ABDELJAWAD, FADI FAEQ. Microstructural Modeling of CSL Grain-Boundary Effects and Crack Growth in F.C.C. Polycrystals. (Under the supervision of Professor Mohammed Zikry.)

A new multiple-slip rate-dependent crystalline constitutive formulation that is coupled to the evolutionary equations of mobile and immobile dislocation densities is developed. Dislocation densities were modeled as internal state variables that provide a more detailed microstructural description of the material’s inelastic deformation and interrelated physical mechanisms that control different failure modes. Specialized microstructurally-based finite-element schemes have been used to investigate the effects of crystallographic orientations of the grains and grain-boundaries (GBs), grain shape and size, (GB) misorientation and the dependency of GB strength and mechanical properties on specific CSL misorientations on the inelastic finite deformation and failure mode mechanisms in f.c.c. polycrystalline aggregates. A Voronoi algorithm was used to generate grains and GBs with random shapes and sizes. The combined effects of GB misorientation, structure and geometry, strain hardening, localized plastic shear slip, intensive regions of crystal lattice rotation and the evolution, interaction and accumulation of dislocation densities on the nucleation and growth of intergranular and transgranular failure modes in f.c.c. polycrystalline aggregates were studied. Results from this study are consistent with experimental observations that microstructures with desired material properties, such as resistivity to crack nucleation, can be achieved by the control of the crystallographic orientation distribution of the grain aggregate and CSL GB orientations. Results from this study show that transgranular failure modes are dominant in aggregates with a high
frequency of $\Sigma 3$ GBs, and intergranular fracture modes dominate the aggregate with a high frequency of $\Sigma 17b$ GBs.
Microstructural Modeling of CSL Grain-Boundary Effects and Crack Growth in F.C.C. Polycrystals

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DEDICATION

To my father and my best friend, Faeq, my beloved mother, Helja, my dear wife, Hanadee, my great siblings, Basil and Karmel. Thanks for all the help, support and dedication. You have paid a lot of attention to me throughout my college career and you have been there for me for all the ups and downs.
BIOGRAPHY

Fadi F. Abdeljawad was born on April 6, 1981 in Amman, Jordan. After finishing middle school in 1996 and achieving an excellent score in an individual scholarship exam, he was awarded a one-year scholarship for Al-OROUBA private high schools. The academic scholarship was renewed to cover the 3-year high school studies. He finished high school in 1999 with an overall average that ranked him among the top 1% students in his class in Jordan. He was admitted to The College of Engineering at the University of Jordan at Amman. After completing the fresh year with an outstanding GPA, Fadi decided to move to the U.S.A. to obtain his college education. He was admitted to the College of Engineering at North Carolina State University in the spring semester of 2001. He was nominated for the honorary society of PI TAU SIGMA in 2002 and PHI KAPPA PHI in 2005. He was elected as an honorary member for the National Society of Collegiate Scholars in 2002. He graduated with a B.S. in Mechanical Engineering in the fall of 2003. He was the receiver of Gordon & Louise Smith Scholarship for the year of 2003-2004. During his undergraduate studies, Fadi was hired by Professor M. Zikry as an undergraduate research assistant. Upon the completion of his B.S. degree, Fadi decided to pursue his Master of Science degree and he was awarded a graduate research assistantship. After graduating with an MS degree in Mechanical Engineering, Fadi was employed by Sikorsky Aircraft in January 2006. Fadi is member of the Society for Automotive Engineers and the American Society for Mechanical Engineers.
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CHAPTER 1
INTRODUCTION

The inelastic finite deformation and the microstructural mechanisms of different failure modes of crystalline metallic materials can be characterized by the constituents of these crystalline aggregates, grains and grain boundaries (GBs). Although the GB width is on average less than two atomic diameters at the microstructural scale, GB networks can control grain bulk properties and the overall behavior of crystalline materials. GBs have a dominant influence on different properties and phenomena (see for example, Randle 1993 and Watanabe 1984), such as grain growth and recrystallisation, creep behavior, solute aggregation and corrosion, chemical reaction and phase transformations, and electrical, magnetic, and mechanical properties.

GB porosity, excess free volume, and the local strain fields adjacent to GB regions are what define the uniqueness of GB structure. GBs can be classified in terms of orientation as either random or special boundaries, such as coincidence site lattice (CSL) GBs, see for example, Mykura (1969) and Priester (1989). This classification of GBs is based on the structure and geometry of these boundaries. In the CSL formalism, certain orientations in space of two neighboring crystal lattices will result in a periodic arrangement of the interfacing lattices. The difference in orientation between two neighboring crystal lattices defines the misorientation at the GB separating them. This CSL formalism can provide a linking bridge between the GB geometry and its properties, but this pure geometrical description of GBs does not predict and estimate special GB properties and its relation to random GBs or grain bulk (Priester 1989, Sutton and Ballufﬁ 1987). This is because GB
properties depend not only on GB orientation, but also on local defect, dislocation, structure, chemistry and electronic bonding (Sutton and Balluffi 1987).

Different experiments have shown that transgranular failure mode can occur in crystalline materials with low-angle CSL boundaries, whereas failure in crystalline aggregates with high-angle CSL boundaries may be characterized by intergranular failure mode (Brosse et al. 1981, Watanabe 1989, and Peralta 2005). Computational analyses at different scales by Zikry and Kao (1996), Ashmawi and Zikry (2003), and several molecular dynamics investigations (Yoo and King 1990, and Caturla, Nieh et al. 2003) have also shown that failure in crystalline metals can be characterized in terms of GB structure and misorientation.

Furthermore, the effects of GB strength and structure on the failure mode mechanisms of polycrystalline aggregates were investigated by Lin and Pope (1992), and Meyers and Ardell (1993). It was found that low-angle boundaries are strong and do not fracture, whereas high-angle boundaries are weaker and have a propensity for fracture. The intrinsic weakness of GBs is what causes the intergranular fracture mode in crystalline metallic materials at low temperatures. Lin and Pope (1992) also determined that fracture strength of special, low, angle GBs is roughly an order of magnitude higher than the fracture strength of high-angle GBs. They also suggested that cracks tend to grow in regions where there is a slightly lower fraction of Σ3 boundaries. Low-angle and Σ3 boundaries are basically ideal lattices with periodically spaced dislocation cores. High angle random boundaries have very different structure in comparison with perfect lattices. High angle random GBs in crystalline materials are characterized by lower cohesion than random low angle boundaries. Since crack propagation may be due to low GB cohesion, cracks may
propagate in an intergranular mode in high-angle GBs, while $\Sigma 3$ and low-angle boundaries may resist crack propagation due to high GB cohesion.

The GB’s surface energy increases as the GB’s misorientation about the tilt axis increases. As noted by Gleiter (1982), this variation in surface energy results in each GB orientation having a different dislocation structure, and this has a direct bearing on the mode of material failure. McLean (1973) found that low-angle GBs have lower energies than average or general high-angle GBs. Experimental observations by Hanada et al. (1985) have shown that intergranular fracture in $Ni_3Al$ samples occurred along random and $\Sigma 5\sim\Sigma 29$ GBs. They observed an evident resistivity of low-angle and $\Sigma 3$ GBs against intergranular cracking. GBs having the coincidence orientation relation ($\Sigma 5\sim\Sigma 29$) and random GBs were preferentially broken under tensile stress. Experiments by Zhang (1999) have shown that secondary slip lines were always activated near large-angle GBs and these GBs act as obstacles to slip deformation since slip bands could not pass through them. Zhang (1999) also found that dislocations transfer through low-angle GBs showing plastic strain compatibility. Atomistic based calculations of Yoo and King (1990) for a pure copper bicrystal with $\Sigma 17b$ GB have shown that intergranular fracture can occur as a result of symmetric double dislocation pile-up.

One of the current challenges is the lack of reliable inelastic crystalline constitutive relations and ductile failure models that can account for high densities of dislocations, which are associated with plastic deformations, within the grain-bulk and the GB interfacial planes. Experiments by Marguiles et al. (2001) and Raabe et al. (2001), on texture evolution of polycrystalline materials, indicate that macroscopic crystalline-plasticity models, such as
those based on Taylor, Sachs, and self-consistent models, generally overestimate texture in f.c.c. and b.c.c. aggregates. This is due to several factors, but the overriding factor is that GB heterogeneities and effects are generally smeared out in these models. Hence, as noted by Davies and Randle (2001), if failure is to be accurately modeled, failure models must account for interfacial effects due to sub-grains, cell walls and GBs. The effects of how GB interactions and mechanisms, such as slip transmission, impedance, and blockage affect void nucleation and growth at different physical scales are not well understood and have not been adequately quantified.

Furthermore, if the mechanical, physical and chemical properties of the GB interfacial planes can be optimized as a function of the spatial orientation (the crystallography of each grain) and the crystallographic orientation distribution, then interfacial properties and behavior response can be tailored for damage tolerant applications. This optimization process is defined as GB Engineering, GBE (Watanabe, 1984). Experimental investigations by Mykura (1969), Miura et al. (1980), Lin et al. (1986), Randle (1994) and Randle et al. (1999), and Watanabe (1989, 1994), and atomistic simulations by Yoo and King (1990) and Mills (1993) have shown that for both solute-free and embrittled metallic and intermetallic aggregates, GB misorientations directly affect the emission and the shielding of dislocations at crack-tips and the nucleation of cracks. These studies show that the initiation and propagation of intergranular and transgranular failure modes in f.c.c. and b.c.c. polycrystals at low and intermediate temperatures are directly related to the GBs' misorientation and interfacial properties.

Hence, microstructures, through the control of GBs and triple junctions, can be potentially engineered and optimized for desired applications. Recent applications of
engineered GB interfaces include, mitigating crack susceptibility and stress corrosion cracking in nickel-based alloys (Aust et al., 1994), increasing strength and ductility of nickel aluminide intermetallics (George et al., 1996 and Watanabe and Tsurekawa, 1999), and enhancing the corrosion and thermal resistance of nickel and iron alloys (Palumbo et al., 1999). These attempts offer the potential for the design of new failure-resistant material systems.

Therefore, crystalline materials with certain types of CSL GBs may result in different failure modes, transgranular or intergranular failure. However, it is not understood how GB distributions, grain sizes and shapes, dislocation-density evolution along crystallographic planes, and accumulated plastic slip affect inhomogeneous deformation patterns and failure in aggregates with a specified distribution of CSL boundaries. Hence, the major objective of this investigation is to obtain a detailed understanding and accurate prediction of the dominant physical mechanisms that can lead to microstructurally induced deformation and crack-growth in crystalline materials with distributions of $\Sigma 3$ and $\Sigma 17b$ CSL GBs in different sized aggregates with and without initial cracks. These CSL boundaries were chosen since they are characterized by well-defined angle and axis of misorientation relationship that can be used to better understand the effects of GB orientations on the inelastic behavior of f.c.c. aggregates. A dislocation-density multiple-slip formulation will be used to account for the inelastic behavior in a representative f.c.c. material. Voronoi tessellation will be used to represent grain shapes and sizes. CSL GB misorientations will be generated based on angle/axis pair and GB normal for different sized aggregates. A microstructurally based failure criteria will be developed to characterize crack behavior as a function of initial specimen geometry, and the interrelated effects of mobile and immobile dislocation density,
multiple-slip behavior, geometrical softening, localized plastic slip, and GB orientation and
distribution will be used to characterize intergranular and transgranular failure in aggregates
of different sizes.

This study is a first step in developing a physically based understanding of
microstructurally induced failure modes in crystalline materials with a high frequency of
CSL GBs. This thesis is organized as follows: The rate-dependent dislocation-density based
crystalline constitutive formulation is introduced in Chapter 2; the numerical method is
outlined in Chapter 3; the results and discussion for aggregates with various grain-sizes and
an outline of the crystallography of grains and GBs are presented in Section 4; Convergence
of numerical analysis is presented in chapter 5; the inelastic behavior and finite deformation
of aggregates with no initial cracks are discussed in chapter 6; the behavior of crystalline
aggregates with a pre-existing crack is presented in Chapter 7; and recommendations for
future research are outlined in Chapter 8.
CHAPTER 2
DISLOCATION-DENSITY BASED MULTIPLE-SLIP
CRYSTALLINE CONSTITUTIVE FORMULATION

The formulation for the finite deformation of multiple-slip crystal plasticity rate-dependent constitutive relations and the derivation of the evolutionary nonlinear equations for the mobile and immobile dislocation densities, which are coupled to the multiple-slip crystal plasticity formulation, are presented in this chapter. The dislocation-density based crystalline formulation presented below is based on work developed by Zikry and Kao (1996), and Zikry and Kameda (1998).

