ABSTRACT

REZVANIAN, OMID. Grain Subdivision and Microstructural Interfacial Scale Effects in Polycrystalline Materials. (Under the direction of Professor Mohammed A. Zikry.)

The major objective of this research is to develop a unified physically-based representation of the microstructure in f.c.c. crystalline materials to investigate finite inelastic deformation and failure modes and scenarios at different physical scales that occur due to a myriad of factors, such as texture, grain size and shape, grain subdivision, heterogeneous microstructures, and grain boundary misorientations and distributions. The microstructurally-based formulation for inelastic deformation is based on coupling a multiple-slip crystal plasticity formulation to three distinct dislocation densities, which pertain to statistically stored dislocations (SSDs), geometrically necessary dislocations (GNDs), and grain boundary dislocations (GBDs). This dislocation density based multiple-slip crystal plasticity formulation is then coupled to specialized finite-element methods to predict the scale-dependent microstructural behavior, the evolving heterogeneous microstructure, and the localized phenomena that may contribute to failure initiation for large inelastic strains. The SSD densities provide a representation of cell-type dislocation microstructures and their related processes. The GND densities provide an understanding of the scale-dependent deformation behavior of crystalline materials as a function of grain and aggregate sizes. The GBD densities are formulated to represent the misfit dislocations that arise due to lattice misorientations across GBs, and to provide a framework to investigate the phenomena associated with the grain boundary orientations and distributions. This provides a local criterion of how GB interfaces, such as triple junctions are potential sites for failure initiation and localized behavior. The
evolution of the GNDs is used to predict and understand how crystallographic and non-crystallographic microstructures relate to intragranular and intergranular deformation patterns and behavior. Furthermore, a clear understanding of how GB strength changes due to microstructural evolution is obtained as a function of microstructural heterogeneities that occur at different physical scales.
GRAIN SUBDIVISION AND MICROSTRUCTURAL INTERFACIAL SCALE EFFECTS IN POLYCRYSTALLINE MATERIALS

by

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A dissertation submitted to the Graduate Faculty of North Carolina State University in partial fulfillment of the requirements for the Degree of Doctor of Philosophy

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APPROVED BY:

__________________________
Chair of Advisory Committee
To my father, and my mother
BIOGRAPHY

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CHAPTER 1

INTRODUCTION, BACKGROUND, AND OBJECTIVES

1.1 INTRODUCTION AND BACKGROUND

Crystalline materials, such as metals and many classes of non-metallic solids, can be categorized by the periodic crystalline pattern of their atoms. The three most common crystalline structures are the body-centered cubic (b.c.c.), face-centered cubic (f.c.c.) and close-packed hexagonal structures (h.c.p). Inelastic deformation is caused by slip on close-packed planes of these crystalline structures. These slip-planes are distinct for each cubic structure.

All crystals contain imperfections, which may be point, line, surface or volume defects. Imperfections can significantly change the properties of crystalline solids by locally disturbing atom arrangements. Differences between theoretical and experimental values of the applied shear stress to plastically deform a single crystal, have led to delineating of the essential role of dislocation motion in crystallographic slip (Taylor, 1934). Under an applied stress, the lattice deforms elastically until the stretched bonds near a dislocation break down, and new bonds are formed, causing crystallographic slip.

Since the ability of a crystalline material to plastically deform by crystallographic slip largely depends on the ability of dislocations to move, impeding dislocation motion will result in the strengthening of material. There are a number of ways to impede dislocation movement, which include controlling the grain size, strain hardening, strain-
gradient hardening, and alloying. Dislocation multiplication or generation during plastic
deformation increases their mutual interactions, which result in dislocations become
pinned or tangled. This will in turn result in a decrease in the mobility of dislocations and
a strengthening or hardening of the material.

Strain hardening is typically due to the presence of two categories of stored
dislocations: statistically stored dislocations (SSDs) associated with plastic strain (see, for
example, Kocks, 1966), and geometrically necessary dislocations (GNDs) associated with
plastic strain gradients (Ashby, 1970). SSDs accumulate by the statistical trapping of
dislocations during plastic slip. Therefore, they are randomly oriented and have no
geometrical consequence. On the other hand, gradients of plastic deformation, due to
material texture and inelastic anisotropy, results in the presence of GNDs, which are
required to preserve the lattice continuity through accommodating lattice misorientations.

