, 0, t) = u_2^{\text{bot}}(x_1, 0, t) = 0) \). The whole square is meshed using 1,600 (40 \times 40)
elements and split into several grains by the four different grain boundary areas, which is indicated by the bold lines as shown in Figure 3.10. For these simulations, the stress-dimensioned scaling constant $\sigma_0$ and the isotropic hardening parameter $\mathcal{H}_0$ are set as 195 $MPa$ and 0 $MPa$ respectively, and the values in Table 3.2 are used again for the rest of the material parameters.

$$ u_1(x_1, L, t) = u_1^i(t), u_2(x_1, L, t) = 0 $$

Figure 3.10. The schematic illustration of the square plate problem with four different grain boundary areas.

$$ u_1(x_1, 0, t) = u_2(x_1, 0, t) = 0 $$

Figure 3.11. The distributions of the accumulated plastic strain and the temperature with: (a) the microhard, and (b) microfree boundary conditions.
The comparison of the microscopic boundary condition is addressed through the single grain in Figure 3.11. Figure 3.11. (a) shows the distributions of the accumulated plastic strain $e^p$ and temperature $\mathcal{T}$ respectively with the microhard boundary condition at the grain boundaries, while Figure 3.11. (b) are those with the microfree boundary condition. The terminologies “NT11” and “UVARM6” in Figure 3.11. (a) indicate the accumulated plastic strain and the temperature respectively, and are used continually in the rest of this work. For this example, $\ell_{en}/L = 0.3$, $\ell_{dis}/L = 0.0$ and $\ell_{N-G}/L = 0.0$ are used. As can be seen in Figure 3.11. (a), each edge of the plate with microhard boundary condition obstructs the dislocation movement, which results in $e^p = 0$, whereas in the case of microfree boundary condition, $e^p$ and $\mathcal{T}$ are evenly spread across the grain.

Figure 3.12 shows the distributions of $e^p$ and $\mathcal{T}$ with no gradient effect. This can be regarded as the reference case for the purpose of the comparison to other cases with the gradient effect.

The effects of the grain boundary area in conjunction with the energetic gradient hardening, dissipative gradient strengthening, GNDs hardening, and no gradient effect are shown in Figure 3.13 through the stress-strain responses. As can be seen in Figure 3.13. (a), no significant hardening or strengthening is observed under the conventional plasticity theory. On the other hand, by considering the gradient effect, the energetic hardening, dissipative strengthening and GNDs hardening is observed respectively in Figure 3.13. (b), (c) and (d) with varying grain boundary areas.
Figure 3.13. The effects of the grain boundary area on the stress-strain response with: (a) no gradient effect ($\ell_{en} = \ell_{dis} = \ell_{N-G} = 0$) (b) the energetic length scale only ($\ell_{en}/W = 0.1$, $\ell_{dis} = \ell_{N-G} = 0$), (c) the dissipative length scale only ($\ell_{dis}/W = 0.05$, $\ell_{en} = \ell_{N-G} = 0$), and (d) the N-G length scale only ($\ell_{N-G}/W = 0.5$, $\ell_{en} = \ell_{dis} = 0$).

(fig. cont’d.)
The effects of the grain boundary area in conjunction with the energetic gradient hardening, dissipative gradient strengthening and GNDs hardening on the distributions of $e^p$ and $T$ are also shown respectively in Figure 3.14, Figure 3.15 and Figure 3.16. For the simulations in Figure 3.14, the energetic length scales vary from 0.1 to 0.3, and the dissipative and N-G length scales are set as zero. It should be noted that the distributions of $e^p$ and $T$ are not identical in all grains since the simple shear loading is applied to the top edge of the plate, and not to each grain individually. It is clearly observed in Figure 3.14 by comparing to Figure 3.12 that the distributions of $e^p$ and $T$ with the energetic hardening are significantly different from those with no gradient effect. This tendency is also observed with the dissipative strengthening effects when comparing
Figure 3.15 with Figure 3.12 as well as with the GNDs hardening effects when comparing Figure 3.16 with Figure 3.12.

(a)

(b)

(c)

(d)

Figure 3.14. The distributions of the accumulated plastic strain and the temperature in conjunction with varying grain boundary areas with the energetic length scale only ($\ell_{dis} = \ell_{N-G} = 0$): (a) $e^p$ with $\ell_{en}/W = 0.1$, (b) $T$ with $\ell_{en}/W = 0.1$, (c) $e^p$ with $\ell_{en}/W = 0.2$, (b) $T$ with $\ell_{en}/W = 0.2$, and (e) $e^p$ with $\ell_{en}/W = 0.3$, and (f) $T$ with $\ell_{en}/W = 0.3$. (fig. cont’d.)
Figure 3.15. The distributions of the accumulated plastic strain and the temperature in conjunction with varying grain boundary areas with the dissipative length scale only ($\ell_{en} = \ell_{N-G} = 0$): (a) $e^p$ with $\ell_{dis}/W = 0.01$, (b) $T$ with $\ell_{dis}/W = 0.01$, (c) $e^p$ with $\ell_{dis}/W = 0.03$, (d) $T$ with $\ell_{dis}/W = 0.03$, (e) $e^p$ with $\ell_{dis}/W = 0.05$, and (f) $T$ with $\ell_{dis}/W = 0.05$.

(fig. cont’d.)
Figure 3.16. The distributions of the accumulated plastic strain and the temperature in conjunction with varying grain boundary areas with the N-G length scale only ($\ell_{en} = \ell_{dis} = 0$): (a) $e^p$ with $\ell_{N-G}/W = 0.1$, (b) $T$ with $\ell_{N-G}/W = 0.1$, (c) $e^p$ with $\ell_{N-G}/W = 0.3$, (d) $T$ with $\ell_{N-G}/W = 0.3$, (e) $e^p$ with $\ell_{N-G}/W = 0.5$, and (f) $T$ with $\ell_{N-G}/W = 0$. 

(FIG. CONT’D.)
3.7 Intermediate (deformable) grain boundary

The schematic illustration of the simple shear problem: (a) the macroscopic, microscopic boundary conditions, and initial conditions (b) $4 \times 4$ grains.

The assumption of two null boundary conditions, microfree and microhard boundary conditions, is used at the grain boundary in the previous two sections. In this section, the governing differential equation is solved by imposing the proposed grain boundary flow rule to account for the deformable grain boundary. Furthermore, the characteristics of the proposed strain gradient plasticity theory incorporating the flow rules of both the grain interior and grain boundary is addressed in this section by solving the shear problem of a square plate with an edge of $L$. The schematic illustration of the problem, the initial conditions, and the macroscopic and microscopic boundary conditions as well as the grain boundary area are shown in Figure 3.17. The parameter
$u^\dagger(t)$ represents the prescribed displacement. The whole square is meshed using 1,600 (40 × 40) elements and split into the 16 (4 × 4) grains by the grain boundary area, which is indicated by the bold lines. The material parameters for the grain interior and grain boundary are presented in Table 3.3.

Table 3.3. The material parameters used in Section 3.7.

<table>
<thead>
<tr>
<th>Grain interior</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$ (GPa)</td>
<td>110</td>
</tr>
<tr>
<td>$\nu$</td>
<td>0.33</td>
</tr>
<tr>
<td>$\mu$ (GPa)</td>
<td>48</td>
</tr>
<tr>
<td>$\rho$ (g · cm$^{-3}$)</td>
<td>8.960</td>
</tr>
<tr>
<td>$c_\varepsilon$ (J/g · °K)</td>
<td>0.385</td>
</tr>
<tr>
<td>$\alpha^\text{th}$ (μm/m · °K)</td>
<td>16.0</td>
</tr>
<tr>
<td>$\dot{p}_1, \dot{p}_2$ (s$^{-1}$)</td>
<td>0.04</td>
</tr>
<tr>
<td>$r$</td>
<td>0.6</td>
</tr>
<tr>
<td>$m_1$</td>
<td>0.05</td>
</tr>
<tr>
<td>$m_2$</td>
<td>0.2</td>
</tr>
<tr>
<td>$T_y$ (°K)</td>
<td>1,358</td>
</tr>
<tr>
<td>$n$</td>
<td>0.3</td>
</tr>
<tr>
<td>$\sigma_0$ (MPa)</td>
<td>195</td>
</tr>
<tr>
<td>$H_0$ (MPa)</td>
<td>0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Grain boundary</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_0^\text{GB}$ (MPa)</td>
<td>195</td>
</tr>
<tr>
<td>$H_0^\text{GB}$ (MPa)</td>
<td>0</td>
</tr>
<tr>
<td>$\rho^\text{GB}$</td>
<td>0.04</td>
</tr>
<tr>
<td>$m^\text{GB}$</td>
<td>1</td>
</tr>
<tr>
<td>$T_y^\text{GB}$</td>
<td>700</td>
</tr>
<tr>
<td>$n^\text{GB}$</td>
<td>0.4</td>
</tr>
</tbody>
</table>

As can be seen from Equation (3.82), the grain boundary may act like a free surface, i.e. microfree boundary condition, when $\ell_{en}^\text{GB} = \ell_{dis}^\text{GB} = 0$. On the other hand, the microhard boundary condition can be compelled under the conditions $\ell_{en}^\text{GB} \to \infty$ and $\ell_{dis}^\text{GB} \to \infty$. Firstly, the validity of these conditions is examined in this section. Next, the direct comparison between the classical plasticity theory ($\ell_{en}/L = \ell_{dis}/L = \ell_{N-G}/L = 0.0$) and the gradient-enhanced plasticity theory ($\ell_{en}/L = \ell_{dis}/L = \ell_{N-G}/L = 0.1$) is given in order to check the ability of the proposed flow rule on the size effect. The numerical results in terms of the accumulated plastic strain profile and the stress-strain curves are shown in Figure 3.18 and Figure 3.19. As can be seen in these figures, the
microfree and microhard boundary conditions are well captured under the classical plasticity theory as well as the gradient-enhanced plasticity theory. In addition, in Figure 3.18. (c), no size effect is observed in the classical plasticity theory with varying normalized material length scales as expected. In Figure 3.19. (c), on the other hand, strain hardening and strengthening are more pronounced as the dimensions of the shear plate height are reduced ($\ell_{en}^GB/L \rightarrow \infty$, $\ell_{dis}^GB/L \rightarrow \infty$). In Figure 3.20, the effects of each material length scale parameter, i.e. $\ell_{en}$, $\ell_{dis}$ and $\ell_{N-G}$, along with the microscopically hard boundary condition are also examined through the profile of accumulated plastic strain. In addition, the contributions of each length scale parameter on the stress-strain responses are shown in Figure 3.20. (c).

Figure 3.18. Classical plasticity theory ($\ell_{en}/L = \ell_{dis}/L = \ell_{N-G}/L = 0.0$). The distributions of the accumulated plastic strain with: (a) the microscopically free ($\rho_{en}^GB = \rho_{dis}^GB = 0$), and (b) microscopically hard boundary conditions ($\rho_{en}^GB \rightarrow \infty$, $\rho_{dis}^GB \rightarrow \infty$), and (c) the stress-strain responses.
Figure 3.19. Strain gradient plasticity theory ($\ell_{en}/L = \ell_{dis}/L = \ell_{N-G}/L = 0.1$). The distributions of the accumulated plastic strain with: (a) the microscopically free ($\ell_{en}^{GB} = \ell_{dis}^{GB} = 0$), and (b) microscopically hard boundary conditions ($\ell_{en}^{GB} \to \infty$, $\ell_{dis}^{GB} \to \infty$), and (c) the stress-strain responses.
Figure 3.20. The distributions of the accumulated plastic strain with the microscopically hard boundary condition \( (\ell_{\text{en}} / L \to \infty, \ell_{\text{dis}} / L \to \infty) \) under: (a) the energetic length scale only \( (\ell_{\text{en}} / L = 0.1, \ell_{\text{dis}} / L = \ell_{N-G} / L = 0.0) \), (b) the dissipative length scale only \( (\ell_{\text{dis}} / L = 0.1, \ell_{\text{en}} / L = \ell_{N-G} / L = 0.0) \), (c) the N-G length scale only \( (\ell_{N-G} / L = 0.1, \ell_{\text{en}} / L = \ell_{\text{dis}} / L = 0.0) \), and (d) the stress-strain responses.
Variations in the stress-strain responses and the evolutions of maximum temperature are investigated for the various values of the normalized energetic and dissipative grain boundary material length scales as shown in Figure 3.21 and Figure 3.22. It is assumed by setting $\ell_{\text{dis}}^{\text{GB}}/\ell_{\text{dis}} = 0$ that all plastic work at the grain boundary is stored as surface energy which depends on the plastic strain state at the surface. In this case, $\rho_{\text{en}}^{\text{GB}}/\ell_{\text{en}}$ reflects the grain boundary resistance to plastic deformation. Figure 3.21. (b) and Figure 3.22. (b) show the size effects on the strain hardening and temperature evolution due to the grain boundary energetic length scale, and it is more pronounced in the more strongly constrained material, i.e. increasing $\ell_{\text{en}}^{\text{GB}}/\ell_{\text{en}}$. On the other hand, by setting $\rho_{\text{en}}/\ell_{\text{en}} = 0$, it is assumed that the work performed at the grain boundary is dissipated in the absence of surface energy. In this case, $\ell_{\text{dis}}^{\text{GB}}/\ell_{\text{dis}}$ reflects the grain boundary resistance to slip transfer. As can be seen in Figure 3.21. (c), the initial yield strength increases without strain hardening as $\ell_{\text{dis}}/\ell_{\text{dis}}$ increases.