2.1. Multiple-Slip Crystal Plasticity Formulation

The material deformation gradient tensor, which defines the mapping function between material orientation vector in the initial and deformed configuration is denoted by $F_{ik}$ and the spatial velocity gradient is denoted by $L_{ij}$ and it is defined in symbolic notation as

$$ L = \dot{F} \cdot F^{-1}. $$

(2.1)

It is assumed that the velocity gradient $L$ can be additively decomposed into symmetric and skew-symmetric parts as follows

$$ L_{ij} = D_{ij} + W_{ij}, $$

(2.2)

where the symmetric portion
\[ D_{ij} = \frac{1}{2} \left( L_{ij} + L_{ji} \right), \]  

(2.3)

is the deformation rate tensor, and the skew-symmetric part

\[ W_{ij} = \frac{1}{2} \left( L_{ij} - L_{ji} \right), \]  

(2.4)

is the spin tensor.

The total deformation rate tensor, \( D_{ij} \), and the total spin tensor, \( W_{ij} \), can be additively decomposed into elastic and inelastic, plastic, components as

\[ D_{ij} = D^{*}_{ij} + D^{p}_{ij}, \]  

(2.5)

\[ W_{ij} = W^{*}_{ij} + W^{p}_{ij}. \]  

(2.6)

The superscript * denotes the elastic component, while the superscript p denotes the plastic component. \( W^{*}_{ij} \) includes the rigid body spin. The elastic component of the velocity gradient,

\[ L^{*}_{ij} = D^{*}_{ij} + W^{*}_{ij}, \]  

(2.7)

\( W^{*}_{ij} \) corresponds to the elastic lattice distortion, which accompanies crystallographic slip.

The inelastic components are defined in terms of the crystallographic slip-rates as

\[ D^{p}_{ij} = \dot{P}^{(\alpha)}_{ij} \gamma^{(\alpha)}, \]  

(2.8)

\[ W^{p}_{ij} = \dot{\omega}^{(\alpha)}_{ij} \gamma^{(\alpha)}, \]  

(2.9)

where \( \alpha \) is summed over all slip-systems, and \( \dot{P}^{(\alpha)}_{ij} \) and \( \dot{\omega}^{(\alpha)}_{ij} \) are symmetric and skew-symmetric second-order tensors and are defined as
\[ P_{ij}^{(\alpha)} = \frac{1}{2} \left( s_i^{(\alpha)} n_j^{(\alpha)} + s_j^{(\alpha)} n_i^{(\alpha)} \right), \]  
\[ \omega_{ij}^{(\alpha)} = \frac{1}{2} \left( s_i^{(\alpha)} n_j^{(\alpha)} - s_j^{(\alpha)} n_i^{(\alpha)} \right), \]

where \( n_i^{(\alpha)} \) is the unit vector normal to the slip plane, and \( s_i^{(\alpha)} \) is the unit vector in the slip direction.

The elastic response can be expressed as follows

\[ \Delta^* \sigma_{ij} = L_{ijkl} D_{kl}^*, \]

where \( L_{ijkl} \) is the elastic modulus fourth-order tensor of the crystal. The objective stress rate used in the analysis is based on Jaumann stress-rate of Cauchy stress, \( \sigma_{ij} \). It is co-rotational with the lattice spin. The objective stress rate used here is given by

\[ \Delta^* \sigma_{ij} = \dot{\sigma}_{ij} - W_{ik}^* \sigma_{kj} - W_{jk}^* \sigma_{ki}, \]

where \( \dot{\sigma}_{ij} \) is a material time-derivative of Cauchy stress.

The Jaumann stress rate co-rotational with the material element can be derived as

\[ \Delta \sigma_{ij} = L_{ijkl} (D_{kl} - D_{kl}^p) - W_{ik}^p \sigma_{kj} - W_{jk}^p \sigma_{ki}, \]

and for the case of elastic isotropy

\[ L_{ijkl} = \mu \left( \delta_{ik} \delta_{jl} + \delta_{jk} \delta_{il} \right) + \lambda \delta_{ij} \delta_{kl}, \]

where \( \lambda \) and \( \mu \) are the lame constants.
For rate-dependent inelastic formulation, the flow rule can be described as a power law relation (Hutchinson, 1976) where the slip rates are expressed in terms of the resolved shear stresses. The power law takes the form

\[
\dot{\gamma}^{(\alpha)} = \dot{\gamma}_{\text{ref}}^{(\alpha)} \left[ \frac{\tau^{(\alpha)}}{\tau_{\text{ref}}^{(\alpha)}} \right]^{1/(1-m)} \]

no sum on \( \alpha \). \tag{2.16}

\( \dot{\gamma}_{\text{ref}}^{(\alpha)} \) is the reference shear strain rate which corresponds to a reference shear stress, \( \tau_{\text{ref}}^{(\alpha)} \). The exponent \( m \) defines the material strain rate sensitivity parameter and is given by

\[
m = \frac{\partial \ln \tau^{(\alpha)}}{\partial \ln \dot{\gamma}^{(\alpha)}}. \tag{2.17}\]

The strain rate sensitivity parameter is much less than one for values of the shear slip rate smaller than a critical value. The rate sensitivity parameter is approximately equal to one for slip rates greater than the critical slip rate. In this case, the flow is assumed to be characterized by drag-controlled dislocation motion. The rate-independent limit is achieved as \( m \) approaches zero. For multiple slip, \( \gamma \) is taken as the sum of the accumulated plastic strains on all slip systems \( n \),

\[
\gamma = \sum_{\alpha=1}^{n} |\gamma^{(\alpha)}| \tag{2.18}\]

\( \tau^{(\alpha)} \) in the power law stated above is the resolved shear stress and is given in terms of the Cauchy stress and Schmid’s factor as

\[
\tau^{(\alpha)} = P^{(\alpha)}_{ij} \sigma_{ij}. \tag{2.19}\]
Temperature evolution relation can be obtained from the balance of energy. With no thermal conduction, the rate of change of temperature is related to the rate of the plastic work by

\[ \dot{T} = \frac{\chi}{\rho c_p} \sigma_{ij}^{\text{dev}} D_{ij}^p, \]

(2.20)

where \( \chi \) is the fraction of the plastic work converted to heat, \( \sigma_{ij}^{\text{dev}} \) is the deviatoric stress, \( \rho \) is the material density, and \( c_p \) is the specific heat of the material.

### 2.2. Evolution equations of mobile and immobile dislocation densities

For an inelastic response, an accurate description of the material’s microstructure can be achieved by introducing state variables that provide a linking bridge between the micro-level phenomena and the macro-level continuum engineering quantities. Internal variables along with the current stress and temperature can describe the local state that determines the strain. If the internal variables are denoted as \( \xi \), then the strain can be given by

\[ \varepsilon = \varepsilon(\sigma, T, \xi). \]

(2.21)

For a rate-dependent inelastic formulation, if the local state that determines the strain is dependent on \( \sigma, T, \xi \), then the rate of evolution of the internal variables can be determined by the local state. Mathematically, the rate equation for the \( i^{th} \) internal variable can be written as

\[ \dot{\xi}_i = g_i(\sigma, T, \xi). \]

(2.22)
In this crystal plasticity rate-dependent formulation, two internal variables are used, which are the immobile and mobile dislocation densities. The rate equations for the mobile and immobile dislocation densities will link the macroscopic description of the inelastic deformation of the body to the microstructural local state of the material and more specifically the dislocation structure in each crystal. In inelastic deformations, the evolution and the characteristics of the microstructure are governed by the mechanisms of dislocation production and dynamics recovery. As the material is strained, immobile dislocations are stored in each crystal, and these dislocations act as obstacles for evolving mobile dislocations. Therefore, the immobile and mobile dislocation densities can be coupled, due to the continuous immobilization of mobile dislocations. Furthermore, by including the mobile dislocation densities as a second internal variable, we can account for the fast (in comparison with the immobile dislocation densities) transients associated with the initiation and propagation of plastic flow (Kubin and Estrin, 1988).

The reference shear stress, which is a measure of slip resistance on each slip system, can be given as a function of \( \rho_{im}^{(\alpha)} \), the immobile dislocation density. In terms of a kinetic equation, the flow stresses on each slip system can be recast using the power law stated above to obtain

\[
\tilde{\tau}^{(\alpha)} = \tau^{(\alpha)}(\rho_{im}^{(\alpha)}, \dot{\gamma}^{(\alpha)})
\]  

(2.23)

The reference shear stress that is used in this analysis is a modification of widely used classical forms (see, for example, Mughrabi, 1987) that relate the reference shear stress to a square-root dependence on the dislocation density as
\[ \tau_{\text{ref}}(\alpha) = \tau_y(\alpha) + Gb \sum_{\eta=1}^{12} a_\eta \sqrt{\rho_{\text{im}}(\eta)}, \] (2.24)

where \( G \) is the shear modulus, \( b \) is the magnitude of burger’s vector, \( \tau_y(\alpha) \) is the static yield stress and the coefficients, \( a_\eta (\eta=1,12) \) are interaction coefficients, and generally have a magnitude of unity. In this study, the reference shear stress has been modified to account for latent and self-hardening mechanisms. In the above reference shear stress equation, if the material coefficients \( a_\eta (\eta=1,12) \) are different from each other, then latent hardening applies. If the coefficients are equal, then self-hardening applies.

Now consider a given state for a deformed material that has a dislocation structure of total dislocation density, \( \rho^{(\alpha)} \). This total dislocation density is assumed to be additively composed, into a mobile dislocation density, \( \rho_m^{(\alpha)} \), and an immobile dislocation density \( \rho_{\text{im}}^{(\alpha)} \), as

\[ \rho^{(\alpha)} = \rho_{\text{im}}^{(\alpha)} + \rho_m^{(\alpha)} \] (2.25)

Following the approach of Gottstien and Argon (1987), we have assumed that during an increment of strain, an immobile dislocation density rate is generated, which will be denoted by \( \dot{\rho}_{\text{im}}^{(\alpha)+} \) and an immobile dislocation density rate is annihilated, which will be denoted by \( \dot{\rho}_{\text{im}}^{(\alpha)-} \) on each slip-system as

\[ \frac{d\rho_{\text{im}}^{(\alpha)}}{dt} = \dot{\rho}_{\text{im}}^{(\alpha)+} + \dot{\rho}_{\text{im}}^{(\alpha)-}. \] (2.26)

The same assumption is made to derive the balance equation for the mobile dislocation density. It is stated as
\[
\frac{d\rho_m^{(\alpha)}}{dt} = \dot{\rho}_m^{(\alpha)+} + \dot{\rho}_m^{(\alpha)-}
\]  

(2.27)

where \(\dot{\rho}_m^{(\alpha)+}\) corresponds to a generation of mobile dislocation densities, and \(\dot{\rho}_m^{(\alpha)-}\) corresponds to an annihilation of mobile dislocation densities.

The balance between dislocation generation and annihilation is the basis for the evolution of mobile and immobile dislocation densities as a function of strain. Plastic deformation of the crystal is assumed to begin with the easy glide stage, stage I. In this stage, most of the dislocations belong to the primary slip-system, and very little slip takes place on secondary slip-systems. In this stage, dislocation densities are comparatively low, and the details of dislocation interaction and accumulation have been substantiated by TEM and other high-resolution methods. In the second stage of hardening (stage II), secondary slip-systems are activated, and dislocation clusters and cell walls begin to form. The third stage of hardening is characterized by the annihilation and the rearrangement of dislocations. For a detailed experimental overview of dislocation emission, interaction, trapping and annihilation for the three hardening stages in f.c.c. materials, see, for example, Mitchell (1964), Anongba et al. (1993), Argon and Haasen (1993).