During straining, dislocations commonly organize themselves into mosaic
patterns consisting of regions of low dislocation density separated by regions of high
dislocation density, which are also called dislocation boundaries. The density of
dislocations, and the spacing of the boundaries have been commonly used as

Microstructures are the result of these heterogeneous distributions of stored
dislocations. In general, two types of dislocation boundaries may result from plastic
deformation of crystalline materials, which subdivide the grains on two size scales (Bay
et al., 1992). At the smallest scale of approximately a few microns, a heterogeneous
distribution of SSDs, subdivide the grains into a cell-type microstructure of
approximately equiaxed and low-density cells, separated by high-density walls also known as incidental dislocation boundaries (IDBs) as noted by Kuhlmann-Wilsdorf and Hansen (1991).

At a larger scale, geometrically necessary boundaries (GNBs) are formed as the result of different active slip systems or different magnitudes of plastic slip among neighboring regions (cell-blocks) of individual grains, which leads to the division of grains into cell-blocks (Hughes, 2001). Dislocations stored in these boundaries are the GNDs needed to accommodate lattice misorientations across the GNBs (see, for example, Hughes, 2001; Hansen et al., 2001; Bay et al., 1992). Different microstructures that can develop from different grain orientations are shown in Fig. 1.1.

In this context, stable and unstable orientations play a critical role. Homogenous microstructures are more likely to occur for stable orientations. The majority of experimental studies on orientation stability are mainly related to the deformation behavior of f.c.c. materials under rolling or channel die compression. Some of the crystal orientations that have been studied are goss orientation under rolling (Driver et al., 1994; Morii and Nakayama, 1985, 1988; Nakayama and Morii, 1982; Wrobel et al., 1988, 1994), copper orientation under rolling (Driver et al., 1994; Morii and Nakayama, 1985; Nakayama and Morii, 1982; Wagner et al., 1995; Zasimchuck and Markashova, 1990), copper orientation under channel die compression (Godfrey et al., 1998a), brass orientation under rolling (Driver et al., 1994; Malin et al., 1981; Nakayama and Morii, 1982), brass orientation under channel die compression (Godfrey et al., 1998b), cube orientation under rolling (Liu and Hansen, 1996, 1998; Malin et al., 1981; Wert et al., 1997; Wrobel et al., 1994), cube orientation under channel die compression (Akef and
Driver, 1991; Butler and Hu, 1989), rotated-cube under rolling (Bauer et al., 1977; Kohlhoff et al., 1981) and rotated-cube under channel die compression (Akef and Driver, 1991; Becker et al., 1990; Butler and Hu, 1989; Humphreys and Ardakani, 1994). Goss, copper and brass are considered to be stable orientations, while cube and rotated-cube are generally regarded as unstable under rolling or channel die compression.

A macroscale grain subdivision can also occur in which a single crystal or a polycrystal with large grains is subdivided into deformation bands, consisting of alternate bands with positive and negative lattice rotations, separated by bands with zero lattice rotation. The rotated bands are referred to as the matrix bands (MBs) and the unrotated bands are referred to as the transition bands (TBs). The subdivision of cube oriented single crystals to deformation bands, under rolling compression, has been the subject of many experimental and analytical studies (see, for example, Hansen and Juul Jensen, 1999; Liu and Hansen, 1998; Wert et al., 1997). Material purity, deformation process, and texture are the major factors affecting the characteristics of this macroscopic subdivision. Cube oriented single crystals, when subjected to plane-strain compression or rolling, would have two pairs of co-directional slip systems, which are equally stressed. If the four slip systems have an equal amount of resistance against slip then the shear amplitudes on all four of them would be equal. Hence, the four slip systems will not be able to induce lattice rotation, unless an asymmetry is introduced. As a result, the idea of shear amplitude imbalance was introduced by Wert et al. (1997). In that approach, it is postulated that if a shear imbalance is applied on the balanced slip-systems of a cube-oriented single crystal, a physically-based asymmetry can evolve, which can lead to the formation of deformation bands.
Crystallographic texture of the crystalline materials causes the plastic deformation and rotations of the grains to be dissimilar, which can lead to intercrystalline deformation inhomogeneities. On the other hand, at the boundaries, at least for athermal deformations where grain boundary sliding is not likely to happen, neighboring grains are forced to have compatible deformations if failure surfaces, such as voids and cracks are not present. This in turn causes intragranular deformation fields to be inhomogeneous. These local deformation inhomogeneities can cause strain localization, which is considered to be a possible initiation point for failure (Harder, 1999).