Figure 3.21. The distributions of the accumulated plastic strain according to the various values of $\ell_{\text{en}}/\ell_{\text{en}}$ and $\ell_{\text{dis}}/\ell_{\text{dis}}$: (a) combined $\ell_{\text{en}}$ and $\ell_{\text{dis}}$, (b) $\ell_{\text{en}}$ only, and (c) $\ell_{\text{dis}}$ only. (fig. cont’d.)
Figure 3.22. The evolutions of the maximum temperature according to the various values of $\ell_{en}/\ell_{en}$ and $\ell_{dis}^{GB}/\ell_{dis}$: (a) combined $\ell_{en}^{GB}$ and $\ell_{dis}^{GB}$, (b) $\ell_{en}^{GB}$ only, and (c) $\ell_{dis}^{GB}$ only.

(fig. cont’d.)
3.8 Conclusions

The two-dimensional finite element analysis for the thermodynamically consistent thermo-mechanical coupled gradient enhanced plasticity model is proposed within the areas of grain interior and grain boundary, and validated by comparing against two sets of small-scale experiments demonstrating the size effects. The proposed formulation is developed based on the concept of dislocations interaction mechanisms and thermal activation energy. The thermodynamic microstresses are assumed to be divided in two components, i.e. the energetic and dissipative components, which in turn, both energetic and dissipative material length scale parameters are incorporated in the governing constitutive equations. These two thermodynamic microstresses can be respectively obtained in a direct way from the Helmholtz free energy and rate of dissipation potential by taking maximum entropy production into account. The concept of GNDs density is additionally employed in this chapter to interpret the microstructural strengthening mechanisms induced by the nonhomogeneous deformation. Correspondingly, the model in this chapter incorporates the terms related to GNDs-induced strengthening and the additional material length scale parameter. Not only the partial heat dissipation due to fast transient time, but also the distribution of the temperature caused by the transition from plastic work to heat, are included into the coupled thermo-mechanical model by deriving a generalized heat equation.

The proposed SGP model and the correspondingly developed finite element code are validated through the comparisons against the experimental measurements from small-scale aluminum and nickel thin film tests. The material parameters for two kinds of metals are also calibrated by using the experimental measurements. The numerical results show good agreement with the experimental measurements in terms of both tests. The simple shear problem and the square plate problem are solved based on the validated model in order to examine size effect in small-scale metallic materials and two null boundary conditions respectively. The energetic hardening, dissipative strengthening and GNDs hardening are well observed respectively with varying \( \ell_{en}, \ell_{dis} \) and \( \ell_{G-N} \). The parametric study is carried out to investigate the effect of the temperature-related parameters on the stress-strain curve, the distributions of the temperature and the accumulated plastic strain, and the temperature evolution. The effect of the microhard boundary condition at the grain boundary on the stress-strain curve, and the distributions of the
plastic strain and the temperature is presented by solving the square plate problem. The strengthening effect due to the microhard boundary condition at the grain boundary is clearly observed with increasing grain boundary areas in this simulation. In addition, the microfree and microhard boundary conditions are well captured by using the proposed grain boundary flow rule. Lastly, the size effects on the stress-strain responses and the evolutions of maximum temperature are well observed with the cases of (a) combined $\ell_{en}^{GB}$ and $\rho_{dis}^{GB}$, (b) $\ell_{en}^{GB}$ only, and (c) $\ell_{dis}^{GB}$ only.
4 THERMODYNAMICALLY CONSISTENT STRAIN GRADIENT PLASTICITY MODELS AND APPLICATIONS FOR FINITE DEFORMATIONS: SIZE EFFECTS AND SHEAR BANDS

4.1 Introduction

A strain localisation is generally shown as a narrow band of intense shearing strain. Needleman (1988) has shown that the conventional rate-independent plasticity model will cause an ill-posed problem during strain softening in finite element analysis. From a theoretical point of view, the strain localisation is related to the change in the characteristics of the governing relations for the rate-independent materials. The forms of the partial differential equations vary from hyperbolic to elliptic or vice versa. The finite element results of the localisation problem, as a result, show the mesh dependent behaviour. Not only the width of the shear bands, but also some characteristics of the materials such as the stiffness deduction are dependent on the mesh size or density, thus the conventional rate-independent models without any regularization cannot be used to solve the shear band problems.

One promising approach to address this phenomenon is to bring in one or more intrinsic material length scales to the conventional plasticity theory. The earliest attempts of this approach are made by Aifantis (1984, 1987) who developed gradient-dependent plasticity theory by integrating the gradient terms into the conventional flow rule. Aifantis (1984, 1987) also shows that the width of the shear bands is strongly related to the coefficients of the gradient terms. Hereafter, the numerous gradient-enhanced plasticity theories have been proposed based on the work of Aifantis (1984, 1987) from a computational viewpoint (Deborst and Muhlhaus, 1992; deBorst and Pamin, 1996; Muhlhaus and Aifantis, 1991). In these works, the higher-order strain gradient terms are directly incorporated to the constitutive relations, thus have been termed as explicit gradient-enhanced approach by Engelen et al. (2003). In order to implement the explicit approaches, it is necessary to involve the nonstandard boundary conditions at the boundary of plastic zone. At the outer boundary or the stationary elasto-plastic boundary areas, the use of nonstandard boundary conditions is comparatively understood well. However, if the plastic zone expands under the inelastic deformation, it turns out to be more complicated (Peerlings, 2007). Furthermore, since the finite element implementation of the explicit approach requires C^1-continuous interpolation functions in the course of processing the discretisation, there exists a considerable challenge in implementing the explicit approach. In order to avoid the use of C^1-continuous two-field interpolation, which is computationally expensive, Pamin (1994) proposed an approach that only requires C^0-continuous interpolation functions in conjunction with a penalty constraint for the gradient of the plastic strain. One disadvantage of this approach is that the total number of degrees of freedom (D.O.F) increases since this involves in a three-field approach. One of the possible solutions for this issue is to employ the constitutive formulations of the viscoplastic theory, in this way, the distinct elasto-plastic boundaries can be avoided (see Gudmundson (2004) as an example).

The implicit gradient-enhanced approach is then introduced as an alternative method with only C^0-continuous requirement in order to overcome a computational inherent difficulty in the explicit approach. In the implicit approach, the Helmholtz-type partial differential equation is obtained, and the nonlocal quantities are calculated in a coupled method based on the equilibrium conditions. The implicit gradient-enhanced approaches have been generally utilized not only to solve the mesh dependency problems (Engelen et al., 2003), but also in modeling of the ductile
damage (Geers, 2004), the quasi-brittle fracture (Peerlings et al., 1996), and the finite deformation problems (Geers, 2004). Recently, a finite deformation gradient-enhanced model for an isotropic elasto-plastic, rate-independent material has been proposed in a thermodynamically consistent framework based on a systematic unification of the implicit approach and micromorphic theory (Anand et al., 2012). In their work, it is concluded that, from a physical point of view, the derivation of the Helmholtz type partial differential equation for the micromorphic variable, which is typically used in implicit approach, is not totally satisfactory. From a numerical point of view, however, an implicit theory is highly practical to regularize the numerical simulations of the strain localisation during strain softening.

Another issue in the implicit approach is the fact that the implicit approach may be incapable of modeling the size effect phenomenon in the strain hardening regime (Engelen et al., 2006; Peerlings et al., 2012). The three existing higher-order strain gradient plasticity theories (two explicit approaches by Fleck and Hutchinson (1997, 2001) and one implicit approach by Engelen et al. (2003)) are compared in Engelen et al. (2006) in order to evaluate their performance to predict the size effect. It is concluded in their work that the size effect cannot be observed in the theory of Engelen et al. (2003) whereas Fleck and Hutchinson theory (Fleck and Hutchinson, 1997, 2001) can capture the strengthening effect as the specimen thickness decreases (see Figure 1 and Table 1 in Engelen et al. (2006)). Peerlings (2007) proposed an implicit approach which can predict the similar size effect as observed in the explicit approach. The gradient-enhanced plasticity-damage theory based on the implicit approach is then constructed in Peerlings et al. (2012) based on a combination of the theories proposed in Engelen et al. (2003) and Peerlings (2007) in order to capture the size effect in hardening plasticity as well as regularize the localisation of deformation due to softening. It should be noted that all the aforementioned works have been done under the small deformation framework (Engelen et al., 2006; Engelen et al., 2003; Peerlings, 2007; Peerlings et al., 2012). To the best of the authors’ knowledge, no attempt has been made to predict the size effect with the implicit gradient theory developed under the finite deformation framework.

Meanwhile, the thermal effect is an important issue in the gradient-enhanced plasticity model. In the nano/micro systems, the classical continuum theories, i.e. Fourier law used in local thermodynamic equilibrium, are not enough to analyze the system, therefore the other theories on the basis of the non-equilibrium thermodynamics need to be considered with the effect of the temperature and its gradient for the fast transient behaviour. If the mean free path is approximately same to medium size, heat transfer is partly ballistic rather than purely diffusive. This is caused by the small depth of the zone influenced by heat or small size of the structure and the non-equilibrium transition of thermodynamic circumstances related to reducing the response time (Tzou and Zhang, 1995). Moreover, when the response time in nano/micro scale materials decreases to the thermalisation time range, it results in the non-equilibrium conversion of thermodynamics state between phonons and electrons (Brorson et al., 1990; Tzou, 1995; Tzou and Zhang, 1995). The conventional heat equation is not capable of capturing the effect of electron-phonon interaction in this time frame, thus the microscopic generalized heat equation has to be employed to interpret these phenomena.

In the author’s previous works (Voyiadjis and Song, 2017; Voyiadjis et al., 2017), the thermodynamically consistent coupled thermo-mechanical strain gradient plasticity (SGP) models to study the characteristics of nano/micro-scale metallic materials were proposed and solved numerically based on one-dimensional finite element implementation. As is well known, there is bound to be a fundamental difference between one-dimensional finite element implementation and two-dimensional one. For example, in one-dimensional case, some special complications, e.g. the
resonance between the physical scale and mesh scale, cannot be considered during the simulation. It should be noted that there is no difference between the different dimensions from the variational point of view, however, the difference exists in the description of the finite dimensional approximation spaces. The finite element implementation in multi-dimension is based on the same principle of the one in one-dimension, thus the piecewise-polynomial functions of low degree with many terms for the accuracy are considered. In the two-dimensional model, it is significantly complicated since the polynomial functions have more variables, and the open sets are much more varied than in one-dimensional model. In terms of the dimensional extension, there is the simple modification from one-dimensional finite element implementation for the strain gradient plasticity model to the two-dimensional one in Voyiadjis and Song (2017). However, the model in that work was developed based on the small deformation framework, and the effects of temperature and its gradient were not considered. The effect of the mechanical component of thermodynamic microforces were addressed in terms of the stress jump phenomenon. In this chapter, two-dimensional numerical simulation for the finite deformation incorporating the temperature effect is developed based on the implicit gradient-enhanced approach, and the proposed model is applied to the simple shear problem to examine the feasibility of the proposed model for showing the size effect during hardening. The uniaxial tension problem is also solved to explore the characteristics of the proposed model on the mesh sensitivity tests.

**Notation:** Hereafter, the vectors or tensors of any order are denoted by the boldface letter, e.g. \( \mathbf{a} = \{a_i\} \), \( \mathbf{b} = \{b_j\} \), \( \mathbf{A} = \{A_{ij}\} \), and \( \mathbf{B} = \{B_{ij}\} \). The symmetric and antisymmetric parts of a tensor \( \mathbf{A} \) are written by \( \text{sym} \mathbf{A} \) and \( \text{asym} \mathbf{A} \) respectively, the norm of a tensor \( \mathbf{A} \) is written by \( |\mathbf{A}| \), the trace and determinant of a tensor \( \mathbf{A} \) is written respectively by \( \text{tr} \mathbf{A} \) and \( \text{det} \mathbf{A} \). The scalar product between tensors or vectors is denoted with as many dots as the number of contracted index pairs, e.g. \( \mathbf{a} \cdot \mathbf{b} = a_i b_i \) and \( \mathbf{A} : \mathbf{B} = A_{ij} B_{ij} \). The upper dot over a symbol indicates its material time derivative, \( \dot{\mathbf{a}} = \frac{d\mathbf{a}}{dt} \). The symbol \( \nabla \) indicates the spatial gradient operator and \( \nabla^2 \) is the Laplacian operator. A superscript \( T \) indicates a transpose of a tensor.

### 4.2 Theoretical formulation of the proposed model

#### 4.2.1 Kinematics

The homogeneous body \( \mathcal{B} \) in the reference (undeformed), intermediate and current (deformed) states is presented in Figure 4.1. The material point is simply denoted by \( \mathbf{X} \), and its Lagrangian coordinates are denoted by \( X_i \) \( (i = 1, 2, 3) \). The point in the current state is denoted by \( \mathbf{x} \), and its Eulerian coordinates are denoted by \( x_i \) \( (i = 1, 2, 3) \). In this figure, the one to one mapping function \( \mathbf{x} = \mathcal{M}(\mathbf{X}, t) \) is used for defining the velocity \( \mathbf{v} \) and the deformation gradient \( \mathbf{F} \) respectively such as \( v_i = \frac{\partial \mathcal{M}_i(X_i, t)}{\partial t} = \mathcal{M}_i \) and \( F_{ij} = \frac{\partial x_i}{\partial X_j} = \frac{\partial \mathcal{M}_i(X_i, t)}{\partial X_j} \). By assuming that the elastic deformation rotates and stretches the body while the plastic deformation only shears the body, a line vector in the undeformed state \( d\mathbf{X} \) is transformed to the deformed state \( d\mathbf{x} \) after the deformation \( \mathbf{u}(\mathbf{X}) \) through the following multiplicative decomposition\(^{10}\)

\[
    dx_i = \frac{F_{ik}^p F_{kj}}{F_{ij}} dX_j
\]

\(^{10}\) As is standard, the superscripts ‘e’ and ‘p’ are used to express the elastic and plastic states respectively.
where $F$ is the deformation gradient, $F^e$ is the elastic distortion and $F^p$ is the plastic distortion. The implicit function theorem $F$ must be non-singular, that is, the Jacobian determinant $J(X, t) \equiv det F(X, t) \neq 0$. The Jacobian determinant is the property of measuring the ratio between deformed ($\Omega$) and undeformed ($\Omega_0$) infinitesimal volumes, that is,

$$d\Omega = J d\Omega_0$$

(4.2)

where $L^e$ and $L^p$ represent the elastic and plastic distortion rate tensors addressed with the elastic and plastic components of the deformation rate tensor $\mathbf{D}$ and the spin rate tensor $\mathbf{W}$, that is, $L^e = D^e + W^e$ and $L^p = D^p + W^p$. The elastic and plastic parts of $\mathbf{D}$ and $\mathbf{W}$ are given by

$$D^e_{ij} = \text{sym} L^e_{ij}, \quad D^p_{ij} = \text{sym} L^p_{ij}, \quad W^e_{ij} = \text{asym} L^e_{ij}, \quad W^p_{ij} = \text{asym} L^p_{ij}$$

(4.4)

Note that the plastic flow does not induce changes in volume, consistently $det F^p = 1$, and $L^p$ and $D^p$ are deviatoric.