In stage I, dipoles and multi-poles are formed after mobile dislocations emitted from a source are trapped by dislocations of opposite signs on parallel slip planes. The back stress at the source is due to the dislocation emitted by the source. If the flow stress is greater than this back stress, the source will continue to emit dislocations, and dislocations that are trapped can break free. A large number of dipoles, multi-poles and loops are formed in easy glide by forest interactions, cross-slip around obstacles and interactions between dislocations on
parallel slip planes. Dipoles and multi-poles occur in well-spaced clusters. Thus allowing primary dislocations to glide over long distances. This can be expressed as

\[ \frac{d\rho_m^{(\alpha)}}{dt} = \text{rate of generation} \] (2.28)

The rate of dislocation generation is proportional to the distance traveled by the emitted dislocations from a dislocation source with density \( \rho_{source}^{(\alpha)} \). This distance, \( y_{back} \), is related to the decrease of the back stress on the dislocation density source, \( \rho_{source}^{(\alpha)} \), after previously emitted dislocations have traveled this distance \( y_{back} \). The rate of generation for the mobile dislocation density can be written as

\[ \frac{d\rho_m^{(\alpha)}}{dt} = \rho_{source}^{(\alpha)} \frac{\bar{v}}{y_{back}}, \] (2.29)

where \( \bar{v} \) is mobile dislocation average velocity. Using Orowan`s equation, \( \dot{\gamma}^{(\alpha)} = \rho_m^{(\alpha)} b \bar{v} \) and (2.29), we obtain the following equation

\[ \frac{d\rho_m^{(\alpha)}}{d\gamma} = g_{source} \left( \frac{\rho_{im}^{(\alpha)}}{b^2} \right), \] (2.30)

where \( b \) is the modulus of the burgers vector.

In stage II, secondary slip-systems are activated. Dipole clusters multiply and join together, so that primary glide dislocations are effectively blocked. Hardening increases in this stage are due to an increase in dislocation tangles. The forest dislocations of these systems serve as obstacles for the primary dislocations. The mobile dislocations are immobilized with a mean free path proportional to \( \rho_{im}^{(\alpha)-1/2} \). Spatially organized forest structures and tangles such as Frank nets, cell walls, or sub-boundaries can act as
immobilization sites at this stage of the deformation. Thermally activated cross-slip can also block the glide dislocations. The rate of trapping of dislocations is related to an increase in rate of growth of immobile dislocations. Therefore, the coupled evolutionary equations for the mobile and immobile dislocation densities for stage II hardening are given by

\[
\frac{d\rho_m^{(\alpha)}}{d\gamma} = -\frac{g_{\text{immob}}}{b} \rho_m^{(\alpha)1/2} - \frac{g_{\text{min}}}{b^2} \exp\left(-\frac{H}{kT}\right),
\]

\[
\frac{d\rho_im^{(\alpha)}}{d\gamma} = \frac{g_{\text{immob}}}{b} \rho_im^{(\alpha)1/2} + \frac{g_{\text{min}}}{b^2} \exp\left(-\frac{H}{kT}\right),
\]

At moderate and large strains, the third stage, stage III, of hardening is characterized by the dynamic recovery. At temperatures lower than 40% of the melting temperature, the main mechanism of recovery is the annihilation of the screw segments of opposite signs on the expanding dislocation loops. The evolution for the immobile density for this stage is

\[
\frac{d\rho_im^{(\alpha)}}{d\gamma} = -g_{\text{recov}} \rho_{im}^{(\alpha)},
\]

By using the chain-rule and Orowan’s equation, equations (2.30)-(2.33) can be combined to obtain a coupled set of nonlinear evolutionary equations for the mobile and immobile dislocation densities, for each slip-system \(\alpha\)

\[
\frac{d\rho_m^{(\alpha)}}{dt} = \gamma^{(\alpha)} \left( \frac{g_{\text{sour}}}{b^2} \left( \frac{\rho_m^{(\alpha)}}{\rho_m^{(\alpha)1/2}} - \frac{g_{\text{min}}}{b^2} \exp\left(-\frac{H}{kT}\right) - \frac{g_{\text{immob}}}{b} \rho_{im}^{(\alpha)1/2} \right) \right),
\]

\[
\frac{d\rho_im^{(\alpha)}}{dt} = \gamma^{(\alpha)} \left( \frac{g_{\text{min}}}{b^2} \exp\left(-\frac{H}{kT}\right) + \frac{g_{\text{immob}}}{b} \rho_{im}^{(\alpha)1/2} - g_{\text{recov}} \exp\left(-\frac{H}{kT}\right) \rho_{im}^{(\alpha)} \right),
\]

where \(H\) is the activation enthalpy, and \(k\) is Boltzmann’s constant. The \(g\) coefficients indicate the following
• \( g_{sour} \): Coefficient pertaining to an increase in the mobile dislocation density due to dislocation sources.

• \( g_{minter} \): Coefficient related to the trapping of mobile dislocations due to forest intersections, cross-slip around obstacles or dislocation interactions.

• \( g_{recoy} \): Coefficient related to the rearrangement and annihilation of immobile dislocations.

• \( g_{immob} \): Coefficient related to the immobilization of mobile dislocation.

As these evolutionary equations indicate, the dislocation activity related to recovery and trapping are coupled to thermal activation. The thermal activation energy temperature is updated using the temperature evolution equation (equation 2.20).

2.3. Determination of the coefficients for the coupled evolutionary equations

To couple the evolutionary equations to the crystal plasticity formulation, the \( g \)-coefficients in equation (2.34) and (2.35) and the enthalpy \( H \) have to be determined as a function of the deformation mode. The enthalpy, \( H \), is determined by defining an exponential ratio of the current temperature to the reference temperature. Two general conditions, pertinent to the evolution of dislocation densities in crystalline materials, have been used to determine the \( g \) coefficients in equations (2.34) and (2.35).

i. The mobile and immobile dislocation densities saturate at large strains

ii. The relaxation of the mobile dislocation density to a quasi-steady state value occurs much faster than the variation of the immobile density.
These conditions are invoked based on the arguments by Mecking and Kocks (1981), Walgraef and Aifantis (1985a,b), and Kubin and Estrin (1988). They used similar arguments to determine coefficients in equations pertaining to the evolution of mobile and immobile dislocation densities. The saturation of both the immobile and mobile dislocation densities at large strains and the relaxation of both the mobile and immobile densities to different quasi-steady values in f.c.c materials have also been experimentally substantiated by several investigators [see, for example, Mughrabi (1987), Hansen (1990), Bay et al. (1992)]. For a detailed presentation of the process used in determining the g coefficients, refer to Zikry and Kao (1996) and Kamada and Zikry (1998).
CHAPTER 3
NUMERICAL METHOD

The numerical algorithm is presented in this chapter; refer to Zikry (1994b) for a detailed presentation. To update the state of stress of the crystalline material, the total deformation-rate tensor, $D_{ij}$, and the plastic deformation-rate tensor, $D_{ij}^p$, are needed. An implicit finite-element analysis has been used to obtain the total deformation-rate tensor, $D_{ij}$. The displacements are obtained by the quasi-Newton solution for the nonlinear static-equilibrium equation. The update formula used in this algorithm is the Broyden-Fletcher-Goldfarb-Shanno (BFGS) formula. The deformation tensor can be calculated once the displacements are obtained. The $\overline{B}$ method has been used in the calculation to overcome numerical problems associated with incompressible deformation. In the $\overline{B}$ method, the deformation gradient is decomposed into volumetric and deviatoric parts; the volumetric part of the deformation tensor is then computed at reduced quadrature points. The resulting volumetric deformation field eliminates spurious modes that can arise due to incompressible deformation. Once the deformation tensor is obtained from the updated nodal displacements, the total deformation-rate tensor, $D_{ij}$, and the total spin tensor, $W_{ij}$, can be calculated at each load level.

The plastic deformation-rate tensor, $D_{ij}^p$, was obtained by taking the time derivative of the resolved shear-stress

$$\dot{\tau}^{(\alpha)} = \frac{d}{dt} (P_{ij}^{(\alpha)} \sigma_{ij}), \quad (3.1)$$
together with the objective stress rate, and the isotropy assumption of the elastic modulus tensor, resulting in the following nonlinear initial value system of equations for the multiple-slip crystalline model.

\[ \dot{\tau}^{(\alpha)} = L_{ijkl} P_{ij}^{(\alpha)} \left[ D_{kl} - D_{kl}^p \right]. \quad (3.2) \]

Using equation (2.8) and the power law in equation (2.16), equation (3.2) above can be written as

\[ \dot{\tau}^{(\alpha)} = 2G \left( P_{ij}^{(\alpha)} D_{ij} - P_{ij}^{(\alpha)} \left[ \sum_{\beta=1}^{12} P_{ij}^{(\beta)} \gamma_{ij}^{(\beta)} \left( \tau_{ij}^{(\beta)} \right)^{\frac{1}{m}} \right] \right). \quad (3.3) \]

It has been assumed in the above derivation that the lattice spin is a function of the elastic spin. Once the resolved shear stresses are obtained from (3.3). The updated plastic deformation-rate tensor can be obtained by inputting the resolved shear stresses from (3.3) in the power law (2.16) to obtain the updated slip-rates, \( \dot{\gamma}^{(\alpha)} \), which will be used in equation (2.8) to obtain updated plastic deformation-rate tensor. The strain-rate sensitivity parameter, \( m \), determines the nonlinearity of the system of differential equations in (3.3). The slip vectors used in the formulation, \( n_i^{(\alpha)} \) and \( s_i^{(\alpha)} \), rotate with the lattice and it was assumed that the rate of change of the unit vectors is a function of the elastic spin

\[ \dot{n}_i^{(\alpha)} = W_{ij}^* n_j, \quad \dot{s}_i^{(\alpha)} = W_{ij}^* s_j, \quad (3.4a,b) \]

where the elastic lattice spin is obtain from the total and plastic spin tensors as follows

\[ W_{ij}^* = W_{ij} - W_{ij}^p. \quad (3.5) \]

The solution to the system of ordinary differential equations, (3.3), is numerically
difficult, not only due to the nonlinearity of the resolved shear stress, but also because the system of equations is numerically stiff in certain time intervals. The different time scales pertaining to the resolved shear stress on each slip system cause the numerical stiffness of system. This results in eigenvalues corresponding to the Jacobian of the initial value problem that are widely varying. This leads to the growth of numerically propagated error, i.e. instability in the solution of the system of differential equations.

Since the system of equations given by (3.3) is only stiff in some regions of the integration domain, an explicit fifth-order accurate Runge-Kutta method is used over most of the time domain. The propagated error is measured by the growth in the local truncation error. If the time-step must be restricted due to stability and not accuracy, a backward Euler method is used. The general form of backward Euler method can be written as follows

\[ y_{n+1} = y_n + hf (y_{n+1}, t_{n+1}), \]  

(3.6)

which can be derived from general multi-step general formula given by

\[ y_{n+1} = \sum_{i=1}^{k} \alpha_i y_{n+1-i} + h \sum_{i=0}^{k} \beta_i f_{n+1-i}, \]  

(3.7)

where \( h \) is the step size, \( k \) is a fixed integer and either \( \alpha_i \) or \( \beta_i \) is not zero. The backward Euler method, which is both A-stable and stiffly stable, is obtained by setting \( \alpha_1 = 1 \) and \( \beta_o = 1 \).