In crystal plasticity models, the effect of dislocation immobilization on slip hardening can be described in two ways. Phenomenological models postulate that the flow stress on each slip system can be related to a strain-hardening process, whereas for physically-based models, the flow stress on each slip system is based on dislocation processes. In these physically-based models, strain-dependent plasticity theories only consider the effect of the SSDs in the hardening formulations, while strain-gradient plasticity theories try to account for the hardening due to plastic strain gradients (see, for example, Aifantis, 1987; Zbib and Aifantis, 1992; Fleck and Hutchinson, 1997).

A number of dislocation density models have been developed based on dislocation-density storage and recovery. One-variable dislocation models account for the evolution of immobile dislocations by assuming that mobile dislocation density is strain independent, and that mobile dislocations move an average distance before they are immobilized or annihilated. The basis of this model is statistical theory of strain hardening by Kocks (1966). More general two-variable models typically describe the evolution of mobile and immobile dislocation densities through the inter-related
dislocation processes (see, for example, Estrin and Mecking, 1984; Kubin and Estrin, 1988; Zikry and Kao 1996). These models can be used to predict the flow stress, up to a saturated limit. Mobile and immobile-density based two-variable models also do not account for the non-uniform distribution of stored dislocations. The increased hardening in large strains can only be described through a cell-type microstructure that occurs as a result of these nonuniform distributions (see, for example, Nes, 1998). Hence, the density of stored dislocations in dislocation cell interiors and walls, and dislocation cell size are critical microstructural parameters that need to be accounted for and understood (Nix et al., 1985; Mughrabi, 1987; Estrin et al., 1998).

As for strain-gradient plasticity formulations, the relationship between plastic strain gradients and the density of dislocations required to accommodate the geometrical consequences of such a gradient originated with the classical work of Nye (1953). Nye’s tensor provides a direct measure of the number of GNDs from the plastic slip gradients. Plastic strain gradients appear either, as the result of the geometry of the loading, or because of the material’s anisotropic plastic properties. The motivation for strain gradient plasticity theory stems from the scale-dependent deformation behavior of materials, observed in a variety of plasticity phenomena that implies a stronger response for smaller sizes. For example, the measured indentation hardness of metallic materials increases by a factor of two as the depth of indentation decreases from 10 to 1 microns (Nix, 1989; De Guzman et al., 1993; McElhaney et al., 1998). In general, when the deformation field’s characteristic length (e.g. diameter of a wire, radius of a void or particle, depth of indentation) becomes comparable to internal material length scale, strain gradient effects may play a dominant role (see, for example, Nix, 1989).
Crystal plasticity models have been incorporated within large-scale finite-element models to obtain a more detailed understanding of material behavior at the grain level. (see, for example, Zikry and Nemat-Nasser, 1990; Becker et al., 1991; Becker and Panchanadeesvaran, 1995; Zikry and Kao, 1996; Dai, 1997; Zikry and Kameda, 1998; Bate, 1999; Mika and Dawson, 1999; Kumar and Dawson, 2000; Beaudoin et al., 2000; Acharya and Beaudoin, 2000; Arsenlis and Parks, 2000; Dawson et al., 2002; Ashmawi and Zikry, 2003; Evers et al., 2004; Rezvanian et al., 2006). Most of these approaches have accounted for microstructural effects, such as texture evolution, microstructure evolution, geometrical softening, and strain hardening.

As noted earlier, some of these crystalline formulations (see, for example, Ashmawi and Zikry, 2003, Evers et al., 2004) have been coupled to the evolution of dislocation densities. However, what has been lacking is a validated and integrated approach that can account for the interrelated microstructural mechanisms that occur on different physical scales that range from the evolution of SSD densities in a heterogeneous microstructure framework that can be coupled to the evolution of GND and GBD densities, such that relevant microstructurally-induced phenomena and mechanisms can be accurately predicted and understood.