The right polar decomposition of a second-order, non-singular tensor $F^e$ can be obtained by the orthogonal rotation tensor $R^e$ and the symmetric, non-negative definite right stretch tensor $U^e$ as

$$F^e_{ij} = R^e_{ik} U^e_{kj}$$

(4.5)

where $U^e = \sqrt{F^e T F^e}$.

The elastic Cauchy-Green deformation tensor $C^e$ can be given by

$$C^e_{ij} = F^e_{ki} F^e_{kj} = U^e_{ij}$$

(4.6)

A useful quantity, the elastic Green-St. Venant strain $E^e$ (hereinafter referred to as elastic strain in this chapter), is defined using Equation (4.6) as follows:
\[ E_{ij}^e = \frac{1}{2} (C_{ij}^e - \delta_{ij}) = \frac{1}{2} (F_{ki}^e F_{kj}^e - \delta_{ij}) = \frac{1}{2} (U_{ij}^e - \delta_{ij}) \]  

(4.7)

where \( \delta_{ij} \) is the Kronecker delta.

Then, the material time derivative of \( C^e \) can be obtained by differentiating Equation (4.6) as follows:

\[ \dot{C}_{ij}^e = \dot{F}_{ki}^e F_{kj}^e + F_{ki}^e \dot{F}_{kj}^e = 2 \text{sym} \left( F_{ki}^e \dot{F}_{kj}^e \right) = 2 \dot{E}_{ij}^e \]

(4.8)

where \( \dot{E}_{ij}^e \) represents the rate of elastic strain \( E_{ij}^e \).

4.2.2 Nonlocal implicit gradient-enhanced theory

The implicit gradient theory is adopted in this chapter because of its algorithmic efficiency compared to other gradient-enhanced approaches, so-called explicit gradient theory (Engelen et al., 2003). The nonlocal effective plastic strain \( \tilde{\varepsilon}^p \), which indicates a weighted average of the local effective plastic strain \( \varepsilon^p \), is introduced and obtained by following partial differential equation with the material length scale parameter \( l_p \) (see Engelen et al. (2003) for more details):

\[ \tilde{\varepsilon}^p - l_p^2 \nabla^2 \tilde{\varepsilon}^p = \varepsilon^p \]

(4.9)

4.2.3 Coupled thermo-mechanical framework

4.2.3.1 Principle of virtual power

Thermodynamically consistent gradient-enhanced theories with incorporating the thermal effect have been developed by Voyiadjis and co-workers based on the principle of virtual power to investigate the behaviour of small-scale metallic materials (Voyiadjis and Faghihi, 2012; Voyiadjis et al., 2014; Voyiadjis and Song, 2017; Voyiadjis et al., 2017). In this section, the fully coupled thermo-mechanical theory is formulated by considering a nonlocal variable \( \tilde{\varepsilon}_p \) in conjunction with the new forms of the free energy and the dissipation potentials.

The elastic deformation power in the deformed state \( \mathcal{P}_{int}^e \) can be given with the Cauchy stress tensor \( \sigma \) and the deformation rate tensor \( D \) by

\[ \mathcal{P}_{int}^e = \int_{\tilde{\Omega}} \sigma_{ij} D_{ij} d\Omega \]  

(4.10)

Since \( \sigma \) is symmetric, \( \sigma : D = \sigma : \mathbf{L} \). Then, by using Equation (4.2), \( \sigma : \mathbf{L} = tr \sigma \tilde{\mathbf{F}} \mathbf{F}^{-1} = (\sigma \mathbf{F}^{-T}) : \tilde{\mathbf{F}} \). Now, \( \mathcal{P}_{int}^e \) can be expressed alternatively by using Equation (4.2) as follows:

\[ \mathcal{P}_{int}^e = \int_{\tilde{\Omega}} J \sigma_{ik} F_{jk}^{-1} \dot{F}_{ij} d\Omega_0 = \int_{\tilde{\Omega}_0} P_{ij} \dot{F}_{ij} d\Omega_0 \]  

(4.11)

where the non-symmetric first Piola-Kirchhoff stress tensor \( P \) can be obtained by performing a Piola transformation on the symmetric Cauchy stress tensor \( \sigma \). Here, another stress quantity \( \sigma^e \) (hereafter, written as the elastic stress) is defined by relating to \( P \) as follows:

\[ \sigma_{ij}^e \equiv P_{lj} F_{lj}^p \]  

(4.12)

Moreover, the substitution of Equation (4.11) into Equation (4.12) gives the following equation for the elastic stress quantity \( \sigma^e \).

\[ \sigma_{ij}^e = J \sigma_{ik} F_{jk}^{-1} P_{lj}^p = J \sigma_{ik} F_{jk}^{-1} \]

(4.13)

Meanwhile, by using Equations (4.11) and (4.12), the elastic deformation power is
expressed as \( \int_{\Omega_0} \sigma_{ij}^e \dot{F}_{ij} \, d\Omega_0 \). Finally, the internal power \( P_{\text{int}} \) can be written with the energy contributions as follows:

\[
P_{\text{int}} = \int_{\Omega_0} \left( \sigma_{ij}^e \dot{F}_{ij}^e + x \varepsilon^p + q_i \ddot{\varepsilon}^p + Q_i \ddot{\varepsilon}^p_i + A \dddot{T} + B \dddot{T}_i \right) \, d\Omega_0 \tag{4.14}
\]

where \( \Omega_0 \) is an arbitrary subregion of the reference body \( \Omega_0 \), \( \dot{F}^e \) is the elastic distortion rate, \( x \), \( q \) and \( Q \) are the microscopic stresses conjugate to the local effective plastic strain rate \( \ddot{\varepsilon}^p \), nonlocal effective plastic strain rate \( \dddot{\varepsilon}^p \) and the gradient of \( \dddot{\varepsilon}^p \) respectively. The last two terms are related to the thermal effect, in which the generalized stresses \( A \) and \( B \) are conjugate to the temperature rate \( \dddot{T} \) and the gradient of \( \dddot{T} \) respectively.

The external power \( P_{\text{ext}} \) is given with the macro- traction \( \mathbf{t} \) and micro- traction \( \mathbf{m} \) on the external surface \( \partial \Omega_0 \) and the body forces acting within \( \Omega_0 \) as follows:

\[
P_{\text{ext}} = \int_{\Omega_0} \left( \sigma_{ij}^e \dot{F}_{ij}^e \right) \, d\Omega_0 + \int_{\partial \Omega_0} \left( t_i \dot{M}_i + m \ddot{\varepsilon}^p + a \dddot{T} \right) \, dS_0 \tag{4.15}
\]

where \( \dot{M} \) is the generalized external body force conjugate to the macroscopic velocity \( \mathbf{v} = \dot{\mathbf{M}} \). Additionally, the external virtual power is assumed to have the term of \( a \) conjugate to \( \dddot{T} \) for the thermal effect.

Meanwhile, by the assumption of the irrotational plastic flow \( (\mathbf{W}^P = 0) \) and the definition of the mapping function \( \mathbf{M}(\mathbf{X}, t) \), Equation (4.3) can be expressed as

\[
\dot{M}_{i,k} F_{kj}^{-1} = \dot{F}_{ik}^e F_{kj}^{-1} + F_{ik}^e P_{km}^p m_{mj}^{-1} \tag{4.16}
\]

Using the assumption that \( \varepsilon^p \) evolves along the plastic stretch, i.e. \( \dot{\varepsilon}^p = |D_{ij}^p| \) with an initial condition \( \varepsilon^p(\mathbf{X},0) = 0 \) and the definition of the plastic flow direction by \( N_{ij}^p = D_{ij}^p / |D_{ij}^p| \), Equation (4.16) can be expressed as

\[
\dot{M}_{i,k} F_{kj}^{-1} = \dot{F}_{ik}^e F_{kj}^{-1} + \varepsilon^p F_{ik}^e N_{km}^p m_{mj}^{-1} \tag{4.17}
\]

By considering \( \dot{M}, \dot{F}^e, \dot{\varepsilon}^p, \dot{\varepsilon}^p \) and \( \dddot{T} \) as the virtual velocity fields with the variations of \( \delta \dot{M}, \delta \dot{F}^e, \delta \dot{\varepsilon}^p, \delta \dot{\varepsilon}^p \) and \( \delta \dddot{T} \) respectively, the internal and external parts of the virtual power are written from Equations (4.14) and (4.15) as follows:

\[
P_{\text{int}}^v = \int_{\Omega_0} \left( \sigma_{ij}^e \delta F_{ij}^e + x \delta \varepsilon^p + q_i \delta \dot{\varepsilon}^p + Q_i \delta \ddot{\varepsilon}^p_i + A \delta \dddot{T} + B \delta \dddot{T}_i \right) \, d\Omega_0 \tag{4.18}
\]

\[
P_{\text{ext}}^v = \int_{\Omega_0} \left( \sigma_{ij}^e \delta F_{ij}^e \right) \, d\Omega_0 + \int_{\partial \Omega_0} \left( t_i \delta \dot{M}_i + m \delta \ddot{\varepsilon}^p + a \delta \dddot{T} \right) \, dS_0 \tag{4.19}
\]

and Equation (4.17) becomes

\[
\delta \dot{M}_{i,k} F_{kj}^{-1} = \delta \dot{F}_{ik}^e F_{kj}^{-1} + \delta \varepsilon^p F_{ik}^e N_{km}^p m_{mj}^{-1} \tag{4.20}
\]

The following relation is established in an arbitrary subregion \( \Omega_0 \) by the fundamental statement of the principle of virtual power:

\[
P_{\text{int}}^v = P_{\text{ext}}^v \tag{4.21}
\]

4.2.3.2 Objectivity of the internal power

After a change in frame defined by a transformation \( \mathbf{Q} \), the quantities in Equation (4.1) become \( d\mathbf{x}' \), \( \mathbf{F}' \) and \( d\mathbf{X}' \) as follows:
\[ \frac{Q_{ik}dx_k}{
abla x_i} = \frac{Q_{ik}F_{kl}}{r_{il}} dX_l \]  

(4.22)

By definition, \(dX\) remains unchanged after a transformation \(Q\) ( \(dX' = dX\)). From Equation (4.22),

\[ F_{lj}' = Q_{lk}F_{kj} \]  

(4.23)

Using Equation (4.1) one obtains,

\[ F_{ik}'F_{kj}' = Q_{ik}F_{kl}'F_{lj}' \]  

(4.24)

The reference and intermediate states are independent of the changes in frame,

\[ F_{lj}' = Q_{lk}F_{kj} \]  

(4.25)

and \(F^p\) is objective. Differentiating Equation (4.25) gives

\[ \hat{F}_{lj}' = \hat{Q}_{lk}F_{kj} + Q_{lk}\hat{F}_{kj} \]  

(4.26)

Similarly, based on the notion of Gurtin et al. (2010), \(L^p\), \(D^p\), \(U^e\) (hence \(E^e\)) and \(C^e\) are objective under a change in frame. This consequence of frame invariance is reserved for later use.

Now, the internal virtual power \(P_{int}^{\text{vir}}\) is assumed to be invariant and it is further assumed that the virtual fields are converted in an identical way to the corresponding non-virtual fields \(P_{int}^{\text{vir}}\). Therefore one obtains,

\[ P_{int}^{\text{vir}} = P_{int}^{\text{vir}'} \]  

(4.27)

Under a change in frame, \(x, q, A, \delta e^p, \delta e^p\) and \(\delta T\) in Equation (4.18) are invariant because all of these terms are scalar fields. \(\delta e^p, \delta T\) also remain unchanged since they are a gradient of \(\delta e^p\) and \(\delta T\) in the reference state. On the other hand, \(\sigma^e, Q\) and \(B\) are converted to \(\sigma^{e'}, Q'\) and \(B'\) respectively, and using Equation (4.26), \(\delta \mathcal{F}^e\) is converted to

\[ \delta F_{lj}' = \hat{Q}_{lk}F_{kj} + Q_{lk}\delta F_{kj} = Q_{lk}(\hat{Q}_{kl}F_{kj} + \delta F_{kj}) \]  

(4.28)

By taking the aforementioned conditions into consideration, \(P_{int}^{\text{vir}'}\) can be given by

\[ P_{int}^{\text{vir}'} = \int_{\Omega_0} \left( \sigma_{ij}'(\hat{Q}_{lk}F_{kj} + Q_{lk}\delta F_{kj}) + x\delta e^p + q\delta e^p + Q_i'\delta e^p + A_i\delta T \right) \]  

\[ + B_i'\delta T_i \right) d\Omega_0 \]  

(4.29)

Equation (4.27) gives that

\[ \{ \sigma_{ij}'(\hat{Q}_{lk}F_{kj} + Q_{lk}\delta F_{kj}) - \sigma_{ij}'\delta F_{kj} \} + (Q_i' - Q_i)\delta e^p + (B_i' - B_i)\delta T_i = 0 \]  

(4.30)

From the last two terms in the LHS of Equation (4.30), the stress quantities \(Q_i\) and \(B_i\) are invariant. Under the assumption that \(Q\) is an arbitrary time-independent transformation \(Q = 0\), the transformation of \(\sigma^e\) can be obtained by

\[ \sigma_{ij}' = Q_{lk}\sigma_{kj}^e \]  

(4.31)

With the further assumption \(Q = I\), after some algebraic manipulation (see Appendix B), Equation (4.30) gives that

\[ \sigma_{ij}^eF_{jk}'\hat{Q}_{lk} = 0 \]  

(4.32)

which indicates that \(\sigma^eF^eT = F^e\sigma^eT\).