This adaptive methodology of solving the system of differential equations is efficient since it controls the accuracy and stability of the solution process by providing automatic time step control that is tied to a stiffness ratio function, which monitors the dispersion of the eigenvalues through a local truncation error function. Fifth-order accuracy is obtained by
using time step doubling on the Runge-Kutta fourth-order method. Two numerical solutions are obtained; the first employs a step size of $2h$ and the second solution with two steps, each of size $h$. The two solutions can be written as

$$\tau(t + 2h) = \hat{\tau}_1 + (2h)^5 \phi + O(h^6) + ...., \quad (3.8)$$

$$\tau(t + 2h) = \hat{\tau}_2 + 2(h)^5 \phi + O(h^6) + ...., \quad (3.9)$$

where $\phi$ is of the order $\tau^5(t)/5!$. The fifth-order accurate solution can be obtained by combining the two fourth-order solutions giving

$$\tau(t + 2h) = \hat{\tau}_2 + \frac{\Delta}{15} + O(h^6) + ...., \quad (3.10)$$

where $\Delta$ is the local truncation error which is used as a measure of the solution approximation at a given time step. Given this error measure, an adjusted time-step is calculated as follows

$$h_{new} = F h_{old} \left| \frac{\Delta_o}{\Delta_1} \right|^{0.20}, \quad (3.11)$$

where $h_{new}$ is the modified, adjusted, time-step, and $h_{old}$ is the initial time-step. The actual accuracy at the current time-step is $\Delta_1$, is measured by the supermum norm as max $|\tau_1 - \tau_2|$, and $\Delta_o$ is the desired accuracy measured by $\varepsilon H$. $\varepsilon$ is the tolerance level supplied by the user and $H$ is a scaling factor for fractional errors for the $i^{th}$ equation given by $|\tau| + h \left| \frac{d\tau}{dt} \right|$, where h is the initial time step. The factor $F$ serves to keep the new time-step small enough to be accepted if the truncation error in the next time-step is growing. It can be concluded from equation (3.11) that the adjusted time-step is increased if the truncation error is smaller
than the desired accuracy and on the contrary, the time-step is decreased if the truncation error is greater than the desired accuracy.

Since Runge-Kutta methods have finite stability regions, there can be a growth in the propagated error. Therefore, the time-step, in certain domains, is restricted due to stability and not due to the accuracy requirement given by $\varepsilon H$, which therefore designates a region of stiff behavior. In this computational scheme, the largest allowable time step is specified, i.e., the time-step on the stability boundary. This indicates that the local errors are of the same magnitude as the accuracy tolerance used in equation (3.11). If the time-step is unduly restricted due to stability, the solution will proceed in time, albeit inefficiently, due to the necessity of using intolerably small time-steps. To correctly identify the regions of numerical stiffness and to distinguish a step reduction due to accuracy from a time-step reduction due to stability, a stiffness ratio, $S_R$, has been defined as

\[
S_R = \frac{\left|\text{Re} \lambda\right|_{\text{max}}}{\left|\text{Re} \lambda\right|_{\text{min}}} \left(\frac{1}{t_2 - t_1}\right),
\]

(3.12)

where $\left|\text{Re} \lambda\right|_{\text{max}}$ and $\left|\text{Re} \lambda\right|_{\text{min}}$ are the greatest and smallest absolute values of the real parts of the eigenvalues of the Jacobian of the system of ordinary differential equations given by (3.3) and $t_2 - t_1$ is the time interval of the integration. A large stiffness ratio, $S_R$, indicates that the ratios of the eigenvalues are dispersed relative to the time scale. When the time-step is restricted due to the presence of these widely varying eigenvalues, this is a stability problem and an indication that the initial-value problem is numerically stiff. An increasing stiffness ratio is an indication that for a specified deformation mode, the slip-rates, $\dot{\gamma}^{(\alpha)}$, are much greater for one slip system than for the other active slip systems - one of the slip
systems may be dominating the deformation process. The domination of one slip system over other active slip systems can occur when macroscopic shear bands form in a crystalline solid material (see Zikry1992 and Zikry 1994). In the present analysis, when stiff behavior is encountered, the integration is automatically switched from explicit Runge-Kutta to the backward Euler scheme. Using the backward Euler method leads to a nonlinear system of algebraic equation for the multiple-slip crystalline model. The algebraic system of nonlinear equations was solved using quasi-Newton method.

The adaptive computational algorithm used to update the plastic deformation-rate tensor, has also been used to update the coupled nonlinear mobile and immobile dislocation density evolutionary equations (2.34) and (2.35).
CHAPTER 4
MICROSTRUCTURAL REPRESENTATION OF GRAIN SHAPES, CRYSTALLINE INTERFACES, GRAIN ORIENTATION, AND GRAIN BOUNDARY MISORIENTATION

4.1. VORONOI TESSELLATION FOR GRAIN SHAPE REPRESENTATION

Realistic microstructures need to be represented, not only by accurately modeling crystalline behavior at different scales, but also by accounting for grain shapes and distributions that are physically representative of polycrystalline aggregates. Hence, Voronoi tessellation is used to generate polygons for different grain sizes and distributions.

If we assume that \( P \) is a discrete set of points in real space, \( P \subseteq \mathbb{R}^n \), and \( \bar{x} \) represents any point in space, then for almost any point \( \bar{x} \), there is always one point of \( P \) to which \( \bar{x} \) is closer than \( \bar{x} \) is to any other point of \( P \). If \( P \) contains two points, \( a_1 \) and \( a_2 \), then the perpendicular bisector of the line segment from \( a_1 \) to \( a_2 \) forms a hyperplane. This unique hyperplane represents the set of all possible points equidistant from \( a_1 \) and \( a_2 \). In general, the set of all possible points in space closer to a point \( a_n \) of \( P \) than to any other point of \( P \) constitutes the interior of a convex polytope, polygons in 2-D. These polygons are referred as the Dirichlet domain or Voronoi cell for \( a_n \). The complete set of these polytopes tessellates the whole space, and this defines the Voronoi tessellation corresponding to the set \( P \). Voronoi tessellation is the decomposition of space determined by distances to a prescribed discrete set of points in space. A detailed description of Voronoi decomposition is given by Okabe et al. (1999) and Lili (2001). Once Voronoi diagram was generated by random points based on a
specimen’s geometry, a finite-element mesh was then used for numerical discretization. The use of Voronoi tessellation to represent the grain morphology provides a physically-based microstructural representation of actual grain shapes. In this study, Voronoi tessellation is used to tessellate the specimen domain resulting in 2-D polygons with each polygon representing a grain.

4.2. REPRESENTATION OF GB GEOMETRY, STRUCTURE AND DEGREES OF FREEDOM

Interfaces play a key role in controlling and influencing the thermo-mechanical, chemical and electrical properties of engineering metallic materials. Polycrystalline aggregates contain a network of GBs separating grains, crystals, of various orientations in space.

The mechanical properties of metallic materials are greatly governed by the properties of the point, line and planar defects contained in the crystalline aggregate. In the case of planar defects such as GBs, the structure and geometry of these boundaries greatly contribute to the properties of these boundaries and the overall properties of the polycrystalline aggregate.

A complete description of the GB geometry can be obtained if the crystal structure, lattice parameters and the eight geometrical degrees of freedom are clearly identified (Wolf, 1992). The eight degrees of freedom are subdivided into five macroscopic and three translational or microscopic ones. The microscopic degrees of freedom correspond to rigid body translations parallel and perpendicular to the GB plane. TEM experiments and
computer simulations, which have been conducted on GBs have shown that microscopic degrees of freedom contribute to a lowering of the excess free energy of the system, and they play a key role during the process of GB migration (Smith, 1980 and Bishop, 1982). The macroscopic degrees of freedom describe a pair of grains joined at a boundary (Goux, 1974 and Wolf, 1992). They characterize the overall orientation change between two grains at a GB (Randle, 1996).

In the misorientation scheme used in the microstructural finite-element simulations, the macroscopic DOF are obtained through a relative rotation between the crystallographic orientations of two interpenetrating crystal lattices. The relative rotation is defined by an angle of rotation (misorientation), in which one lattice is rotated about a defined axis of rotation, which is common to both neighboring lattices. Specifically, an angle/axis pair defines the misorientation scheme, as shown in Figure 4.1, for a general GB. The misorientation scheme provides three of the five macroscopic DOF, the remaining two DOF define the boundary plane with reference to one of the interfacing lattices.

When two neighboring crystal lattices interpenetrate and for certain combinations of orientation relationships, a proportion of crystal lattice sites can coincide producing a periodic array of lattice sites. A high density of coincident sites indicates a good fit between the two neighboring grains. This forms the basis of the coincident site lattice (CSL). In CSL models, the reciprocal density of the coinciding lattice points is denoted by the symbol $\Sigma$, and the GB plane is considered a plane running through the CSL, therefore the CSL is only valid physically at the boundary itself (Randle, 1996). CSL models are used to describe the GB geometry because they provide a well-defined set of grain orientations needed to represent GB misorientations.
4.3. GRAIN ORIENATIONS AND GB MISORIENATIONS

In polycrystalline metallic materials, slip is characterized by dislocation motion, or glide, on the closest packed planes in the crystal, and in preferred crystallographic directions, which have the highest linear density. The planes on which slip occurs are called slip planes and the directions in slip planes where dislocations move are called slip directions. In f.c.c. materials, slip occurs on the family of \{111\} octahedral closed packed planes and in the \langle110\rangle directions. There are eight \{111\} planes in the f.c.c. unit cell. However, \{111\} planes of opposite faces of the octahedral are parallel to each other, and this reduces the planes to four. Each one of the four \{111\} octahedral planes contains three \langle110\rangle directions and noting that the reverse directions are neglected, since shear slip can carry on a positive or negative value. As a result, there are 12 possible closed packed slip systems in f.c.c. metallic materials, 4 - \{111\} planes with 3 -\langle110\rangle directions for each plane.

The slip systems in each grain are oriented with respect to a global coordinate system depending on initial grain orientations. This can be achieved by applying the appropriate transformation laws to the unit vectors, \(\mathbf{n}\) and \(\mathbf{s}\), defining each slip system, where \(\mathbf{n}\) is the unit vector normal to the slip plane and \(\mathbf{s}\) is the unit vector that lays on the slip plane in the slip direction. The unit vectors defining slip systems are transformed as follows

\[
\hat{n}_i = M_{ij}n_j, \tag{4.1}
\]

\[
\hat{s}_i = M_{ij}s_j, \tag{4.2}
\]
where \( \hat{n}_i \) and \( \hat{s}_i \) are the transformed unit vectors defining the slip system for each grain, \( n_j \) and \( s_j \) are the unit vectors defining the slip system in the global coordinate system and \( M_{ij} \) is the misorientation matrix.

### 4.3.1 Euler Angles

Grain orientations are defined by a specified set of Euler angles. Any rotation in space can be generated by three sequential rotations through certain angles. These angles are referred as Euler angles (Randle, 1993). In the misorientation context of GBs, the two interpenetrating crystal grains will have two sets of crystal axes, \( x_1y_1z_1 \) for grain 1 and \( x_2y_2z_2 \) for grain 2. Assuming that the crystal axes for grain 1 are in the reference position, three rotations are required to align the crystal axes of grain 2 with the crystal axes of the reference grain, grain1. These rotations can be obtained as follows:

Rotation 1 = \( m_1 = \varphi_1 \) about axis \( z_2 \);

Rotation 2 = \( m_2 = \Phi \) about axis \( x'_2 \);

Rotation 3 = \( m_3 = \varphi_2 \) about axis \( z_1 \).