1.2 RESEARCH OBJECTIVES

The major objective of this work is to provide a unified formulation that accounts for grain subdivision phenomena in f.c.c. polycrystals that ranges from the scale of dislocation cells to cell-blocks and macroscale grain subdivision. Dislocation densities
associated with SSDs, GNDs, and GBDs will be coupled to a multiple-slip crystalline plasticity formulation to track intergranular and intragranular microstructural evolution, and to understand how this is related to collective grain behavior, grain subdivision, and GB orientation and distribution.

This dislocation density based multiple-slip crystal plasticity formulation is coupled to specialized finite-element methods to predict the scale-dependent microstructural behavior, the evolving heterogeneous microstructure, and the localized phenomena that may contribute to failure initiation. Voronoi tessellation is used to generate physically realistic random grain shapes. The incorporation of the SSDs provides a physical representation of a cell-type dislocation microstructure and its related processes. The GNDs provide a framework for understanding of the scale-dependent deformation behavior of crystalline materials as a function of grain and aggregate size and shape. The GBD densities are obtained based on the density of misfit dislocations that are formed due to the lattice misorientations across the GBs. Therefore, the phenomena associated with the GB orientations and distribution of low and high-angle GBs can be investigated. This can provide a local criterion of how GB interfaces, such as triple junctions are potential sites for failure initiation and localized behavior. This study provides a physically-based validated methodology that can be used to track dominant deformation and failure scenarios at different physical scales that occur due to myriad factors, such as texture, grain size and shape, grain subdivision, type of microstructure, and GB orientations and distributions.

The outline of the dissertation is as follows: chapter 1 presents the introduction and an overview of the background of the subject. In chapter 2, the microstructural
formulation for inelastic deformation and subdivision of crystalline grains that is based on coupling a multiple-slip crystal plasticity formulation to three distinct dislocation density formulations, which pertain to SSDs, GNDs, and GBDs, is presented. In chapter 3, the microstructurally-based computational finite-element schemes are outlined. In chapter 4, the modeling and experimental validation of subdivision of a cube oriented aluminum single crystal under rolling compression to deformation bands is presented. In Chapter 5, the behavior of a polycrystal with random grain shapes under tension is presented for a formulation that only considers SSDs. In chapter 6, the effect of GBD and GND densities are investigated for polycrystalline aggregates. In chapter 7, scale-dependent behavior is investigated by scaling the polycrystalline sample of chapter 6, to a smaller size. In chapter 8, low-angle GBs are investigated. In Chapter 9, future research recommendations are outlined.
Figure 1.1. Microstructure type as a function of the grain orientation
CHAPTER 2
MICROSTRUCTURAL REPRESENTATION OF GRAIN
DEFORMATION AND SUBDIVISION

The microstructural formulation for inelastic deformation and subdivision of crystalline grains is based on coupling a multiple-slip crystal plasticity to three distinct dislocation density formulations, which pertain to statistically stored dislocations (SSD), geometrically necessary dislocations (GND), and grain boundary dislocations (GBD). This interrelated formulation is presented in this chapter.

2.1 MULTIPLE-SLIP CRYSTAL PLASTICITY FORMULATION

The crystal plasticity kinematics that is used here is based on that developed by Zikry and Kao (1996) and Kameda and Zikry (1998). The velocity gradient tensor $L$ can be obtained from the deformation gradient tensor $F$ and the rate of change of it $\dot{F}$ as

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

(2.1)

The velocity gradient can then be decomposed into its symmetric and skew-symmetric parts; the symmetric part being the deformation-rate tensor $D$ and the skew-symmetric part being the spin tensor $W$. The total deformation-rate tensor and the total spin tensor can then be additively decomposed into elastic and plastic components as

$$ D_{ij} = D_{ij}^* + D_{ij}^p, \quad W_{ij} = W_{ij}^* + W_{ij}^p. $$

(2.2a-b)
The * superscript denotes the plastic component and $P$ superscript denotes the elastic component.