4.2.3.3 Balance equations

By assuming \(\delta e^p = 0\) and \(\delta e^p = 0\), and using the description of the tensor \(P\) given in Equation (4.11), the equations for the local macroscopic surface traction conditions, the balance of the macroscopic linear momentum and the balance of the generalized stresses \(A\) and \(B\) can be
represented respectively as follows:

\[ t_i = P_{ij} n_j \]  \hspace{2cm} (4.33)
\[ P_{ij} + \delta_i = 0 \]  \hspace{2cm} (4.34)
\[ a = B_i n_i \]  \hspace{2cm} (4.35)
\[ B_{il} - \mathcal{A} = 0 \]  \hspace{2cm} (4.36)

where \( n \) is the outward unit normal vector to \( \partial \Omega_0 \).

Next, by assuming \( \delta \mathcal{M} = 0 \), \( \delta \varepsilon^p = 0 \) and \( \delta T = 0 \), and after some algebraic manipulations, the equations for the first microscopic force balance and the nonlocal microscopic traction conditions are given by

\[ Q_{il} - q_l = 0 \]  \hspace{2cm} (4.37)
\[ m = Q_{il} n_i \]  \hspace{2cm} (4.38)

Lastly, by assuming \( \delta \mathcal{M} = 0 \), \( \delta \varepsilon^p = 0 \) and \( \delta T = 0 \), and defining
\[ M^e_{ij} \equiv F_{ik}^e \sigma^e_{kj} \]  \hspace{2cm} (4.39)
\[ \bar{\sigma} \equiv M^e_{ij} N^p_{ij} \]  \hspace{2cm} (4.40)

the second microscopic force balance can be obtained by

\[ x = \bar{\sigma} \]  \hspace{2cm} (4.41)

where \( M^e \) represents the elastic Mandel stress, which is given by

\[ M^e_{ij} = \mathcal{J} F_{kl}^e \sigma^e_{kl} F_{ji}^{e-1} \]  \hspace{2cm} (4.42)

and \( \bar{M}^e \) is the deviatoric part of the Mandel stress, i.e. \( \bar{M}^e_{ij} = M^e_{ij} - M^e_{kk} \delta_{ij} / 3 \). For more details about this section, see Appendix C.

4.2.3.4 Laws of thermodynamics

The first law of thermodynamics is considered here to derive the thermodynamically consistent formulation to account for the rate-independent small-scale behaviour of the metallic volumes during the fast transient process. The adiabatic inelastic deformation for metals is affected by the initial temperature and the evolution of temperature caused by the transition from plastic work to heat. The enhanced gradient theory is employed for the mechanical part of the formulation, whereas the micromorphic model is employed for the thermal part as follows (see the work of Forest and Amestoy (2008)):

\[ \rho \dot{\varepsilon} = \sigma^e_{ij} \dot{f}^e_{ij} + \sigma^p \dot{e}^p + q \dot{e}^p + Q \dot{\varepsilon}^p + \mathcal{A} \dot{T} + B_i \dot{T}_i - q_i + \rho \mathcal{H}_{EXT} \]  \hspace{2cm} (4.43)

where \( e \) is the specific internal energy, \( q \) is the thermal flux vector, and \( \mathcal{H}_{EXT} \) is the specific heat from the external source. \( \rho \) is the mass density.

The second law of thermodynamics introduces the physical base accounting for the distribution of GNDs in the body. The following entropy production inequality can be obtained based on the second law in conjunction with the specific entropy \( s \) and the micromorphic approach by Forest (2009):

\[ -\rho \dot{\varepsilon} + \rho s T + \sigma^e_{ij} \dot{f}^e_{ij} + \sigma^p \dot{e}^p + q \dot{e}^p + Q \dot{\varepsilon}^p + \mathcal{A} \dot{T} + B_i \dot{T}_i - q_i + \frac{T_i}{T} \geq 0 \]  \hspace{2cm} (4.44)

By following Coleman and Noll (1963), the entropy production vector in this chapter is assumed to be equal to the thermal flux vector divided by the temperature.

4.2.4 Energetic and dissipative thermodynamic forces
By taking the time derivative of the Helmholtz free energy (per unit volume), defined as \( \Psi = e - T s \), and equating it into Equation (4.44), the following Clausius-Duhem inequality can be derived.

\[
\sigma_{ij}^e \dot{F}_{ij}^e + x \dot{e}^p + q_i \dot{e}_i^p + Q_i \dot{e}_i^p + \mathcal{A} \dot{T} + \mathcal{B}_i \dot{J}_i - \rho \dot{\Psi} - \rho s \dot{T} - q_i \frac{J_i}{T} \geq 0
\]  
(4.45)

From Equations (4.26) and (4.31), it is evident that both \( \sigma^e \) and \( \dot{F}^e \) are not objective under a change in frame. Thus, the elastic stress power is most conveniently represented through the objective elastic stress rate \( \dot{E}^e \) (Gurtin et al., 2010). To accompany this, the second Piola-Kirchhoff elastic stress \( \textbf{P}^e \) is defined such as

\[
\text{\( P_{ij}^e \equiv JF_{ik}^{e-1} \sigma_{kl}^e F_{lj}^{e-1} \)}
\]  
(4.46)

Accordingly, by Equation (4.13), \( \textbf{P}^e \) can be expressed with \( \sigma^e \) as

\[
\text{\( P_{ij}^e = F_{ik}^{e-1} \sigma_{kj}^e \)}
\]  
(4.47)

Note that by using the definitions of \( \textbf{M}^e \) and \( \textbf{P}^e \) given respectively in Equations (4.42) and (4.46), the relationship between \( \textbf{M}^e \) and \( \textbf{P}^e \) can be obtained by

\[
M_{ij}^e = C_{ik}^e P_{kj}^e
\]  
(4.48)

Equations (4.25), (4.31), (4.32) and (4.47) yield that \( \textbf{P}^e \) is symmetric and objective under a change in frame. Finally, the elastic stress power \( \sigma^e : \dot{\textbf{F}}^e \) can be converted to the new form with the objective tensors \( \textbf{P}^e \) and \( \dot{\textbf{E}}^e \) as follows:

\[
\sigma_{ij}^e \dot{F}_{ij}^e = F_{ik}^e P_{kj}^e \dot{F}_{ij}^e = P_{ij}^e (F_{ik}^e \dot{F}_{kj}^e) = P_{ij}^e \dot{E}_{ij}^e
\]  
(4.49)

Substituting Equation (4.49) into Equation (4.45) gives that

\[
P_{ij}^e \dot{E}_{ij}^e + x \dot{e}^p + q_i \dot{e}_i^p + Q_i \dot{e}_i^p + \mathcal{A} \dot{T} + \mathcal{B}_i \dot{J}_i - \rho \dot{\Psi} - \rho s \dot{T} - q_i \frac{J_i}{T} \geq 0
\]  
(4.50)

Meanwhile, the Helmholtz free energy function in this chapter is required to be smooth with respect to \( E_{ij}^e, e^p, e^p, e_i^p, T \) and \( J_i \) to explain the effect of non-uniform microdefects distribution in company with the temperature on the homogenized material response.

\[
\Psi = \Psi(E_{ij}^e, e^p, e_i^p, e_i^p, T, J_i)
\]  
(4.51)

In the process of developing the constitutive equations, the plastic dissipation work must be non-negative. By using Equations (4.50) and (4.51), one can obtain the following inequality:

\[
\left( P_{ij}^e - \rho \frac{\partial \Psi}{\partial E_{ij}^e} \right) \dot{E}_{ij}^e + \left( x - \rho \frac{\partial \Psi}{\partial e^p} \right) \dot{e}^p + \left( q_i - \rho \frac{\partial \Psi}{\partial e_i^p} \right) \dot{e}_i^p + \left( Q_i - \rho \frac{\partial \Psi}{\partial e_i^p} \right) \dot{e}_i^p
\]  
(4.52)

\[
+ \left( A - \rho s - \rho \frac{\partial \Psi}{\partial T} \right) \dot{T} + \left( B_i - \rho \frac{\partial \Psi}{\partial J_i} \right) \dot{J}_i - q_i \frac{J_i}{T} \geq 0
\]

One now assumes that the thermodynamic conjugate microstress quantities \( x, q_i, Q_i \) and \( A \) are decomposed into the energetic and the dissipative components as follows (Voyiadjis and Deliktas, 2009b; Voyiadjis and Faghihi, 2012):

\[
x = x_e^{en} + x_e^{dis}; \quad q_i = q_i^{en} + q_i^{dis}; \quad Q_i = Q_i^{en} + Q_i^{dis}; \quad A = A^{en} + A^{dis}
\]  
(4.53)

By using Equations (4.52) and (4.53), the energetic microstresses are defined as follows:

\[
P_{ij}^e = \rho \frac{\partial \Psi}{\partial E_{ij}^e}; \quad x_e^{en} = \rho \frac{\partial \Psi}{\partial e^p}; \quad q_i^{en} = \rho \frac{\partial \Psi}{\partial e_i^p}; \quad Q_i^{en} = \rho \frac{\partial \Psi}{\partial e_i^p}; \quad A^{en}
\]  
(4.54)

\[\text{\( B_i \) is assumed to be strictly energetic in this work.}\]
The dissipation density per unit time $\mathcal{D}$ is then obtained as
\[ \mathcal{D} = x^{dis} \dot{\varepsilon}^p + q_i^{dis} \dot{\varepsilon}^p + Q_i^{dis} \dot{\varepsilon}^p + \mathcal{A}^{dis} \dot{T} - \frac{q_i}{T} T_i \geq 0 \] (4.55)

The dissipative counterparts of the thermodynamic microstresses are obtained from the dissipation potential $\mathcal{D} = \mathcal{D}(\dot{\varepsilon}^p, \dot{\varepsilon}^p, \dot{T}, T_i)$ as follows:
\[ x^{dis} = \frac{\partial \mathcal{D}}{\partial \varepsilon^p}; \quad q_i^{dis} = \frac{\partial \mathcal{D}}{\partial \varepsilon^p}; \quad Q_i^{dis} = \frac{\partial \mathcal{D}}{\partial \dot{\varepsilon}^p}; \quad \mathcal{A}^{dis} = \frac{\partial \mathcal{D}}{\partial \dot{T}}; \quad -\frac{q_i}{T} T_i = \frac{\partial \mathcal{D}}{\partial T_i} \] (4.56)

4.2.5 Helmholtz free energy and energetic thermodynamic forces

The free energy per unit volume is put forward with three main counterparts, i.e., elastic energy $\Psi^e$, defect energy $\Psi^d$, and thermal energy $\Psi^T$ as follows:
\[ \Psi(\varepsilon^e, \varepsilon^p, \varepsilon^p, \varepsilon^p, \varepsilon^p, \varepsilon^p, T, T_i) = \Psi^e(\varepsilon^e, T) + \Psi^d(\varepsilon^e, \varepsilon^p, \varepsilon^p, T) + \Psi^T(T, T_i) \] (4.57)

4.2.5.1 Elastic free energy

The constitutive equations take a special form when the continuum is isotropic in the undeformed state. In such a case, the elastic free energy density function $\Psi^e$ depends on $\varepsilon^e$ through a set of the principal invariants of $\varepsilon^e$ such as
\[ \Psi^e = \bar{\Psi}^e(I, II, III, T) = \bar{\Psi}^e(\lambda_1^e, \lambda_2^e, \lambda_3^e, T) = \bar{\Psi}^e(E_1^e, E_2^e, E_3^e, T) \] (4.58)

where $\lambda_\alpha^e$ and $E_\alpha^e$ ($\alpha = 1, 2, 3$) indicate the positive eigenvalues of $U^e$ and $E^e$ respectively, and the invariants $I$, $II$ and $III$ are given by
\[ I = \text{tr} C^e = C_{kk}^e \]
\[ II = \frac{1}{2} \left[ (\text{tr} C^e)^2 - \text{tr} C^e \right] = \frac{1}{2} \left[ C_{ii}^e C_{jj}^e - C_{ij}^e C_{ji}^e \right] \]
\[ III = \det C^e = \frac{1}{6} \epsilon_{ijk} \epsilon_{lmn} C_{il}^e C_{jm}^e C_{kn}^e \] (4.59)

The spectral decompositions of $\varepsilon^e$ and $U^e$ are given by
\[ \varepsilon^e = \sum_{\alpha=1}^{3} \lambda_\alpha^e N_\alpha^e \otimes N_\alpha^e \] (4.60)
\[ U^e = \sum_{\alpha=1}^{3} \lambda_\alpha^e N_\alpha^e \otimes N_\alpha^e \] (4.61)

where $N_\alpha^e$ ($\alpha = 1, 2, 3$) are the orthonormal eigenvectors of $C^e$.