The first rotation is about the \( z_2 \) axis with an angle of \( \varphi_1 \) whereas the second rotation is one about axis \( x'_2 \), which is the new direction of \( x_2 \) after rotation 1, with an angle of \( \Phi \) and finally the third rotation is one about axis \( z_1 \) with an angle of \( \varphi_2 \). Figure 4.2 illustrates these three rotations. The total misorientation matrix that results from the above three rotations is given by
\[M = \mathbf{m}_3 \mathbf{m}_2 \mathbf{m}_1,\] (4.3)

where \(M\) is the misorientation matrix, and the elements of this matrix can be obtained as a function of Euler angles as follows

\[
M = \begin{bmatrix}
\cos \varphi_1 \cos \varphi_2 - \sin \varphi_1 \sin \varphi_2 \cos \Phi & \sin \varphi_1 \cos \varphi_2 + \cos \varphi_1 \sin \varphi_2 \cos \Phi & \sin \varphi_2 \sin \Phi \\
-\cos \varphi_1 \sin \varphi_2 - \sin \varphi_1 \cos \varphi_2 \cos \Phi & -\sin \varphi_1 \sin \varphi_2 + \cos \varphi_1 \cos \varphi_2 \cos \Phi & \cos \varphi_2 \cos \Phi \\
\sin \varphi_1 \sin \Phi & -\cos \varphi_1 \sin \Phi & \cos \Phi
\end{bmatrix}.\] (4.4)

4.3.2. THE GB MISORIENTATION SCHEME

The geometrical description of the GB geometry can be defined using the misorientation scheme by specifying an angle of misorientation, \(\theta\), an axis of misorientation with UVW indices, and a vector \(\mathbf{N}\) corresponding to the normal of the GB plane as shown in figure 4.1. The orthogonal misorientation matrix \((M)\) that defines the orientation difference between two neighboring grains is obtained in terms of the angle/axis pair as

\[
M = \begin{bmatrix}
U^2(1-\cos \theta) + \cos \theta & \cos \theta & \cos \theta \\
UV(1-\cos \theta) - W \sin \theta & V^2(1-\cos \theta) + \cos \theta & V \cos \theta \\
WU(1-\cos \theta) - V \sin \theta & VW(1-\cos \theta) + U \sin \theta & W^2(1-\cos \theta) + \cos \theta
\end{bmatrix}.\] (4.5)
Figure 4.1: Illustration of the misorientation scheme for the GB geometry
Figure 4.2: Definition of Euler Angles
CHAPTER 5

CONVERGENCE OF NUMERICAL SIMULATIONS

In this study, different polycrystalline aggregates were constructed using Voronoi tessellation. A polycrystalline solid consisting of 11 grains (figure 5.1) was used in the convergence analysis; the specimen aspect ratio was set to be 1:2 with dimensions of $100 \times 200 \, \mu m^2$. Symmetric boundary conditions were used for the bottom and left edges of the specimen, the model represents the top right quarter of a larger polycrystalline aggregate. Monotonic quasi-static loading was applied in which the specimen was strained in tension along the [001] direction (figure 5.2) with a net applied strain rate of $7.143 \times 10^{-4} \, s^{-1}$.

Material properties used in this analysis are representative of austenitic stainless steel, which has an f.c.c. crystalline structure even at room temperatures. Table 5.1 lists material properties used in the simulations. GB regions were given the same material properties as the grain bulk. Euler angles defining grain orientations were assigned randomly with a maximum misorientation of $15^\circ$.

Table 5.1: Material properties used in the mesh convergence analysis

<table>
<thead>
<tr>
<th>Material Properties</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s Modulus</td>
<td>193 GPa</td>
</tr>
<tr>
<td>Static Yield Stress</td>
<td>207 MPa</td>
</tr>
<tr>
<td>Poisson’s Ration</td>
<td>0.3</td>
</tr>
<tr>
<td>Reference Strain Rate</td>
<td>0.001</td>
</tr>
<tr>
<td>Critical Strain Rate</td>
<td>$10^4$</td>
</tr>
<tr>
<td>Reference Shear Stress Interaction Coefficients</td>
<td>0.3</td>
</tr>
<tr>
<td>Strain Rate Sensitivity Parameter</td>
<td>0.01</td>
</tr>
</tbody>
</table>
Three different FEM meshes for the 11-grain polycrystalline aggregate model were obtained with 1175 elements (1254 nodes) for the first mesh, 2217 elements (2325 nodes) for the second mesh and 3296 elements (3401 nodes) for the third mesh. The stress-strain curve and deformed mesh were obtained for all three simulations. The nominal axial stress for the numerical results is obtained as follows

\[
\sigma_{\text{nominal}} = \frac{1}{A} \int \sigma_{2i} n_i dA,
\]

(5.1)

where \(A\) is the initial non-deformed cross-sectional area of the specimen, \(n_i\) is the unit normal vector, \(\sigma_{2i}\) is the surface traction on the top surface (top boundary) of the specimen.

The mesh convergence of the 11-grain polycrystalline aggregate is investigated by comparing the nominal stress-strain response (figure 5.3) and the deformed mesh (figure 5.4) for the three FEM meshes- 1175, 2217 and 3296 elements.

There was no variation in the final deformed configuration of the specimen between all three FEM meshes, 1175, 2217 and 3296 elements. The stress-strain response was also identical for all three FEM meshes, which indicates the convergence of the three meshes. Based on this analysis, an FEM mesh with 2217 elements will be utilized for most of the simulations. However, more refined FEM meshes will be used for aggregates with pre-existing cracks.
Figure 5.1: 11-grain polycrystalline aggregate
Figure 5.2: Loading and geometrical configurations
Figure 5.3: Nominal stress-strain curves for the 11-grain model with three FEM meshes
Figure 5.4: Deformed mesh for the 11-grain model for (a) 1175 elements (b) 2217 elements (c) 3296 elements
CHAPTER 6

POLYCRYSTALLINE AGGREGATE MODELS WITH CSL GBs

The multiple-slip crystal plasticity finite element based constitutive formulation that is coupled to the evolutionary equations of mobile and immobile dislocation densities were employed to investigate the inelastic deformations and material failure modes in f.c.c. polycrystalline materials with different CSL GBs. It has been shown experimentally that GB misorientation can greatly affect its properties, such as strength (Meyers and Ardell 1993), energy (McLean 1973) and resistance to crack nucleation and corrosion (Watanabe 1983).

In this chapter, $\Sigma 3$ and $\Sigma 17b$ CSL GBs were implemented in polycrystalline aggregate models with a number of grains that ranged from 11 to 50 grains. The choice of implementing $\Sigma 3$ and $\Sigma 17b$ CSL models in the formulation is based on different experimental observations and numerical simulations (Yoo and King 1990, and Lin and Pope 1992) on f.c.c. metallic materials, which suggest that single dislocation pile-ups result in transgranular failure modes in low angle CSL GBs and symmetric double dislocation pile-ups result in intergranular failure modes in high angle CSL GBs.

Three distinct aggregate models were used in this study and the developed Voronoi tessellation algorithm was used to generate specimen models with 11, 25 and 50 grains. The specimen aspect ratio used in all aggregate models was set to be 1:2 with dimensions of $100 \times 200 \, \mu m^2$. Monotonic quasi-static loading was applied, and specimens were displaced in tension along [001] direction with symmetric boundary conditions.
In this study, GBs, which characterize the interfacial region between two neighboring grains, are defined as separate regions with unique material and geometrical properties. Since GB regions are generally smaller in comparison with the bulk dimensions of the grains, the width of these GB regions was assigned to be equal or less than 10% of the grain diameter, which ranged from 32 $\mu m$ for the 11-grain model to 12 $\mu m$ for the 50-grain model. The GB regions were generated as follows: 2-D polygons tessellate a domain with a prescribed boundary with each one of the generated polygons representing a grain. All lines defining the polygons, which are within the specimen boundary, domain, were selected during the meshing process for the quadrilateral elements corresponding to the GB region. The GBs were generally modeled with refined meshes, in comparison with the grain interior, to account for the higher dislocation densities and stresses that would arise at GB regions.

The CSL models were implemented in the polycrystalline aggregate models by controlling crystal lattice orientations; each two neighboring grains were oriented in space such that the total misorientation at the GB separating the two neighboring grains will satisfy the CSL criteria. Grain orientations were defined using the misorientation scheme (angle/axis pair), as indicated in Table 6.1 for the $\Sigma 3$ and $\Sigma 17b$ CSL GBs.

<table>
<thead>
<tr>
<th>CSL Model</th>
<th>UVW</th>
<th>$\theta$ (Degrees)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Sigma 3$</td>
<td>111</td>
<td>60</td>
</tr>
<tr>
<td>$\Sigma 17b$</td>
<td>110</td>
<td>86.63</td>
</tr>
</tbody>
</table>

Table 6.1: Angle/axis pair for $\Sigma 3$ and $\Sigma 17b$ CSL GBs
Crystal lattice orientations needed to generate the CSL GB misorientations were obtained as follows: If an angle/axis pair of $\theta / \langle{U VW}\rangle$ is needed to generate a specific CSL model, each two neighboring grains were oriented about the same misorientation axis (UVW) needed to generate the CSL GB between the two grains. The first grain of the two neighboring grains was oriented by angle ($\frac{\theta}{2}$) about the axis UVW while the other grain was oriented by angle ($-\frac{\theta}{2}$) about the same axis (UVW). This process was repeated for every two neighboring grains in the polycrystalline aggregate. Due to geometrical compatibilities and to prevent having two neighboring grains with the same exact orientation, a polycrystalline aggregate will not have all of its grain orientations satisfying any CSL orientation, therefore grains, which did not satisfy a specified CSL boundary misorientation, were assigned random orientations that are close to the misorientation angle $\theta$. Therefore, the percentage of CSL GBs to the total GBs in the models ranged between 60% -73% for the 11, 25 and 50 grain models. Figure 6.1 illustrates the process of orienting two neighboring grains for the generation of CSL boundary. The distribution of the population of CSL GBs and the resulting grain connectivity in the aggregate models used in this study are shown in figure 6.2. The polycrystalline aggregate models employed in the analysis are shown in Figure 6.2 and the same polycrystalline aggregate models with the elements representing the GB network colored in blue are shown in figure 6.3. The material properties used here are representative of austenitic stainless steel. Austenitic steels have an f.c.c. atomic structure, which provides more slip planes for dislocation motion. In typical carbon steel, cooling transforms the steel structure from austenite to a mixture of ferrite and cementite. For austenitic steels, the nickel and chrome contents maintain the austenite phase and slow down
the transformation process. The high chrome and nickel content suppress the transformation keeping the structure fully austenite when cooling. Material properties, which are representative of austenitic stainless steel, with nickel and chromium contents ranging between 8-11% and 18-20%, respectively are used. For the analysis in this chapter, it was also assumed that dislocations in the grain bulk and the GB region are of the same kind and have the same initial values.

Table 6.2 lists all parameters and material properties for the grain bulk and GB region used in the analysis of the 11, 25 and 50-grain models with $\Sigma$ 3 and $\Sigma$ 17b CSL GBs. The specimens were loaded monotonically in tension by applying a macroscopic nominal extension along [001] direction with a strain-rate of $7.143 \times 10^{-4}$ s$^{-1}$. The final nominal extension was set to be 15%.

Table 6.2: Material properties for the grain bulk and GB region

<table>
<thead>
<tr>
<th>Property</th>
<th>Grain bulk</th>
<th>GB region</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial Mobile Dislocation Density</td>
<td>$10^7$</td>
<td>$10^7$</td>
</tr>
<tr>
<td>Initial Immobile Dislocation Density</td>
<td>$10^{10}$</td>
<td>$10^{10}$</td>
</tr>
<tr>
<td>Young’s Modulus</td>
<td>193 GPa</td>
<td>193 GPa</td>
</tr>
<tr>
<td>Static Yield Stress</td>
<td>207 MPa</td>
<td>207 MPa</td>
</tr>
<tr>
<td>Poisson’s Ration</td>
<td>0.3</td>
<td>0.3</td>
</tr>
<tr>
<td>Reference Strain Rate</td>
<td>0.001</td>
<td>0.001</td>
</tr>
<tr>
<td>Critical Strain Rate</td>
<td>$10^4$</td>
<td>$10^4$</td>
</tr>
<tr>
<td>Reference Shear Stress Interaction Coefficients</td>
<td>0.3</td>
<td>0.3</td>
</tr>
<tr>
<td>Strain Rate Sensitivity Parameter</td>
<td>0.01</td>
<td>0.01</td>
</tr>
</tbody>
</table>

Sections in this chapter are organized as follows: $\Sigma$ 3 CSL GBs for the 11, 25 and 50-grain models were investigated and discussed in section 6.1, $\Sigma$ 17b CSL GBs for the 11, 25 and 50-grain models are presented in section 6.2. Section 6.3 discusses the importance of
accounting for the variation of GB strength and mechanical properties as a function of misorientation. In section 6.3, Σ3 CSL GB properties were modified for the 25-grain model and compared with the one with the Σ17b CSL boundaries. Conclusions and summary are presented in section 6.4.

6.1. Σ3 CSL GBs IN F.C.C. POLYCRYSTALLINE AGGREGATES

The Σ3 CSL model is used to represent GB geometry for different polycrystalline aggregate models. Nominal stress-strain curves for 11, 25 and 50-grain models with Σ3 CSL GBs are shown in figure 6.4. It can be seen that the global stress-strain response for the 11, 25 and 50-grain Σ 3 CSL models is approximately the same. This supports the assumption by Schmitz et al. (1989) that bicrystals separated by low-angle tilt boundaries can be treated as single crystals, and hence the orientation of these low-angle boundaries, in the absence of solutes or other impurities at the GB, may not be one of the main mechanisms resulting in material instabilities and failure. Although the global response is almost identical for all models, the formulation is able to capture all local differences in plastic shear slip, lattice rotation and normal stress between all models. At 15% nominal strain, the maximum lattice rotation of approximately $14^\circ$ in the 11-grain model occurs inside one of the grains located in the middle of the specimen (figure 6.5(a)). It should also be noted that the larger lattice rotation region did not occur over the whole entire grain and a portion of that grain rotated with a value of $-8^\circ$ (clockwise rotation). For the 50-grain model and at 15% nominal strain, lattice rotation ranged between $-8^\circ$ and $18^\circ$ with the maximum value attained at the free
surface inside one of the grains (figure 6.5(b)). The same observation can be seen in the 50-grain aggregate, a certain portion of the grain had the larger rotation region, while lattice rotation in the other portion of the grain did not exceed $-4^\circ$. Contours of accumulated plastic shear slip for the 11 and 50-grain models are shown in figures 6.6(a)-(b) respectively. The maximum accumulated plastic shear slip in the 11-grain model was 0.5 (figure 6.6(a)). Regions of intensive plastic shear slip are located inside the grains near the free surface and they extend towards the GB. A shear slip band started to form in another location, it occurred at the free surface and extended towards the inside grains along the GBs. For the 50-grain model and at 15% nominal strain, the maximum accumulated plastic shear slip is 0.5. Regions of high plastic shear slip occurred near the free surface in two different regions. Also, a region of high shear slip occurred on the left free surface of the specimen, where the symmetric boundary conditions are enforced. Contours of the normal stress, $\sigma_{yy}$, normalized by the macroscopic yield stress of the aggregate are shown in figures 6.7(a)-(b) for the 11 and 50-grain respectively. For the 11-grain aggregate (figure 6.7(a)), the maximum stress, $\sigma_{yy}$, is approximately $8 (8\sigma_{yield})$. Traces of high stress occurred at the free surface and extended inside the aggregate. These traces are concentrated inside one of the grains near the GB region. The maximum stress, $\sigma_{yy}$, in the 50-grain model is approximately 8.5. Bands of high normal stress can be identified; these bands extend from the free surface of one side of the aggregate to the free surface on the other side at angle of approximately $45^\circ$ to the loading direction.

Activity of dislocation densities on different slip systems was investigated in order to gain a more detailed understanding of the microstructural features and how it can be related
to the global response of the models under study. For the 11-grain model, the most active slip
systems were identified as (111)[\overline{T}01], (111)[\overline{T}10], (\overline{T} \overline{T} 1)[011] and (1 \overline{T} 1)[011]. Contours
of the immobile dislocation densities for the most active slips systems are shown in figures
6.8(a)-(d). The maximum immobile dislocation densities for slip systems (111)[\overline{T}01],
(111)[\overline{T}10], (\overline{T} \overline{T} 1)[011] and (1 \overline{T} 1)[011] were approximately $9 \times 10^{16} \text{m}^{-2}$, $1.5 \times 10^{17} \text{m}^{-2}$,
$1.1 \times 10^{17} \text{m}^{-2}$ and $1.3 \times 10^{17} \text{m}^{-2}$ respectively. In all active slip systems, immobile densities
attained their maximum values near the GBs; this can indicate slip immobilization at the GB
due to accumulation and pile-ups of immobile densities. Immobile dislocation density pile-
ups at the GBs as seen in figure 6.8(a)-(d) result in stress concentration near the GB, this can
be observed in the normal stress, $\sigma_{YY}$, contour for the 11-grain model (figure 6.7).

For the 50-grain aggregate model, the most active slip systems were identified as
(111)[\overline{T}01], (111)[\overline{T}10], (\overline{T} \overline{T} 1)[011] and (1 \overline{T} 1)[011]. The maximum attained
immobile densities were $1.1 \times 10^{17} \text{m}^{-2}$, $1.5 \times 10^{17} \text{m}^{-2}$, $1.3 \times 10^{17} \text{m}^{-2}$ and
$2.0 \times 10^{17} \text{m}^{-2}$ respectively. Contours of the immobile densities are shown in figure 6.9(a)-(d).
Immobile densities on active slip systems were higher for the 50-grain model than the 11-
grain one. Dislocation densities attained its maximum at the GBs; these pile-ups as to the 11-
grains model are an indication of slip immobilization at the GB. Regions of high immobile
densities occur also near the free surface at the GBs, these regions are characterized with
extensive lattice rotations (figure 6.5(b)).
6.2. Σ 17b CSL GBS IN F.C.C. POLYCRYSTALLINE AGGREGATES

In this section, planar deformation fields in f.c.c. polycrystalline aggregates with Σ17b CSL GBs were simulated. The same procedure, which was used in section 6.1 to simulate models with Σ3 CSL GBs, was utilized to generate models with Σ17b CSL GBs. The angle/axis pair needed to generate a Σ17b CSL boundary is given in table 6.1.

Nominal stress-strain curves for 11, 25 and 50-grain models are shown in figure 6.10. The stress is normalized by the macroscopic yield stress of the aggregate. At nominal strain of 15%, the maximum global stress is approximately 6.89, 7.19 and 7.50 for the 11, 25 and 50-grain models respectively. Contours of crystal lattice rotation for the 11 and 50-grain models are shown in figure 6.11(a)-(b). In the 11-grain model, lattice rotation ranged between −6° and 7°. Bands of high lattice rotation occur in the aggregate along the GBs, some of these bands occur at the free surface at extend to the GBs. At the free surface of the 11-grain model, there exist two regions separated by a GB where lattice rotations are equal in magnitude and opposite in sign across the GB. Lattice rotation contour for the 50-grain model is shown in figure 6.11(b), rotations ranged between −9° and 6° and traces of extensive lattice rotation occur throughout the aggregate. Most of these traces occur at the free surface and extend inside the aggregate. For the 11-grain model, the maximum accumulated plastic shear slip is 0.7 (figure 6.12(a)) whereas for the 50-grain model, the maximum plastic shear slip was 0.75 (figure 6.12(b)). Regions and bands of plastic shear slip are more localized for the 11-grain model than the 50-grain one. Localized regions of accumulation in the 11-grain model occur at the free surface. Contours of normal stress,
are shown in figure 6.13(a)-(b) for the 11 and 50-grain models respectively. Stress values are normalized by the yield stress of the aggregate. Normal stress, \( \sigma_{yy} \), attained a maximum value of 14 in the 11-grain model and approximately 15 in the 50-grain one. In both models (11 and 50 grains), GB regions are characterized by low stress, \( \sigma_{yy} \), values. Regions of high normal stress, \( \sigma_{yy} \), are observed for both models, these regions are located on the left free surface of the aggregates.

Active slip systems for the 11-grain model were identified as \((111)[\overline{1}0]\), \((\overline{11}1)[\overline{1}0]\), \((\overline{1}11)[101]\) and \((\overline{1}1\overline{1})[101]\). Contours of Immobile dislocation densities for these active systems for the 11-grain aggregate are shown in figure 6.14(a)-(d). Immobile densities attained maximum values of \(4.0 \times 10^{17} \text{ m}^{-2}\), \(2.8 \times 10^{17} \text{ m}^{-2}\), \(2.2 \times 10^{17} \text{ m}^{-2}\) and \(1.8 \times 10^{17} \text{ m}^{-2}\) for each one of the active slip systems respectively. The maximum immobile density of \(4.0 \times 10^{17} \text{ m}^{-2}\) on slip system \((111)[\overline{1}0]\) occurred near the free surface at the GB. Accumulation of immobile densities for the 11-grain model with \(\Sigma17b\) boundaries occurred on smaller and more local regions than the ones for the 11-grain aggregate with \(\Sigma3\) GBs.

For the 50-grain model, active slip systems were \((111)[\overline{1}01]\), \((111)[\overline{1}10]\), \((\overline{1}1\overline{1})[\overline{1}0]\) and \((\overline{1}1\overline{1})[101]\). Maximum immobile densities were \(2.2 \times 10^{17} \text{ m}^{-2}\), \(4.2 \times 10^{17} \text{ m}^{-2}\), \(4.0 \times 10^{17} \text{ m}^{-2}\) and \(2.2 \times 10^{17} \text{ m}^{-2}\) for each one of the active slip systems respectively. Regions of immobile dislocation density accumulation occurred near the free surface on all active slip systems. Immobile densities on slip systems \((111)[\overline{1}10]\) and \((\overline{1}1\overline{1})[\overline{1}0]\) could result in a double symmetric pile-up of immobile density. This region of
potential double symmetric accumulation of immobile density corresponds to a region of localized normal stress, $\sigma_{yy}$, which makes it a potential crack site, which will nucleate and propagate at the immobile density pile-up site along the GB. Crack growth along the GBs is a characteristic of intergranular failure modes observed in high angle boundaries (see, for example, Watanbee, 1983).

6.3. GB STRENGTH AND MISORIENTATION

The orientation and structure of the GB are crucial factors in the characterization of deformation modes and failure mechanisms in polycrystalline metallic materials. Dislocation characteristics, grain and GB properties, topological effects of the internal microstructure, and the cohesive strength of internal properties are intricately related to GB misorientation. Different experimental studies have indicated that GB properties including the mechanical properties vary as function of GB geometry and misorientation, (Wolf, 1992, Lin and Pope 1992 and Meyers and Ardell 1993).

In this section, the effects of GB strength and properties on the planar deformation and failure mode mechanisms of polycrystalline aggregate were investigated. The variation of GB strength and properties as a function of misorientation has been accounted for by specifying the material properties of GB regions. The $\Sigma3$ and $\Sigma17b$ CSL GBs were implemented in the polycrystalline aggregate model with 25 grains. The $\Sigma3$ CSL, which is a low-angle CSL GB, is characterized by its strength and high fracture toughness in comparison with the $\Sigma17b$ CSL GB. Therefore, transgranular cracks can have a tendency to
nucleate and grow in low angle CSL GBs whereas intergranular cracks can be dominant in high-angle CSL GBs (Meyers and Ardell 1993 and Peralta, year). Hence, a comparison between different deformation and failure modes for a $\Sigma 3$ CSL aggregate and a $\Sigma 17b$ aggregate has been conducted. Crystallographic misorientations needed to generate CSL boundaries are given in table 6.1. It is assumed that the elastic modulus and the yield strength for the $\Sigma 3$ CSL GB regions are one and a half times larger than $\Sigma 17b$ CSL GB regions. Material properties are representative of austenitic stainless steel. Table 6.3 lists material properties for the $\Sigma 3$ and $\Sigma 17b$ CSL GB regions. This assumption is based on observations by Lin and Pope (1992) that $\Sigma 3$ GBs are stronger than $\Sigma 17b$ ones.