Applying the chain rule to Equation (4.54) gives $P^e$ as
\[ P^e = \rho \frac{\partial \Psi^e}{\partial \varepsilon^e} = \rho \sum_{\alpha=1}^{3} \frac{\partial \bar{\Psi}^e(\lambda_1^e, \lambda_2^e, \lambda_3^e, T)}{\partial \lambda_\alpha^e} \frac{\partial \lambda_\alpha^e}{\partial \varepsilon^e} \] (4.62)

Using the relation $\varepsilon^e = 2E^e + I$ and the derivatives of the stretch $\lambda_\alpha^e$ with respect to $C^e$, i.e., $\partial \lambda_\alpha^e / \partial C^e = (1/2 \lambda_\alpha^e) N_\alpha^e \otimes N_\alpha^e$, Equation (4.62) becomes
\[ P^e = 2\rho \sum_{\alpha=1}^{3} \frac{\partial \bar{\Psi}^e(\lambda_1^e, \lambda_2^e, \lambda_3^e, T)}{\partial \lambda_\alpha^e} \frac{\partial \lambda_\alpha^e}{\partial \varepsilon^e} = \rho \sum_{\alpha=1}^{3} \frac{1}{\lambda_\alpha^e} \frac{\partial \bar{\Psi}^e(\lambda_1^e, \lambda_2^e, \lambda_3^e, T)}{\partial \lambda_\alpha^e} N_\alpha^e \otimes N_\alpha^e \] (4.63)

Next, substituting Equations (4.60) and (4.63) into Equation (4.48) gives the following equation of the elastic Mandel stress.
\[
M^e = \rho \sum_{\alpha=1}^{3} \lambda^e_{\alpha} \frac{\partial \Psi^e}{\partial \lambda^e_{\alpha}} N^e_{\alpha} \otimes N^e_{\alpha}
\]  

(4.64)

The definition of elastic strain \(E^e\) is given in the logarithmic form as follows:

\[
E^e = \ln U^e = \sum_{\alpha=1}^{3} E^e_{\alpha} N^e_{\alpha} \otimes N^e_{\alpha}
\]

(4.65)

where \(E^e_{\alpha}\) is related to \(\lambda^e_{\alpha}\) as follows:

\[
E^e_{\alpha} = \ln \lambda^e_{\alpha} \ (\alpha = 1, 2, 3)
\]

(4.66)

From Equation (4.64) one obtains,

\[
M^e = \rho \sum_{\alpha=1}^{3} \frac{\partial \Psi^e}{\partial E^e_{\alpha}} N^e_{\alpha} \otimes N^e_{\alpha}
\]

(4.67)

The quadratic form of the classical isotropic elastic strain energy function as discussed by Anand (1986) is considered below in conjunction with the linear coupled thermo-elastic free energy:

\[
\Psi^e (E^e, T) = \frac{\mu}{\rho} |E^e|^2 + \frac{\kappa}{2\rho} (tr E^e)^2 - \frac{\kappa \alpha^{th}}{\rho} (T - T_r) tr E^e
\]

(4.68)

where \(E^e\) is the deviatoric elastic strain, i.e. \(E^e_{ij} = E^e_{ij} - E^e_{kk} \delta_{ij}/3\), \(T_r\) is the reference temperature, \(\alpha^{th}\) is the thermal expansion coefficient, and \(\mu > 0\) and \(\kappa > 0\) are the shear and bulk moduli respectively.

The substitution of Equation (4.68) into Equation (4.67) gives the elastic Mandel stress as follows:

\[
M^e = 2\mu |E^e| + \kappa (tr E^e) I - \kappa \alpha^{th} (T - T_r) I
\]

(4.69)

where \(I\) is the identity tensor.

4.2.5.2 Defect free energy

The coupled thermo-elastic free energy \(\Psi^d\) is put forward in terms of the generalized strain quantity \(\bar{\varepsilon}^p = (\varepsilon^p - \bar{\varepsilon}^p)\), hence combines the macro- and micromorphic variables (Forest, 2009). For incorporating the effect of the material length scale in the isotropic gradient plasticity model, another contribution to the defect free energy is additionally put forward as the quadratic functions of \(\varepsilon^p\) and \(\varepsilon^p_{,i}\) as follows:

\[
\Psi^d (\bar{\varepsilon}^p = (\varepsilon^p - \bar{\varepsilon}^p), \varepsilon^p_{,i}, T) = \frac{h_{en}}{2\rho} \bar{\varepsilon}^p 2\left(1 - \left(\frac{T}{T_y}\right)^n\right) + \frac{\mu l_p^2 \varepsilon^p \varepsilon^p_{,i}}{2\rho}
\]

(4.70)

where \(h_{en}\) is the material parameter related to the nonlocal energetic contribution to the flow resistance, \(l_p\) is the plastic material length scale parameter and \(n\) and \(T_y\) are the thermal material parameters.

By substituting Equation (4.70) into Equation (4.54), the energetic thermodynamic microstress quantites \(x^{en}\), \(q^{en}\), and \(Q^{en}_l\) can be obtained as follows:

\[
x^{en} = h_{en} \bar{\varepsilon}^p \left(1 - \left(\frac{T}{T_y}\right)^n\right)
\]

(4.71)

\[
q^{en} = -h_{en} \bar{\varepsilon}^p \left(1 - \left(\frac{T}{T_y}\right)^n\right)
\]

(4.72)
\[ Q_i^{en} = \mu l_P^2 \varepsilon_i^p \] (4.73)

4.2.5.3 Thermal free energy

The purely thermal part of the free energy is given by

\[ \Psi^T(T_i, T_{ij}) = -\frac{1}{2\rho} \left[ \frac{c_e}{T_r} (T - T_r)^2 + a T_{ij} T_{ij} \right] \] (4.74)

where \( c_e \) denotes the specific heat capacity at constant stress. The material constant \( a \) accounts for the interaction between energy carriers such as phonon-electron.

The thermodynamic forces \( \mathcal{A}^{en} \) and \( \mathcal{B}_i \) can be obtained using the definitions in Equation (4.54) along with the free energy density functions given in Equations (4.68), (4.70) and (4.74) as follows,

\[ \mathcal{A}^{en} = \rho \mathcal{S} - \kappa \alpha^th (T - T_r) tr E^p - \frac{h_{en} \dot{\varepsilon}_p^p n}{2} \left( \frac{T}{T_y} \right)^{n-1} - \frac{c_e}{T_y} (T - T_r) \] (4.75)

\[ \mathcal{B}_i = -a T_{ij} \] (4.76)

4.2.6 Dissipation potential and dissipative thermodynamic forces

It is assumed here that the dissipation potential function is composed of two parts, the mechanical part which is dependent on the plastic strain and plastic strain gradient, and the thermal counterpart which shows the purely thermal effect such as the heat conduction. Additionally, by following the statement by Gurtin and Anand (2009) in terms of Aifantis-type formulation that the origin of the nonlocal term in the yield condition of Aifantis (1984, 1987) can be justified only if it is energetic, and not dissipative, the following functional form of the dissipation potential density per unit time is put forward with the assumption \( q^{dis} = Q_i^{dis} = 0 \).

\[ \mathcal{D}(\dot{\varepsilon}_p^p, \dot{T}_i, T_{ij}) = \left[ \sigma_y(T) + \left( \sigma_y^\xi(T) - \sigma_y^0(T) \right) \left( 1 - e^{-\varphi_1 \varepsilon^p} \right) + \mathcal{H}(T) \varepsilon^p \right. \\
+ h_{dis} \dot{\varepsilon}_p^p \left( 1 - \left( \frac{T}{T_r} \right)^n \right) \left( 1 - \frac{m}{2} \dot{T}_i^2 - \frac{k(T)}{T} T_{ij} T_{ij} \right) \geq 0 \] (4.77)

where \( h_{dis} \) is the material constant for the nonlocal dissipative contribution to the flow resistance, \( m \) is the material constant for the energy exchange between phonon and electron, \( k(T) \) is the thermal conductivity coefficient, and \( \varphi_1 \) is the material parameter. The temperature dependent material parameters \( \sigma_y^0(T) > 0 \), \( \sigma_y^\xi(T) \geq \sigma_y^0 \) and \( \mathcal{H}(T) \geq 0 \) are defined as

\[ \sigma_y^0(T) = \sigma_y^0 \left[ 1 - \theta_0 (T - T_r) \right] \] (4.78)

\[ \sigma_y^\xi(T) = \sigma_y^\xi \left[ 1 - \theta_{\varphi_1} (T - T_r) \right] \] (4.79)

\[ \mathcal{H}(T) = \mathcal{H} \left[ 1 - \theta_{\mathcal{H}} (T - T_r) \right] \] (4.80)

as outlined in Simo and Miehe (1992), where \( \theta_0 \) is the flow stress softening parameter and \( \theta_{\varphi_1} \) is the hardening/softening parameter.

Using Equation (4.77) along with Equations (4.56) and (4.78)-(4.80), and the assumption \( k(T)/T = k_0 = constant \), the dissipative thermodynamic microstress quantities are obtained as

\[ x^{dis} = \left[ \sigma_y^\xi (\varepsilon^p, T) + h_{dis} \varepsilon^p \right] \left( 1 - \left( \frac{T}{T_y} \right)^n \right) \geq 0 \] (4.81)

\[ \mathcal{A}^{dis} = -m \dot{T}_i \] (4.82)

\[ q_i = k_0 T_i T_{ij} \] (4.83)
with
\[ \sigma^v_\gamma (\varepsilon^p, \mathcal{T}) = \sigma^0_\gamma (\mathcal{T}) \left( \sigma^\varepsilon_\gamma (\mathcal{T}) - \sigma^p_\gamma (\mathcal{T}) \right) \left( 1 - e^{-\varphi_1 \varepsilon^p} \right) + \mathcal{H} (\mathcal{T}) \varepsilon^p \] (4.84)

4.2.7 Thermo-mechanical coupled heat equation

Heat flow is controlled by the first law of thermodynamics, i.e. the energy conservation law, given in Equation (4.43). The temperature field is governed by the heat flow generated through the inelastic dissipation and thermo-mechanical coupling effect. By considering the law of energy conservation given in Equation (4.43) along with the dissipation potential given in Equations (4.55) and (4.77) in conjunction with the equations for the energetic and dissipative components of the thermodynamics microforces given respectively by Equation (4.54) and Equation (4.56), the relationship for the evolution of the entropy, which describes the irreversible process, can be derived as follows:
\[ \rho \dot{s} \mathcal{T} = \mathcal{D} + \rho \mathcal{H}_{ext} \] (4.85)

By using Equation (4.75) for solving the rate of the entropy \( \dot{s} \) and assuming the specific heat capacity at the constant volume \( c_v = \text{constant} \equiv (c_e \mathcal{T} / \mathcal{T}_r) \), the temperature evolution can be obtained as follows:
\[ c_v \dot{\mathcal{T}} = x^\text{dis} \dot{\varepsilon}^p - \dot{\mathcal{A}} \mathcal{T} - \kappa \alpha^\text{th} \text{tr} \mathbf{E}^e \mathbf{f} \mathcal{T} - \frac{m}{2} \dot{\mathcal{J}}^2 - \frac{1}{2} \frac{k(\mathcal{T})}{\mathcal{T}} \mathcal{T}_i \mathcal{T}_l + \rho \mathcal{H}_{ext} \] (4.86)

with
\[ \dot{\mathcal{A}} = \dot{\mathcal{A}}^en + h_{en} \varepsilon^p \frac{n}{\mathcal{T}_y} \left( \frac{\mathcal{T}}{\mathcal{T}_y} \right)^{n-1} \dot{\varepsilon}^p + \frac{h_{en} \varepsilon^p}{2(n-1)} \frac{n}{\mathcal{T}_y} \left( \frac{\mathcal{T}}{\mathcal{T}_y} \right)^{n-2} \dot{\mathcal{J}} \] (4.87)

As can be seen in Equation (4.86), the temperature evolution involves the rate of change in energy caused by the irreversible mechanical process, thermo-plastic coupling, thermo-elastic coupling, heat conduction, and the external heat source. By substituting the constitutive equations of the dissipative micro forces into Equation (4.86) and using the assumption that the external heat source is absent, the temperature evolution is consequently obtained as
\[
\begin{align*}
\left[ c_v + \frac{m}{2} \dot{\mathcal{J}} + \kappa \alpha^{th} \text{tr} \mathbf{E}^e \mathcal{T} + \frac{h_{en} \varepsilon^p}{2(n-1)} \frac{n}{\mathcal{T}_y} \left( \frac{\mathcal{T}}{\mathcal{T}_y} \right)^{n-2} \right] \dot{\mathcal{J}} & \\
= \left[ \sigma^0_\gamma (\mathcal{T}) + (\sigma^\varepsilon_\gamma (\mathcal{T}) - \sigma^p_\gamma (\mathcal{T})) \left( 1 - e^{-\varphi_1 \varepsilon^p} \right) + \mathcal{H} (\mathcal{T}) \varepsilon^p \right. \\
+ h_{dis} \varepsilon^p \left. \right( 1 - \left( \frac{\mathcal{T}}{\mathcal{T}_y} \right)^n \right) \dot{\varepsilon}^p - \left( \dot{\mathcal{A}}^en + h_{en} \varepsilon^p \frac{n}{\mathcal{T}_y} \left( \frac{\mathcal{T}}{\mathcal{T}_y} \right)^{n-1} \dot{\varepsilon}^p \right) \mathcal{T} - \frac{1}{2} \frac{k(\mathcal{T})}{\mathcal{T}} \mathcal{T}_i \mathcal{T}_l
\end{align*}
\] (4.88)

4.2.8 Yield function

In general, the implicit gradient theory is well known for its computational strength since the nonlocal operator is not required in this theory as mentioned earlier. However, it is revealed by Engelen et al. (2006) that the implicit gradient theory cannot predict the size effect behaviour in the strain hardening regime. Peerlings et al. (2012) proposed the implicit gradient plasticity damage theory which is able in describing the size effect during strain hardening as well as regularising the localisation of plastic deformation during strain softening by combining the
authors’ earlier work on implicit plasticity and damage theories for strain hardening and softening. 