**Table 6.3:** Material properties for the $\Sigma 3$ and $\Sigma 17b$ GB region

<table>
<thead>
<tr>
<th>Property</th>
<th>$\Sigma 3$ CSL</th>
<th>$\Sigma 17b$ CSL</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial Mobile Dislocation Density</td>
<td>$10^7$</td>
<td>$10^7$</td>
</tr>
<tr>
<td>Initial Immobile Dislocation Density</td>
<td>$10^{10}$</td>
<td>$10^{10}$</td>
</tr>
<tr>
<td>Young’s Modulus</td>
<td>289.5 GPa</td>
<td>193 GPa</td>
</tr>
<tr>
<td>Static Yield Stress</td>
<td>310.5 MPa</td>
<td>207 MPa</td>
</tr>
<tr>
<td>Poisson’s Ration</td>
<td>0.3</td>
<td>0.3</td>
</tr>
<tr>
<td>Reference Strain Rate</td>
<td>0.001</td>
<td>0.001</td>
</tr>
<tr>
<td>Critical Strain Rate</td>
<td>$10^4$</td>
<td>$10^4$</td>
</tr>
<tr>
<td>Reference Shear Stress Interaction Coefficients</td>
<td>0.3</td>
<td>0.3</td>
</tr>
<tr>
<td>Strain Rate Sensitivity Parameter</td>
<td>0.01</td>
<td>0.01</td>
</tr>
</tbody>
</table>

The global stress-strain response for the aggregate models with the CSL boundaries is shown in figure 6.16. Higher global stresses are attained in the aggregate with $\Sigma 17b$ GBs, despite the fact that Young’s modulus and the yield strength for GBs are higher for the $\Sigma 3$ CSL model than the one with $\Sigma 17b$ GBs. Contours of lattice rotation for the models with
CSL GBs are shown in figures 6.17(a)-(b). For the Σ3 CSL model, figure 6.17(a), certain grains were characterized by high rotation whereas other grains had very little rotations. Lattice rotation ranged between $-10^\circ$ and $6^\circ$. For the 25-grain model with Σ17b GBs maximum lattice rotation exists near the free surface and collective grain rotations can not be clearly identified as the model with Σ3 GBs. Lattice rotation ranged between $-6^\circ$ and $5^\circ$.

Accumulated plastic shear slip contours are shown in figures 6.18(a)-(b). For the aggregate model with Σ3 GBs, the maximum plastic shear slip was 0.6 and it occurred at the top right corner of the specimen. Also, localized regions of accumulation exist throughout the specimen. The maximum plastic shear slip for the aggregate with Σ17b GBs was 0.7 and localized regions of plastic strain exist at the free surface of the specimen only.

Contours of the normal stress, $\sigma_{yy}$, normalized by the aggregate yield strength are shown in figures 6.19(a)-(b). The normal stress for the aggregate with Σ3 GBs is shown in figure 6.19(a), traces of high stress occur at the GB. This is because the GB strength was set to be higher the grain bulk strength. These traces of high stress exist in bands along GBs and they are aligned with the loading axis, this can be indication that GBs that are aligned with the loading axis can be the primary carrier of the external loading. The maximum normal stress, $\sigma_{yy}$, was approximately 11 ($11\sigma_{Yield}$). For the aggregate model with Σ17b GBs, traces of high normal stress did not occur along GB regions and the maximum normal stress was 13. The maximum normal stress is localized in a small region near the top right corner of the specimen.

The most active slip systems were identified for each model, and the dislocation densities were calculated on each of the active slip systems. For the aggregate with Σ3 GBs,
the most active slip systems were \((111)[\bar{T}01]\), \((111)[T10]\), \((\bar{T}T1)[011]\) and \((1\bar{T}1)[011]\). Contours of Immobile dislocation densities for each one of the active slip systems are shown in figures 6.20(a)-(d). Immobile densities attained maximum values of \(1.7 \times 10^{17} \text{ m}^{-2}\), \(1.8 \times 10^{17} \text{ m}^{-2}\), \(1.5 \times 10^{17} \text{ m}^{-2}\) and \(1.5 \times 10^{17} \text{ m}^{-2}\) for each one of the active slips systems mentioned above respectively. Collective grain behavior can be observed in which certain grains having orientations that are favorable for slip had high densities of immobile dislocations. For slip system \((111)[\bar{T}10]\), the accumulation of immobile dislocation densities can be observed on multiple grains, these regions of accumulation regions occur near the GBs. immobile densities accumulated on one grain only for the slip system \((111)[\bar{T}10]\). Accumulation of immobile densities for slip systems \((\bar{T}T1)[011]\) and \((1\bar{T}1)[011]\) occurred at the free surface only and immobile density activity was less in the interior grains. Accumulation of immobile dislocation densities at the GBs can be an indication of immobile density pile-ups at these GBs, which can result from slip immobilization at the GBs. For the aggregate model with \(\Sigma 17b\) GBs, the most active slip systems were \((111)[\bar{T}01]\), \((\bar{T}T1)[\bar{T}10]\), \((\bar{T}11)[101]\) and \((1\bar{T}1)[\bar{T}01]\) with a maximum immobile dislocation densities of \(1.6 \times 10^{17} \text{ m}^{-2}\), \(2.4 \times 10^{17} \text{ m}^{-2}\), \(1.2 \times 10^{17} \text{ m}^{-2}\) and \(1.3 \times 10^{17} \text{ m}^{-2}\)(figures 21(a)-(d)). Collective grain behavior can be observed for the immobile densities on system \((\bar{T}11)[101]\) and \((1\bar{T}1)[\bar{T}01]\) whereas accumulation of immobile densities occurred at the top right corner of the specimen for systems \((111)[\bar{T}01]\) and \((\bar{T}T1)[\bar{T}10]\).
6.4. CONCLUSIONS AND SUMMARY

The multiple-slip crystalline constitutive formulation that is coupled to the evolutionary equations of mobile and immobile dislocation densities was used to investigate the effects of grain shape, size and orientation, on the inelastic finite deformation and failure modes mechanisms in f.c.c. metallic aggregates with different distributions of CSL GBs.

Aggregates with the $\Sigma 3$ GBs are characterized by their strength and resistivity to crack nucleation as evidenced by the higher local stresses and accumulation of dislocation-densities at the GB regions. The local resolved shear stresses were lower in the grain interior and along the most active slip-systems, which may be an indication that transgranular modes may dominate for this orientation. For the aggregate with $\Sigma 17b$ GBs, the normal stress and dislocation-densities were lower in comparison with the stresses in the grain-interiors. Hence, this may indicate that intergranular failure modes may be dominant for aggregates with $\Sigma 17b$ GBs.

Inelastic deformation fields and different mechanisms of material failure modes for polycrystalline aggregates with $\Sigma 3$ GBs. were discussed in section 6.1. The global stress-strain response was identical for the 11 and 50-grain models, this can be an indication that aggregates with high frequency of low-angle CSL GBs behave like single crystals regardless of the number of grains (Schmitz et al., 1989). For both aggregates (11 and 50 grains), the maximum lattice rotation occurred inside the grain near the free surface. It was also noted that the maximum lattice rotation for both models did not occur over the whole entire grain but a certain portion of it and the other portion had less intense lattice rotations.
Potential failure paths can be predicted for the Σ3 aggregate models based on contours of normal stress, $\sigma_{yy}$, plastic shear slip, and immobile dislocation density on most active slip systems. For the 11-grain model, regions of accumulation of immobile dislocation densities on slip systems $(111)[T10]$ and $(1\bar{T}1)[011]$ occurred inside the grains and near the GB regions. Also, these accumulation sites correspond to regions of high normal stress, $\sigma_{yy}$. This can be an indication of slip immobilization at the GBs, which resulted in stress concentration. Potential failure paths for the 11-grain model with Σ3 GBs are shown in figure (6.22).

For the 50-grain model, immobile dislocation density on slip systems $(111)[T10]$ and $(1\bar{T}1)[011]$ were the highest. Accumulation regions of immobile densities occurred inside the grains and at the free surface and they also corresponded to stress concentration sites that could have resulted from pile-ups of immobile densities. Figure (6.23) shows the potential crack sites and their projected paths for the 50-grain aggregate with Σ3 GBs.

Polycrystalline aggregates with Σ17b GBs were investigated in section 6.2. Differences in the global stress-strain response appear for the 11, 25 and 50-grain models. This is because of the large variations of the crystal lattice initial orientations and the subsequent lattice rotations during the coarse of deformation. For the 11-grain model, lattice rotation was symmetric about one of the CSL GBs located at the left free surface of the specimen. This GB region corresponds to a stress concentration site and immobile dislocation density activity on slip systems $(\bar{T}\bar{T}1)[\bar{T}10]$ and $(\bar{T}11)[101]$ which can form double symmetric accumulation and pile-ups along this GB region. These potential regions
of accumulation are accompanied by high stress concentration at the GB region. For the 50-grain model, regions of accumulated plastic shear slip occur at the free surface of the specimen, these regions of accumulation are accompanied by high lattice rotation along the GBs and accumulation of immobile dislocation densities on four active slip systems. Figures (6.24 and 6.25) show potential failure paths for the 11 and 50-grain models with Σ17b GBs.

In section 6.3, the mechanical properties for the 25-grain model with Σ3 CSL GBs were artificially modified based on experimental observations by Lin and Pope (1992), and Meyers and Ardell (1993), which suggest that Σ3 GBs are stronger and have higher fracture strength than Σ17b GBs. The aggregate with Σ17b GBs was at higher state of stress than the one with Σ3 GBs (figure 6.16). Collective grain behavior for the crystal lattice rotations can be seen for the aggregate with Σ3 GBs. Regions of intensive plastic shear slip can be seen for the aggregate with Σ3 GBs, these regions of intensive accumulation occurred inside the grains near the GBs and immobile dislocation density activity on four slip systems can be observed at these regions. Figure (6.26) shows the suggested failure paths for the aggregate with Σ3 GBs.

For the aggregate with Σ17b GBs, lattice rotations are less than the aggregate with Σ3 GBs. regions of localized intensive plastic shear slip are located at the specimen’s free surface and they correspond to regions of high immobile density along the GBs. Potential cracks nucleation sites for the specimen with Σ17b GBs are shown in figure (6.27).
Figure 6.1: Crystal lattice orientation for two neighboring grains and the resulted CSL GB
Figure 6.2: Clusters of grains in 3 different aggregate models with (a) 11 grains (b) 25 grains (c) 50 grains

Red lines denote CSL GBs locations
Figure 6.3: GB network in aggregates with (a) 11 grains (b) 25 grains (c) 50 grains
Figure 6.4: Nominal stress-strain curves for the 11, 25 and 50-grain models with $\Sigma 3$
Figure 6.5: Lattice rotation contours at 15% nominal strain for models with Σ 3

(a) 11 grains (b) 50 grains
Figure 6.6: Accumulated plastic shear slip contours at 15% nominal strain for models with $\Sigma$

3 (a) 11 grains (b) 50 grains
Figure 6.7: Normalized stress, $\sigma_{yy}$, contours at 15% nominal strain for models with $\Sigma 3$ (a) 11 grains (b) 50 grains
Figure 6.8: Immobile dislocation density for the 11-grain aggregate with $\Sigma$ 3 at 15% nominal strain for slip systems (a) (111)[\overline{1}01]  (b) (111)[\overline{1}10]  (c) (\overline{1} \overline{1} 1)[011]  (d) (1 \overline{1} 1)[011]
Figure 6.9: Immobile dislocation density for the 50-grain aggregate with Σ 3 at 15% nominal strain for slip systems (a) (111)[101] (b) (111)[10] (c) (1 1 1)[011] (d) (1 1 1)[011]
Figure 6.10: Nominal stress-strain curves for the 11, 25 and 50 grain aggregates with Σ 17b
Figure 6.11: Lattice rotation contours at 15% nominal strain for models with $\Sigma$ 17b (a) 11 grains (b) 50 grains
Figure 6.12: Accumulated plastic shear slip contours at 15% nominal strain for models with \( \Sigma 17b \) (a) 11 grains (b) 50 grains
Figure 6.13: Normalized stress, $\sigma_{yy}$, contours at 15% nominal strain for models with $\Sigma$ 17b