Thus, the following yield criterion is adopted in this chapter based on Peerlings et al. (2012):

\[ f = \bar{\sigma} - \left(1 - \emptyset\right)\left[\sigma_0^\gamma(T) + \left(\sigma_0^\gamma(T) - \sigma_0^\beta(T)\right)\left(1 - e^{-\varphi_1 \varepsilon^p}\right) + H(T) \varepsilon^p\right]
+ h_{dis} \varepsilon^p\right]\left(1 - \left(\frac{T}{T_0}\right)^{n_u}\right) \]  

(4.89)

where \(\emptyset\) is the damage variable which is given by \(\emptyset = 1 - e^{-\varphi_2 \varepsilon^p}\) with the material parameter \(\varphi_2\). The softening theory without any gradient effect in hardening can be retrieved by setting \(h_{dis} = 0\), and the deformation is fully localised on the complete failure (\(\emptyset = 1\)).

4.3 Finite element implementation

The finite element (FE) analysis for the proposed strain gradient plasticity theory is performed with the two in-plane displacement fields \((u_1, u_2)\) and the nonlocal effective plastic strain field \(\varepsilon^p\) as independently discretized nodal degrees of freedom via the commercial FE package ABAQUS/standard (2012). The 2D plane strain problems are then solved to evaluate the capability of showing the size effects during hardening and the strain localisation during softening. The increments in nodal displacements and nodal effective plastic strain can be computed by solving the global system of linear equations given in Equation (4.90) based on Newton-Raphson iterations.

\[
\begin{bmatrix}
K_{uu}^{el} & K_{u\varepsilon^p}^{el} \\
K_{\varepsilon^p u}^{el} & K_{\varepsilon^p \varepsilon^p}^{el}
\end{bmatrix}
\begin{bmatrix}
\Delta U_u^\xi \\
\Delta \varepsilon_p^\xi
\end{bmatrix}
= 
\begin{bmatrix}
(\mathcal{R}_u)^\xi \\
(\mathcal{R}_{\varepsilon^p})^\xi
\end{bmatrix}
\]  

(4.90)

where \(K^{el}\) is the Jacobian matrix, and \(U_u^\xi, \varepsilon_p^\xi\) and \((\mathcal{R}_u)^\xi, (\mathcal{R}_{\varepsilon^p})^\xi\) are the nodal values and the nodal residuals of the displacement and the plastic strain at node \(\xi\) respectively.

Meanwhile, when solving the finite deformation plasticity problem within the context of finite element method, the choice of the stress rate is important since the requirement of the material objectivity must be met. In this chapter, the Jaumann objective stress rate is employed for the stress update since it is relatively simple from a computational viewpoint.

4.4 Numerical examples

The simple shear problem of the infinitely long plate is firstly solved in this section to investigate the capacity of the proposed nonlocal implicit gradient approach for predicting the size effect during strain hardening regime. The simple tension problem of the rectangular plate is then solved to show the mesh-insensitive responses of the proposed model on the strain localisation during strain softening regime.

4.4.1 Microscopic boundary condition

In the implicit gradient-enhanced approaches, the additional boundary conditions for \(\varepsilon^p\) are needed only on the exterior surface region of the body to solve the partial differential equation, Equation (4.9). This is in contrast with the explicit gradient-enhanced approach which requires such additional boundary conditions on the elastic-plastic boundary. These boundary conditions
are typically applied to the prescribed subsurface in terms of either the normal derivative of $\bar{\varepsilon}^p$ or $\bar{\varepsilon}^p$ itself as introduced by Engelen et al. (2003). Forest (2009) showed, in the micromorphic approach, that Equation (4.9) can be considered as the nonstandard additional force balance. The following equation is taken to be the micro-free boundary condition on a prescribed subsurface in this chapter

$$\bar{\varepsilon}^p_i n_i = 0 \quad (4.91)$$

or equivalently, in terms of the traction condition,

$$Q_i n_i = 0 \quad (4.92)$$

The other condition on $\bar{\varepsilon}^p$, which is called the micro-hard boundary condition, is given as follows:

$$\bar{\varepsilon}^p = 0 \quad (4.93)$$

It is worth mentioning that these boundary conditions have been commonly used in many works for solving Equation (4.9), e.g. see Anand et al. (2012) and Peerlings et al. (2012).

### 4.4.2 Size effect

Hereafter, the conventional implicit gradient theory which has been proven that is unable to capture the size effect is referred to as CIGT, and the revised version of implicit gradient theory is referred to as RIGT for convenience. The schematic illustration of an infinitely long plate geometry, the initial conditions, and the macroscopic and microscopic boundary conditions under the simple shear is shown in Figure 4.2. The parameter $u^\dagger(t)$ at the top edge represents the prescribed displacement in the $x_1$ direction at time $t$ which increases monotonically, and eventually causes an average shear strain $\gamma = u^\dagger/L$. It is further assumed that the displacements do not occur toward the $x_1$ and $x_2$ directions at the bottom edge, i.e. $u_1(x_1, 0, t) = 0$ and $u_2(x_1, 0, t) = 0$, and $x_2$ direction at the top edge, $u_2(x_1, L, t) = 0$. The material properties for these simulations are provided in Table 4.1. The values for these material properties are taken from the previous work of the author (Voyiadjis and Song, 2017), and the literature (Anand et al., 2012; Simo and Miehe, 1992). Note that the value of $h_{dis}$ is assumed to be much larger than the one of $h_{en}$ in this chapter since it is widely accepted that the plastic deformation is largely a dissipative process. This issue is also discussed in Anand et al. (2012) with regard to the energetic and dissipative contributions to the strain hardening. The C$^0$-continuous interpolation functions are employed for the displacement and nonlocal effective plastic strain fields.
Figure 4.2. The schematic illustration of the simple shear problem including the geometry, macroscopic and microscopic boundary conditions, and initial conditions.

Table 4.1. Material properties used for the numerical simulations (Size effect)

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Units</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu$ Shear modulus</td>
<td>Pa</td>
<td>70.0E9</td>
</tr>
<tr>
<td>$\kappa$ Bulk modulus</td>
<td>Pa</td>
<td>150.0E9</td>
</tr>
<tr>
<td>$\rho$ Density</td>
<td>$g \cdot cm^{-3}$</td>
<td>8.902</td>
</tr>
<tr>
<td>$h_{\text{en}}$ Energetic flow resistance parameter</td>
<td>Pa</td>
<td>1.0E0</td>
</tr>
<tr>
<td>$h_{\text{dis}}$ Dissipative flow resistance parameter</td>
<td>Pa</td>
<td>5.0E9</td>
</tr>
<tr>
<td>$\sigma_y^0$ Initial yield strength for hardening/softening function</td>
<td>Pa</td>
<td>200.0E6</td>
</tr>
<tr>
<td>$\sigma_y^s$ Initial strain hardening parameter for hardening/softening function</td>
<td>Pa</td>
<td>1000.0E6</td>
</tr>
<tr>
<td>$\mathcal{H}$ Initial strain softening parameter for hardening/softening function</td>
<td>Pa</td>
<td>1.0E9</td>
</tr>
<tr>
<td>$\varphi_1$ Material parameter for hardening/softening function</td>
<td>—</td>
<td>20.0</td>
</tr>
<tr>
<td>$\varphi_2$ Material parameter for damage variable</td>
<td>—</td>
<td>20.0</td>
</tr>
<tr>
<td>$\alpha^{th}$ Thermal expansion coefficient</td>
<td>$\mu m/m \cdot K$</td>
<td>16.4</td>
</tr>
<tr>
<td>$T_r$ Reference temperature</td>
<td>$K$</td>
<td>298</td>
</tr>
<tr>
<td>$n$ Temperature sensitivity parameter</td>
<td>—</td>
<td>0.7</td>
</tr>
<tr>
<td>$T_y$ Thermal material parameter</td>
<td>$K$</td>
<td>1,358</td>
</tr>
<tr>
<td>$c_s$ Specific heat capacity at constant stress</td>
<td>$J/g \cdot K$</td>
<td>0.385</td>
</tr>
<tr>
<td>$\theta_0$ Flow stress softening parameter</td>
<td>$K^{-1}$</td>
<td>0.002</td>
</tr>
<tr>
<td>$\theta_{\mathcal{H}}$ Hardening/softening parameter</td>
<td>$K^{-1}$</td>
<td>0.002</td>
</tr>
</tbody>
</table>

The three different normalised material length scale parameters $l_p/L = 0.25$, 0.5 and 1.0
are used for these numerical simulations. An increase in these normalised parameters means a decrease of the height of the shear plate. The micro-free boundary condition given in Equation (4.91) is applied to the external surface for CIGT, on the other hand, the micro-hard boundary condition given in Equation (4.93) is applied for RIGT. The direct comparison between CIGT and RIGT is given in Figure 4.3 in terms of the stress-strain behaviours. As it is shown in Figure 4.3. (a), no size effect is observed in CIGT with varying normalised material length scales as expected. In Figure 4.3. (b), on the other hand, strain hardenings is more pronounced as the dimensions of the shear plate height are reduced. In other words, the significant size effect phenomena, the “smaller is stronger” trend, is observed in RIGT during strain hardening. This result is in contrast with the generally accepted idea that the size effect is unable to be captured by using the implicit gradient approach (Anand et al., 2012; Engelen et al., 2006), but is in agreement with Peerlings et al. (2012).

Figure 4.3. The comparison between the conventional implicit gradient theory (CIGT) and revised implicit gradient theory (RIGT) on the stress-strain responses: (a) CIGT and (b) RIGT (plastic material length scale \( l_p/L = 0.25, 0.5 \) and 1.0).

Figure 4.4. Figure 4.5 and Figure 4.6 show the distributions of the local effective plastic strain \( \varepsilon^p \), nonlocal effective plastic strain \( \bar{\varepsilon}^p \), and the difference between those two plastic strain measures \( \bar{\varepsilon}^p = \varepsilon^p - \bar{\varepsilon}^p \) along the height of the plate respectively with varying normalised material length scale parameters \( l_p/L \) for both CIGT and RIGT. The essential boundary conditions \( \bar{\varepsilon}^p = 0 \) at the top and bottom edges for RIGT are well observed in Figure 4.5. (b) as expected. In RIGT, the non-uniform plastic strain measures (\( \varepsilon^p \) and \( \bar{\varepsilon}^p \)) are present as shown in Figure 4.4. (b) and Figure 4.5. (b), and the differences between \( \varepsilon^p \) and \( \bar{\varepsilon}^p \) become larger as \( l_p/L \) increase (Figure 4.6. (b)). On the other hand, in CIGT, \( \varepsilon^p \) and \( \bar{\varepsilon}^p \) are uniformly distributed across the plate with the same value because of the unrestricted plastic flow at the boundaries, correspondingly \( \bar{\varepsilon}^p \) vanishes for all different values of \( l_p/L \) as shown in Figure 4.6. (a). From this results and Equation (4.9), the second gradient of \( \varepsilon^p \), which is typically used in the explicit gradient approach, can be obtained approximately with \( \bar{\varepsilon}^p \) and the material length scale. Consequentially the size effect cannot be captured in CIGT due to vanishing of \( \bar{\varepsilon}^p \).

Meanwhile, non-vanishing \( \bar{\varepsilon}^p \), which arises from the micro-hard boundary condition on \( \varepsilon^p \), gives rise to the additional hardening in RIGT in combination with the hardening parameter.
as shown in Equation (4.89). The magnitude of this hardening is dependent on $l_p/L$, consequently results in the size dependent behaviour in the material. The size effect observed in Figure 4.3. (b) is obviously generated by the different levels of $\bar{\varepsilon}^p$ with varying normalised plastic material length scale $l_p$ as shown in Figure 4.6. (b).

Figure 4.4. The distributions of the local effective plastic strain $\varepsilon^p$ across the height of the plate with varying plastic material length scale $l_p/L = 0.25$, 0.5 and 1.0: (a) CIGT and (b) RIGT.

Figure 4.5. The distributions of the nonlocal effective plastic strain $\bar{\varepsilon}^p$ across the height of the plate with varying plastic material length scale $l_p/L = 0.25$, 0.5 and 1.0: (a) CIGT and (b) RIGT.
Figure 4.6. The distributions of the difference between the local and nonlocal plastic strain measures \( \varepsilon^p - \bar{\varepsilon}^p \) across the height of the plate with varying plastic material length scale \( l_p/L = 0.25, 0.5 \) and 1.0: (a) CIGT and (b) RIGT.

The distributions of the temperature along the height of the plate for CIGT and RIGT are presented in Figure 4.7. The material length scale \( l_p \) is not involved directly in the temperature evolution as shown in Equation (4.88). However \( l_p \) has an effect on the temperature evolution in an indirect way since it affects the profiles of \( \varepsilon^p \) and \( \bar{\varepsilon}^p \), and the levels of \( \bar{\varepsilon}^p \). Consequently, the size dependent responses on the temperature profiles are shown in RIGT, whereas no size dependent response is observed in CIGT.

Figure 4.7. The distributions of the temperature across the height of the plate with varying plastic material length scale \( l_p/L = 0.25, 0.5 \) and 1.0: (a) CIGT and (b) RIGT.

4.4.3 Shear band

The schematic illustration of the uniaxial plane strain tension problem to explore the mesh-sensitivity characteristics of the proposed model during strain softening is presented in Figure 4.8. To do this, the three different mesh sizes, i.e. Mesh 1: 500, Mesh 2: 1125 and Mesh
3: 2000 elements are used in this subsection. The parameter $u^\parallel(t)$ at the top edge represents the prescribed displacement in the $x_2$ direction at time $t$ which increases monotonically, and eventually causes an average normal strain $\varepsilon = u^\parallel / L$. It is further assumed that no displacements are allowed toward the $x_1$ direction at the top and left edges ($u_1(x_1, L, t) = 0$ and $u_1(0, x_2, t) = 0$) and $x_2$ direction at the bottom edge ($u_2(x_1, 0, t) = 0$). At all edges, the microscopic free boundary condition is imposed. To generate the strain localisation at the left-bottom corner of the rectangular plate, the artificial imperfection is enforced by reducing the shear and bulk moduli by 10%. The commonly used material properties for this section are presented in Table 4.2. The direct comparison between the classical plasticity model without the gradient effect and the proposed gradient-enhanced plasticity model is conducted in the following subsections.

![Diagram](image_url)

**Figure 4.8.** The schematic illustration of the simple uniaxial plane tension problem: (a) the geometry, the boundary conditions, and initial conditions, (b) Mesh 1: $10 \times 50 = 500$, Mesh 2: $15 \times 75 = 1,125$ and Mesh 3: $20 \times 100 = 2,000$ elements.
Table 4.2. Material properties used for the numerical simulations (shear bands)

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Units</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu$</td>
<td>Pa</td>
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4.4.3.1 Classical plasticity model with no gradient effect

The stress-strain responses, the evolutions of maximum local effective plastic strain $\varepsilon^p$, the distributions of $\varepsilon^p$ along the path (as shown in Figure 4.8. (a)) and the profiles of $\varepsilon^p$ at a time step of 5 s under the classical plastic model (no gradient regularisation) are shown in Figure 4.9 for three mesh sizes. The material length scale parameters for all simulations are set to zero since no gradient effect is incorporated. The mesh dependent responses of the material in the softening regime are well observed in Figure 4.9. (a), (b) and (c). Note that the maximum values of $\varepsilon^p$ occur at the node of the left-bottom corner because of the imposed imperfection. It is well known that, when the classical plasticity model is employed for modeling the inelastic deformation, the transversal width of the shear band is forced to be directly proportional to the element size. This fact is also well observed in Figure 4.9. (d), consequently the width of the shear bands decreases as the mesh density increases. Furthermore, the maximum value of the local effective plastic strain drastically increases as the mesh density increases. One possible solution for such a mesh-sensitivity problem is to include the viscosity effect in the current rate-independent constitutive model, so that the regularisation effect can be incorporated in the model. However, this issue is beyond the scope of this work.
Figure 4.9. The numerical results of the uniaxial plane strain tension problem under the classical plasticity model: (a) the stress-strain responses, (b) the evolutions of the local effective plastic strain $\varepsilon^p$, (c) the distributions of $\varepsilon^p$ along the path at 5 s time step, and (d) the profiles of local effective plastic strain $\varepsilon^p$ at 5 s time step with Mesh 1, Mesh 2 and Mesh 3.

(fig. cont’d.)
4.4.3.2 Gradient plasticity model with gradient regularisation
Figure 4.10. The numerical results of the uniaxial plane strain tension problem under the gradient-enhanced plasticity model: (a) the stress-strain responses, (b) the evolutions of the local effective plastic strain $\varepsilon^p$, (c) the distributions of $\varepsilon^p$ along the path at 10 s time step, and (d) the profiles of local effective plastic strain $\varepsilon^p$ at 10 s time step with Mesh 1, Mesh 2 and Mesh 3.

(fig. cont’d.)
In this subsection, the material length scale parameters for all simulations are set by \( l_p/L = 0.005 \). The stress-strain responses, the evolutions of maximum local effective plastic strain \( \varepsilon^p \), the distributions of \( \varepsilon^p \) along the path and the profiles of \( \varepsilon^p \) under the proposed gradient enhanced plasticity model are shown in Figure 4.10 for three mesh sizes. Note that Figure 4.10.
(c) and (d) present the numerical results at a time step of 10 s. Contrary to the classical plasticity model, the widths of the shear bands are consistent with each other and the ranges of $\varepsilon^p$ are also observed to be similar to each other as shown in the contour plots. This mesh independent behaviours can be also shown in Figure 4.10. (a), (b) and (c).

4.5 Conclusions

The thermodynamically consistent constitutive model for the coupled thermo-mechanical strain gradient plasticity theory is constructed in the finite deformation context. For the purpose of the computational efficiency, the implicit gradient-enhanced approach which introduces the nonlocal effective plastic strain through the Helmholtz-type partial differential equation is employed in the spirit of the micromorphic theory. One well-known drawback of the implicit approach is that it does not have the capability of capturing the size effect during strain hardening. In order to overcome this issue, Peerlings et al. (2012) proposed the gradient-enhanced plasticity-damage theory by combining the authors’ previous works in Engelen et al. (2003) and Peerlings (2007). These three works were conducted under the small deformation theory. In some ways, the current work is an extension of Peerlings et al. (2012) in a version of finite deformation theory since the main objective of this study is to prove the capability of the proposed model on the size effect issue. Another important objective is to prove that the proposed model is free from the mesh sensitivity problem which typically appears in the classical plasticity theory.

In order to fulfil these objectives, the two-dimensional finite element algorithm for the proposed model is developed via the commercial package ABAQUS/standard (2012) user-defined subroutine UEL. In this numerical algorithm, the nonlocal effective plastic strain field is treated as the additional degree of freedom.

The plane strain shear problem is considered in conjunction with the two specific microscopic boundary conditions to investigate the size effects during strain hardening. The revised version of the implicit gradient approach is directly compared to the original version. In RIGT, it is well observed that the material responses during hardening is stiffer as the sizes of the specimen get smaller, viz. the size effect. On the other hand, in CIGT, it is shown that the material responses do not depend on the specimen size. The main factor of this difference is the micro-hard boundary condition. This condition describes the complete blockage of the dislocation movements at the prescribed external boundary (not at elastic-plastic boundary), and results in the harder boundary layer, e.g. passivation layer (see Lele and Anand (2008); Voyiadjis and Song (2017)). This effect is more significant when the proportion of the boundary layer on the specimen is large. Therefore, the differences between the local and nonlocal effective plastic strains become larger as the sizes of the specimen get smaller, and this results in more significant gradient effect according to Equation (4.9). Consequently, the material responses become stiffer.

The mesh-sensitivity of the proposed model on the strain localisation during strain softening is also examined in this chapter. In the classical plasticity model with no gradient regularisation, it is well observed that the widths of the shear band drastically vary according to the mesh size, whereas the mesh-independent material responses are obtained in the propose model.
5 CONCLUSIONS AND FUTURE WORKS

Thermo-mechanical modeling of metallic components becomes more complex when their size reduces to the order of a few hundreds of nanometers and they are subjected to inhomogeneous plastic flow under short elapsed time during a transient. Since conventional continuum plasticity and heat transfer theories, based on the local thermodynamic equilibrium, do not account for the microstructural characteristics of materials, they cannot be used to adequately address the observed mechanical and thermal response of the micro-scale metallic structures.

This dissertation explores an important and under-researched topic on the multi-scale modeling in which the careful characterization of mechanical and thermal responses of the materials require that the developed continuum model representing these events occur at the micro-scale. Computational simulations are used to numerically investigate the capability of the proposed models to address the small scale material responses with respect to size effect, mesh-sensitivity and nonequilibrium heat transfer.

In Chapter 2, a phenomenological thermodynamic-based higher order gradient plasticity theory for a single grain is proposed and applied to the stretch-surface passivation problem for investigating the material behaviour under the non-proportional loading condition. The microstructural interface (grain boundary) effect between two grains is also incorporated into the formulation, such that the developed grain boundary flow rule is able to account for the energy storage at the grain boundary caused by the dislocation pile up as well as the energy dissipation through the grain boundary caused by the dislocation transfer. Two cases of the SGP theory with and without the dissipative higher order microstress quantities are proposed with the new forms of the free energy and the dissipation potentials for eliminating an elastic loading gap and the corresponding finite element solution for the stretch-surface passivation problem is developed in order to investigate and compare the responses from two cases under the non-proportional loading condition by using the commercial finite element package ABAQUS/standard (2012) via the user-subroutine UEL. There are a number of conclusions worth mentioning here namely:

1. The magnitude of the stress jump significantly increases as the dissipative length scale increases, on the other hand, the stress jump phenomena disappear as the dissipative length scale comes closer to zero,
2. The slopes of the very first response $E$ immediately after the passivation also increase as the dissipative length scales increase,
3. The stress jump phenomenon is highly correlated with the dissipative higher order microstress quantities $S_{ij}^{dis}$, in addition, the very first responses immediately after the passivation also make a substantial difference with varying passivation points,
4. The hardening material parameter $h$ does not affect the stress jump significantly in the case of the SGP model with $S_{ij}^{dis} \neq 0$,
5. Both the slope of the very first response immediately after the passivation and the corresponding magnitude of the stress jump substantially increase as the non-negative rate sensitivity parameter $m$ increases in the case of the SGP model with $S_{ij}^{dis} \neq 0$,
6. As the temperature-related parameters for the bulk such as the temperature sensitivity parameter $n$ and the thermal material parameter $T_y$ increase, the slope of the very first response immediately after the passivation decreases and the corresponding magnitude of the stress jump increases in the case of the SGP model with $S_{ij}^{dis} \neq 0$. 
(7) the slope of the very first response after the passivation, the corresponding magnitude of the stress jump increase and the variations along with the cases are shown more drastically by decreasing the temperature-related parameters for the interface, such as the interfacial temperature sensitivity parameter $n^I$ and the interfacial thermal material parameter $T'_Y$ in the case of the SGP model with $\delta_{ijk}^{\text{dis}} \neq 0$, and finally

(8) no stress jump is observed in all cases with $\delta_{ijk}^{\text{dis}} = 0$.

In Chapter 3, two-dimensional finite element analysis for the thermodynamically consistent thermo-mechanical coupled gradient enhanced plasticity model is proposed based on small deformations within the areas of grain interior and grain boundary, and validated by comparing against two sets of small-scale experiments demonstrating the size effects. The thermodynamic microstresses are assumed to be divided in two components, i.e. the energetic and dissipative components, which in turn, both energetic and dissipative material length scale parameters are incorporated in the governing constitutive equations. The concept of GNDs density is additionally employed in this chapter to interpret the microstructural strengthening mechanisms induced by the nonhomogeneous deformation. The simple shear problem and the square plate problem are solved based on the validated model in order to examine size effect in small-scale metallic materials and two null boundary conditions respectively. The followings are the selected conclusions based on Chapter 3:

(1) the energetic hardening, dissipative strengthening and GNDs hardening are well observed respectively with varying $\ell_{\text{en}}$, $\ell_{\text{dis}}$ and $\ell_{\text{N-G}}$,

(2) the strengthening effect due to the microhard boundary condition at the grain boundary is clearly observed with increasing grain boundary areas,

(3) the microfree and microhard boundary conditions are well captured by using the proposed grain boundary flow rule, and

(4) the size effects on the stress-strain responses and the evolutions of maximum temperature are well observed with the cases of (a) combined $\rho_{\text{en}}^{\text{GB}}$ and $\rho_{\text{dis}}^{\text{GB}}$, (b) $\rho_{\text{en}}^{\text{GB}}$ only, and (c) $\rho_{\text{dis}}^{\text{GB}}$ only.

In Chapter 4, the thermodynamically consistent constitutive model for the coupled thermo-mechanical strain gradient plasticity theory is constructed in the finite deformation context. For the purpose of the computational efficiency, the implicit gradient-enhanced approach which introduces the nonlocal effective plastic strain through the Helmholtz-type partial differential equation is employed in the spirit of the micromorphic theory. One well-known drawback of the implicit approach is that it does not have the capability of capturing the size effect during strain hardening. In order to overcome this issue, the revised version of the implicit approach is examined in this chapter by considering two null boundary conditions. The followings are the selected conclusions based on Chapter 4:

(1) In the revised version, it is well observed that the material responses during hardening is stiffer as the sizes of the specimen get smaller, viz. the size effect,

(2) on the other hand, in the old version, it is shown that the material responses do not depend on the specimen size,

(3) the differences between the local and nonlocal effective plastic strains become larger as the sizes of the specimen get smaller, and this results in more significant gradient effect, and

(4) the mesh dependent material responses are obtained with the classical plasticity model with no gradient regularisation, whereas in the proposed strain gradient plasticity model, the mesh independent results are obtained.
5.1 Future works

The followings are suggested future works:

· 3D finite element implementation of the proposed model is needed.
· The current model is purely phenomenological. The physically-based gradient-enhanced coupled damage-plasticity model for various metal structures (e.g. FCC, BCC, metal alloys) is needed to be developed instead of a phenomenological one. In most existing strain gradient plasticity theories including the author’s previous works, the plastic strain gradient is calculated as the gradient of plastic strain. That is, these two variables are closely related to each other. However, in fact, the physical origins of these two variables have nothing to do with each other, for this reason, they should be treated as independent variables.
· The single phenomenological material length scale is used in Chapter 4, which deals with finite deformations, for both the hardening and softening regimes. For more elaborate modeling of the gradient-enhanced plasticity theory, the multiple material length scales are needed.
· Moreover, the physically-based temperature and rate dependent material length scale model (Voyiadjis et al., 2011; Voyiadjis and Zhang, 2015; Zhang and Voyiadjis, 2016) or the calibrated length scale via the nanoindentation tests, e.g. Gomez and Basaran (2007); Zhang and Voyiadjis (2016) will be incorporated in future work.
· The application of the proposed strain gradient plasticity model to the high strain rates problem is highly desirable. In this case, thermo-mechanical coupling is very important since the penetration causes considerable heat change.