(a) 11 grains (b) 50 grains
Figure 6.14: Immobile density for the 11-grain aggregate with $\Sigma$ 17b at 15% nominal strain for slip systems (a) $\langle 111 \rangle[\bar{T}10]$ (b) $\langle \bar{T} \bar{T} \bar{T} \rangle\langle \bar{T}10 \rangle$ (c) $\langle \bar{T} \bar{T} \bar{T} \rangle[101]$ (d) $\langle \bar{T}11 \rangle[101]$
Figure 6.15: Immobile density for the 50-grain aggregate with $\Sigma$ 17b at 15% nominal strain for slip systems (a) $(111)[\overline{T}01]$ (b) $(111)[\overline{T}10]$ (c) $(\overline{T}T1)[\overline{T}10]$ (d) $(\overline{T}T1)[101]$
Figure 6.16: Nominal stress-strain curves for the 25–grain model with Σ3 and Σ 17b GBs
Figure 6.17: Lattice rotation contours at 15% nominal strain for the 25-grain model with (a) $\Sigma 3$ CSL (b) $\Sigma 17b$ CSL
Figure 6.18: Accumulated plastic shear slip contours at 15% nominal strain for the 25-grain model with (a) $\Sigma$ 3 CSL (b) $\Sigma$ 17b CSL
Figure 6.19: Normalized stress, $\sigma_{YY}$, contours at 15% nominal strain for the 25-grain model with (a) $\Sigma$ 3 CSL (b) $\Sigma$ 17b CSL
Figure 6.20: Immobile density for the 25-grain aggregate with Σ 3 at 15% nominal strain for slip systems (a) (111)[T01] (b) (111)[T10] (c) (T T1)[011] (d) (1 T1)[011]
Figure 6.21: Immobile density for the 25-grain aggregate with Σ 17b at 15% nominal strain for slip systems (a) (111)[T01] (b) (1 T 1)[T 10] (c) (T 1 1)[101] (d) (1 T 1)[T01]
Figure 6.22: Potential failure paths for the 11-grain model with Σ3 GBs

Figure 6.23: Potential failure paths for the 50-grain model with Σ3 GBs
Figure 6.24: Potential failure paths for the 11-grain model with Σ17b GBs

Figure 6.25: Potential failure paths for the 50-grain model with Σ17b GBs
Figure 6.26: Potential failure paths for the 25-grain model with Σ3 GBs

Figure 6.27: Potential failure paths for the 25-grain model with Σ17b GBs
CHAPTER 7
MICROSTUCTURAL ANALYSIS OF CRACK GROWTH IN F.C.C. METALLIC MATERIALS

The dislocation density-based multiple crystalline formulation is utilized to investigate the effects of grain orientation and the distribution of different CSL GBs on the deformation behavior and crack tip activity in f.c.c. aggregates. In this chapter, the evolution of finite deformation fields, crack tip activity, and plastic zone, and how they evolve in an aggregate with different combinations of $\Sigma 3$ and $\Sigma 17b$ GBs will be investigated. This analysis will relate how grain shape and size, aggregate size, and crystalline structure are related to the GB effects, and how this affects crack-growth behavior.

7.1. POLYCRYSTALLINE AGGREGATE MODELS WITH CSL GBs AND A PRE-EXISTING CRACK

The crystallography of the microstructure is characterized by grain orientations and GB misorientation, which is represented by the distribution of CSL GBs. An f.c.c. polycrystalline aggregate with 25 grains is used in the analysis, the dimensions of the specimen were chosen as $100 \times 200 \mu m^2$. An edge crack is introduced in the aggregate (figure 7.1), the entire crack extends within one grain, and it is located $100 \mu m^2$ from the bottom side of the specimen. Crack length to the specimen width ratio ($\frac{a}{w}$) is 0.2. The crack is initially a slit with zero crack tip opening displacement, CTOD. The crack, under monotonic loading, was gradually opened by releasing the nodes behind the crack-tip. As the
load was applied, the nodes were incrementally moved to new locations. These new locations were tracked to monitor crack location, and to ensure that the crack surfaces are traction free. This process is shown in figure 7.2.

A mesh of 2165 elements is used in the analysis, and the specimen was loaded in tension in a quasi-static manner with an applied strain-rate of $4.76 \times 10^{-4} \text{s}^{-1}$. The final macroscopic nominal strain was 10%. Material properties, which are representative of f.c.c. austenitic steel and used for the grain bulk and GB regions are given in tables 6.2 and 6.3. For the aggregate with $\Sigma^3$ GBs, the elastic modulus and yield strength for the GB regions were one and a half times larger than $\Sigma^{17b}$ GB regions.

The nominal stress-strain response is shown in Figure 7.3 for the crack model with $\Sigma^3$ and $\Sigma^{17b}$ GBs. The model with the $\Sigma^{17b}$ GBs has a higher stress response than the aggregate with the $\Sigma^3$ GBs. Contours of Lattice rotation at 10% nominal strain are shown in Figure 7.4. For both aggregates, there is extensive lattice rotation adjacent to the crack tip. For the crack model with $\Sigma^3$ GBs, lattice rotation attained a maximum of $18^\circ$ and the upper side of the crack front had a positive (counterclockwise) lattice rotation, whereas the bottom side of the crack rotated clockwise. Lattice rotation for the model with $\Sigma^{17b}$ GBs ranged between $-20^\circ$ and $15^\circ$.

Accumulated plastic shear slip contours are shown in Figure 7.5. For the aggregate with the $\Sigma^3$ GBs, the maximum plastic shear slip is 0.7 and it occurred at the tip of the crack. Localized shear slip bands emanate from the crack-tip, and they extend through the grains and GBs. Plastic shear slip attained a maximum of 1.0 in the model with $\Sigma^{17b}$ model and it occurred at the crack tip. For the crack aggregate the $\Sigma^3$ GBs, the final CTOD at 10%
nominal strain was \(8.135 \mu m\). For the aggregate with \(\Sigma 17b\) GBs, the final CTOD at 10% nominal strain was \(9.667 \mu m\) respectively.

Contours of the normal stress, \(\sigma_{yy}\), normalized by the macroscopic yield strength of the specimen are shown in Figure 7.6. The maximum normal stress at the crack tip for the model with \(\Sigma 3\) GBs was 13 and of the highest normal stresses occurred at the GB regions near the crack tip. The normal stress attained a maximum normalized value of 14 near the crack tip for the aggregate with \(\Sigma 17b\) GBs. The region of concentrated normal stress ahead of the crack tip was larger in size for the aggregate with \(\Sigma 17b\) GBs than it was for the aggregate with \(\Sigma 3\) GBs.

The most active slip systems for the aggregate with \(\Sigma 3\) GBs were \((111)[\overline{1}0]\), \((\overline{1}11)[101]\), \((\overline{1}11)[0\overline{1}1]\) and \((1\overline{1}1)[011]\). Dislocation density contours for these active slip systems are shown in Figure 7.7. For the aggregate with \(\Sigma 3\) GBs, the maximum density activity occurred at the tip of the crack for all active slip systems with a maximum attained density of \(3.6 \times 10^{17} m^{-2}\) for slip-system \((\overline{1}11)[101]\). The high density of immobile dislocations at the crack tip can be an indication that the crack tip can emits dislocations (dislocation source), which could result in crack blunting (Rice and Thomson, 1974). For the aggregate with \(\Sigma 17b\) GBs, the most active slip systems were \((111)[\overline{1}0]\), \((\overline{1}11)[101]\), \((1\overline{1}1)[011]\) and \((1\overline{1}1)[\overline{1}01]\). The maximum immobile dislocation density was \(4.5 \times 10^{17} m^{-2}\), which corresponds to slip-system \((111)[\overline{1}0]\). For the aggregate with \(\Sigma 17b\) GBs, the maximum immobile density for the slip system \((1\overline{1}1)[\overline{1}01]\) did not occur at
the crack tip while the maximum immobile densities on the other three active slip systems occurred at the crack tip. For the slip system (T\{\overline{1}1\}1\{01\}) in the $\Sigma_{17b}$ aggregate, the immobile density had its maximum at the crack-tip, and high immobile density emanate from the crack tip. Values of the final CTOD along with the maximum values for the immobile dislocation densities could indicate that the crack for the aggregate with the $\Sigma_{17b}$ GBs had more blunting than the aggregate with $\Sigma_{3}$ GBs. This is evident because immobile density on the most active slip system had a maximum of $4.5\times10^{17}$ $m^{-2}$ at the crack tip for the aggregate with the $\Sigma_{17b}$ GBs, while for the aggregate with the $\Sigma_{3}$ GBs, the maximum immobile density was $3.6\times10^{17}$ $m^{-2}$. This is also evident from the deformed crack surfaces, as seen in Figure 7.6.

7.2. CONCLUSIONS AND SUMMARY

In this chapter, the behavior of aggregates with $\Sigma_{3}$ and $\Sigma_{17b}$ CSL GBs were investigated. For the aggregate with $\Sigma_{3}$ GBs, the normal stress and plastic shear slip at the crack tip were lower than the aggregate with the $\Sigma_{17b}$ GBs. There was more crack-blunting associated with the aggregate with the $\Sigma_{17b}$ GBs, this can be due to higher dislocation-densities and the larger plastic zone ahead of the crack-tip for this aggregate. Furthermore, the normal stresses at the GBs were lower in comparison with the aggregate with the $\Sigma_{3}$ GBs, which indicates that crack growth in this case can be intergranular due to the lower resistance at the GBs. For the aggregate with the $\Sigma_{3}$, there was less dislocation-density and plastic zone activity ahead of the crack-tip, which resulted in less crack blunting. This was also evident
from the CTODs and the deformed crack profiles, which would indicate sharper crack
growth, at least in comparison with the aggregate with the Σ17b GBs. This crack growth
could be crystallographic (transgranular) because of the preferentially oriented slip-systems
near the crack-tip, and because of the higher strength of these GBs, in comparison with the
aggregate with the Σ17b GBs, which can act as barriers to crack growth.

Based on the maximum attained normal stress, immobile dislocation density
accumulation around the crack tip and intensive regions of plastic shear slip, potential crack
growth paths for the 25-grain model with Σ3 and Σ17b CSL GBs were shown in Fig. 7.9 and
7.10 respectively.
**Figure 7.1:** The geometry of the crack model

**Figure 7.2:** The process of generating a crack with zero initial COD
Figure 7.3: Nominal Stress-strain curves for the crack model with CSL GBs
Figure 7.4: Lattice rotation contours at 10% nominal strain for the crack model with (a) $\Sigma 3$ CSL (b) $\Sigma 17b$ CSL
Figure 7.5: Accumulated plastic shear slip contours at 10% nominal strain for the crack model with (a) $\Sigma$ 3 CSL (b) $\Sigma$ 17b CSL
Figure 7.6: Normalized $\sigma_{yy}$ contours at 10% nominal strain for the crack model with (a) $\Sigma 3$ CSL (b) $\Sigma 17b$ CSL.
Figure 7.7: Immobile density for the crack model with $\Sigma$ 3 GBs at 10% nominal strain for slip systems (a) (111)[\{110\}] (b) (\{111\})[\{101\}] (c) (\{111\})[\{01\}] (d) (\{11\})[\{011\}].
Figure 7.8: Immobile density for the crack model with Σ 17b GBs at 10% nominal strain for slip systems (a) \((111)[\overline{T}10]\) (b) \((\overline{T}11)[101]\) (c) \((1\overline{T}1)[011]\) (d) \((1\overline{T}1)[\overline{T}01]\)
Figure 7.9: Potential crack path for the 25-grain model with $\Sigma 3$ GBs

Figure 7.10: Potential crack path for the 25-grain model with $\Sigma 17b$ GBs
CHAPTER 8
RECOMMENDATIONS FOR FUTURE STUDY

The following are recommendations for the future research, based on the current findings of this investigation:

- Extend the crystalline formulation to three dimensions to account for a full-field analysis.
- Account for dynamic effects in the formulation such that wave propagation and shock problems can be modeled.
- Extend the computational algorithm to model aggregates with different crystalline structures such as b.c.c and h.p.c. structures.
- Obtain an accurate description that relates GB strength and material properties to its orientation and incorporate this description in the numerical algorithm.
- Incorporate object-oriented finite element codes in which images of real microstructures can be modeled (true representation of microstructures).
- Use hierarchical modeling schemes that link the FEM predictions with molecular dynamic simulations.
CHAPTER 9

REFERENCES


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