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Quinney, H., Taylor, G.I., 1937. The emission of the latent energy due to previous cold working when a metal is heated. Proceedings of the Royal Society of London Series a-Mathematical and Physical Sciences 163, 0157-0181.


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APPENDIX A. DERIVING THE BALANCE EQUATIONS

The total strain rate \( \dot{\varepsilon}_{ij} \) is defined as follows:

\[
\dot{\varepsilon}_{ij} = \frac{1}{2}(\ddot{u}_{i,j} + \ddot{u}_{j,i})
\]  \hspace{1cm} (A.1)

with the velocity gradient \( \ddot{u}_{i,j} = \partial \ddot{u}_i / \partial x_j \).

By substituting Equation (3.2) into Equation (3.8), one obtains

\[
P^{\text{int}} = \int_{\Omega_0} \left( \sigma_{ij} \dot{\varepsilon}_{ij} - \sigma_{ij} \dot{\varepsilon}_{ij}^p + x \dot{e}^p + Q_i \dot{e}^p_i + A \dot{T} + B_i \dot{T}_i \right) dV
\]  \hspace{1cm} (A.2)

From the plastic incompressibility (\( \varepsilon_{kk}^p = 0 \)), \( \sigma_{ij} \dot{\varepsilon}_{ij}^p = \bar{\sigma}_{ij} \dot{\varepsilon}_{ij}^p \). The divergence theorem can be used here in Equation (A.2) together with Equation (A.1) to obtain the following expression:

\[
P^{\text{int}} = \int_{\partial \Omega_0} \left( \sigma_{ij} n_j \ddot{u}_i + Q_i n_i \dot{e}^p + B_i n_i \right) dS
\]  \hspace{1cm} (A.3)

By equating the external power given in Equation (3.9) to the internal power (\( P^{\text{int}} = P^{\text{ext}} \)), the following expression is obtained:

\[
\int_{\partial \Omega_0} \left\{ \left( \sigma_{ij} n_j - t_i \right) \ddot{u}_i + \left( Q_i n_i - m \right) \dot{e}^p + \left( B_i n_i - a \right) \right\} dS
\]  \hspace{1cm} (A.4)

Here, \( \ddot{u}_i \), \( \dot{e}^p \) and \( \dot{T} \) can be designated randomly when the following conditions are satisfied:

\[
\begin{align*}
\sigma_{ij,j} + \sigma_i &= 0 \hspace{1cm} (A.5) \\
\bar{\sigma}_{ij} &= (x - Q_{kk}) N_{ij} \hspace{1cm} (A.6) \\
B_{ii} - A &= 0 \hspace{1cm} (A.7) \\
t_j &= \sigma_{ij} n_i \hspace{1cm} (A.8) \\
m &= Q_i n_i \hspace{1cm} (A.9) \\
a &= B_i n_i \hspace{1cm} (A.10)
\end{align*}
\]
**APPENDIX B. FRAME INDIFFERENCE OF THE ELASTIC STRESS $\sigma^e$**

Under the assumption that $Q$ is an arbitrary time-independent transformation ($\dot{Q} = 0$), Equation (4.30) gives

$$
\sigma^e_{ij}' \left( \dot{Q}_{lk}^e F^e_{kj} + Q_{lk}^e \delta F^e_{kj} \right) = \sigma^e_{ij} \delta F^e_{ij}
= Q_{lk}^e \sigma^e_{kj}' \delta F^e_{ij} = \sigma^e_{ij} \delta F^e_{ij}
\Rightarrow Q_{lk}^e \sigma^e_{kj}' = \sigma^e_{ij}
\Rightarrow \sigma^e_{kj}' = Q_{kl}^e \sigma^e_{ij}
\Rightarrow \sigma^e_{ij}' = Q_{lk}^e \sigma^e_{kj}

\text{or } \sigma^e = Q \sigma^e
\quad \text{(B.1)}
$$

With the further assumption $Q = I$, from Equation (B.1), $\sigma^e = \sigma^e$. Then, Equation (4.30) gives

$$
\sigma^e_{ij}' \left( \dot{Q}_{lk}^e F^e_{kj} + Q_{lk}^e \delta F^e_{kj} \right) = \sigma^e_{ij} \delta F^e_{ij}
= \sigma^e_{ij}' \left( Q_{lk}^e F^e_{kj} + \delta F^e_{ij} \right) = \sigma^e_{ij} \delta F^e_{ij}
\Rightarrow \sigma^e_{ij}' F^e_{jk} \dot{Q}_{lk}^e + \sigma^e_{ij} \delta F^e_{ij} = \sigma^e_{ij} \delta F^e_{ij}
\Rightarrow \sigma^e_{ij} F^e_{jk} \dot{Q}_{lk}^e = 0
\quad \text{or } (\sigma^e F^e)^T \dot{Q} = 0
\quad \text{(B.2)}
$$
By assuming the microscopic virtual velocity field $\delta \varepsilon^p$ and $\delta \varepsilon^p$ to be zero, Equation (4.20) becomes

$$
\delta M_{i,k} F_{kj}^{-1} = \delta F_{ik} F_{kj}^{-1}
$$

$$
\Rightarrow \delta M_{i,k} F_{km}^{-1} F_{mj} = \delta F_{im} F_{mj}^{-1}
$$

$$
\Rightarrow \delta M_{i,k} F_{kj}^{-1} = \delta F_{ij}^e
$$

(Sub. 1.1)

Substituting Equation (C.1) into Equation (4.18), and applying Equation (4.21) give that

$$
\int_{\Omega_0} \left( \sigma_{ij}^e \delta M_{i,k} F_{kj}^{-1} + \mathcal{A} \delta T + \mathcal{B}_i \delta T_i \right) \, d\Omega_0
$$

$$
= \int_{\Omega_0} (\delta i \delta M_i) \, d\Omega_0 + \int_{\partial \Omega_0} (\tau_i \delta M_i + a \delta T) \, d\Omega_0
$$

$$
\Rightarrow \int_{\Omega_0} \left( \sigma_{ij}^e F_{kj}^{-1} \delta M_{i,k} - \delta i \delta M_i \right) \, d\Omega_0 + \int_{\Omega_0} (\mathcal{A} \delta T + \mathcal{B}_i \delta T_i) \, d\Omega_0
$$

$$
= \int_{\partial \Omega_0} \tau_i \delta M_i \, d\Omega_0 + \int_{\partial \Omega_0} a \delta T \, d\Omega_0
$$

By using the divergence theorem, the above equation becomes

$$
\int_{\partial \Omega_0} P_{ik} n_k \delta M_i \, dS_0 - \int_{\Omega_0} P_{ik,k} \delta M_i \, d\Omega_0 - \int_{\Omega_0} \delta i \delta M_i \, d\Omega_0 + \int_{\Omega_0} \mathcal{A} \delta T \, d\Omega_0
$$

$$
+ \int_{\partial \Omega_0} \mathcal{B}_i n_i \delta T \, dS_0 - \int_{\Omega_0} \mathcal{B}_i \delta T \, d\Omega_0
$$

$$
= \int_{\partial \Omega_0} (\tau_i \delta M_i + a \delta T) \, dS_0
$$

$$
\Rightarrow \int_{\partial \Omega_0} \left( (P_{ik} n_k - \tau_i) \delta M_i + (\mathcal{B}_i n_i - a) \delta T \right) \, dS_0
$$

$$
- \int_{\Omega_0} \left( (P_{ik,k} + \delta i) \delta M_i + (\mathcal{B}_{i,i} - \mathcal{A}) \delta T \right) \, d\Omega_0 = 0
$$

(C.2)

Note that Equation (C.2) must be satisfied for all $\delta M$ and $\delta T$, and the principle of virtual power must hold for the generalized stresses $\mathcal{A}$ and $\mathcal{B}$ in the spirit of the micromorphic approach. To this end, the equations for the local macroscopic surface traction conditions, the balance of macroscopic linear momentum and the balance of the generalized stresses $\mathcal{A}$ and $\mathcal{B}$ can be represented respectively as follows:

$$
\tau_i = P_{ij} n_j \tag{C.3}
$$

$$
P_{ij,i} + \delta_i = 0 \tag{C.4}
$$

$$
a = \mathcal{B}_i n_i \tag{C.5}
$$

$$
\mathcal{B}_{i,i} - \mathcal{A} = 0 \tag{C.6}
$$

where $\mathbf{n}$ is the outward unit normal vector to $\partial \Omega_0$.
Equations (4.18), (4.19) and (4.20), the following relation is given as
\[ \int_{\Omega_0} \left( q \delta \varepsilon^p + Q_i \delta \varepsilon^p_i \right) d\Omega_0 = \int_{\partial \Omega_0} m \delta \varepsilon^p dS_0 \]  
(C.7)

By using the divergence theorem, the above equation becomes
\[ \int_{\Omega_0} q \delta \varepsilon^p d\Omega_0 + \int_{\partial \Omega_0} Q_i n_i \delta \varepsilon^p dS_0 - \int_{\Omega_0} Q_{i,i} \delta \varepsilon^p d\Omega_0 - \int_{\partial \Omega_0} m \delta \varepsilon^p dS_0 = 0 \]
\[ \Rightarrow \int_{\partial \Omega_0} (m - Q_i n_i) \delta \varepsilon^p dS_0 + \int_{\Omega_0} (Q_{i,i} - q) \delta \varepsilon^p d\Omega_0 = 0 \]  
(C.8)

Since Equation (C.8) must be satisfied for all \( \delta \varepsilon^p \), the equations for the first microscopic force balance and the nonlocal microscopic traction conditions can be obtained as follows:
\[ Q_{i,i} - q = 0 \]  
(C.9)
\[ m = Q_i n_i \]  
(C.10)

Lastly, assume the virtual velocity fields \( \delta \mathbf{M}, \delta \varepsilon^p \) and \( \delta T \) to be zero. Then, Equation (4.20) becomes
\[ \delta F^e_{i,k} F^{-1}_{k,j} = -\delta \varepsilon^p F^e_{k,i} N^p_{k,m} F^{-1}_{m,j} \]
\[ \Rightarrow \delta F^e_{i,j} = -\delta \varepsilon^p F^e_{k,i} N^p_{k,j} \]
\[ \Rightarrow \sigma^e_{i,j} \delta F^e_{i,j} = -\delta \varepsilon^p F^e_{k,i} \sigma^e_{i,j} N^p_{k,j} = -\delta \varepsilon^p M^e_{k,j} N^p_{k,j} \]  
(C.11)

where \( \mathbf{M}^e \) represents the Mandel stress, which is given by
\[ M^e_{k,j} = J F^e_{k,i} \sigma^e_{i,j} F^{-1}_{j,l} \]  
(C.12)

From Equation (C.11), the resolved stress quantity \( \mathbf{\bar{\sigma}} \) is defined with the deviatoric part of the Mandel stress \( \mathbf{\bar{M}}^e \) \( \bar{M}^e_{i,j} = M^e_{i,j} - M^e_{k,k} \delta_{i,j}/3 \) as follows:
\[ \bar{\sigma} \equiv \bar{M}^e_{i,j} N^p_{i,j} \]  
(C.13)

Since \( \mathbf{N}^p \) is deviatoric,
\[ \sigma^e_{i,j} \delta F^e_{i,j} = -\delta \varepsilon^p M^e_{i,j} N^p_{i,j} = -\delta \varepsilon^p \bar{M}^e_{i,j} N^p_{i,j} = -\bar{\sigma} \delta \varepsilon^p \]  
(C.14)

Substituting Equation (C.14) into Equation (4.18), and applying Equation (4.21) give that
\[ \int_{\Omega_0} (x - \bar{\sigma}) \delta \varepsilon^p d\Omega_0 = 0 \]  
(C.15)

Since Equation (C.15) must be satisfied for all \( \delta \varepsilon^p \), the second microscopic force balance can be obtained by
\[ x = \bar{\sigma} \]  
(C.16)
APPENDIX D. COPYRIGHT DOCUMENTATION

VITA

Yooseob Song was born in Nonsan, South Korea in June, 1981. He graduated from Anyang High School in February, 2000. Following high school, he began his college education at Hanyang University. In February of 2006, he received his Bachelor of Science degree in Civil Engineering with a structural engineering emphasis. After that, he joined the Hanyang University graduate program and received his Master of Science in the area of structural engineering under the guidance of Professor Taehyo Park in February, 2008. Afterwards, he worked with TESO Engineering Co., Ltd., Seoul, South Korea from 2008-2011 as a structural engineer, where he was involved in the various construction projects including Korea Train eXpress Honam High-Speed Railway, Seoul Metro Line no.9, Incheon Metro Line no.2 and Suseo-Pyeongtaek 4th sector KTX station. After four years’ industry experience, he joined Hanyang University working as a research fellow in the Department of Civil and Environmental Engineering with specialization in high performance cluster computing (HPCC), numerical analysis of extreme loading events, and piezoelectric energy harvesting. Yooseob Song began his doctoral study in 2014 at Louisiana State University (LSU) in the United States under the supervision of Boyd Professor George Z. Voyiadjis. Four years later he completed the research presented in this dissertation with a 4.0 GPA. At LSU, he has been involved in researches in several areas, such as computational solid mechanics, strain gradient plasticity theory, mechanics of materials, fracture and damage mechanics, and multiscale modeling of metals. He has several publications that have been published in several prestigious journals in the field of engineering mechanics. He has also participated in a number of international and national conferences. Yooseob Song got married Minjeong Kim in April, 2015 in Seoul, South Korea.