The plastic components can be defined in terms of the crystallographic slip-rates as

$$D_{ij}^p = \sum_\alpha P_{ij}^{(\alpha)} \gamma^{(\alpha)}, \quad W_{ij}^p = \sum_\alpha \omega_{ij}^{(\alpha)} \gamma^{(\alpha)},$$

(2.3a-b)

where $\alpha$ is summed over all slip-systems, and $P^{(\alpha)}$ and $\omega^{(\alpha)}$ are defined as

$$P_{ij}^{(\alpha)} = \frac{1}{2} \left( \hat{s}_i^{(-\alpha)} n_j^{(\alpha)} - \hat{s}_j^{(-\alpha)} n_i^{(\alpha)} \right), \quad \omega_{ij}^{(\alpha)} = \frac{1}{2} \left( \hat{s}_i^{(-\alpha)} n_j^{(\alpha)} - \hat{s}_j^{(-\alpha)} n_i^{(\alpha)} \right).$$

(2.4a-b)

$\hat{n}^{(\alpha)}$ is the unit vector normal to the slip plane of slip system $\alpha$, and $\hat{s}^{(\alpha)}$ is the unit vector in the slip direction.

The relation between crystallographic slip rates and a material’s microstructure at a given stress state and temperature can be described by constitutive equations that are based on kinetic behavior. In crystallographic slip, the glide of mobile dislocations is impeded by two sources: short-range barriers and long-range stress fields (Kocks et al., 1975). Short-range barriers of a slip system are basically points, where other slip systems’ stored dislocations intersect the plane of that slip system. Stored dislocations could be either statistically or geometrically stored. Long-range stress fields arise due to the formation of dislocation boundaries. Therefore, for slip to occur, the resolved shear stress on a specific slip system, should overcome these two sources of resistance.

A general power-law relation for crystallographic slip rate, which accounts for thermal activation, can be postulated as
\[
\frac{\dot{\gamma}^{(\alpha)}}{\dot{\gamma}_0} = \left( \frac{\tau_{eff}^{(\alpha)}}{\dot{\sigma}^{(\alpha)}} \right) \frac{1}{m} \cdot \exp \left( -\frac{\Delta F}{k T} \left( 1 - \frac{\tau_{eff}^{(\alpha)}}{\tau^{(\alpha)}} \right) \right) \cdot \text{sign}(\tau^{(\alpha)}),
\]

(2.5)

where \( m \) is the strain-rate sensitivity parameter, \( \dot{\gamma}_0^{(\alpha)} \) is the reference strain rate, \( k \) is the Boltzmann’s constant, \( T \) is the absolute temperature, and \( \Delta F \) is the activation energy. \( \tau_{eff}^{(\alpha)} \) is the net deriving force on slip system \( \alpha \), which is the difference between the resolved shear stress \( \tau^{(\alpha)} \) and the resolved back stress \( \tau_b^{(\alpha)} \), which is resulted from the long-range stress fields. \( \tau^{(\alpha)} \) is obtained by the projection of the applied stress tensor on slip system \( \alpha \), and \( \tau_b^{(\alpha)} \) is obtained by the projection of the back-stress tensor \( \tilde{\sigma}_b \) on slip system \( \alpha \) (Harder, 1999), as

\[
\tau_b^{(\alpha)} = \tilde{\sigma}_b \cdot \tilde{n}^{(\alpha)}.
\]

(2.6)

\( \tilde{\tau}^{(\alpha)} \) is the threshold resistance to slip on slip system \( \alpha \), and it can be postulated as the sum of the static yield stress \( \tau_y \) and a function of the density of the obstacles to glide of mobile dislocations, on slip system \( \alpha \), \( \rho_o^{(\alpha)} \), as

\[
\tilde{\tau}^{(\alpha)} = \tau_y + f(\rho_o^{(\alpha)}).
\]

(2.7)

A generally accepted assumption (see, for example, Mughrabi, 1983) for the influence of dislocation interactions on hardening behavior is that slip system strength is proportional to the square root of the density of the obstacles \( \rho_o^{(\alpha)} \) as

\[
f(\rho_o^{(\alpha)}) = c b G \sqrt{\rho_o^{(\alpha)}},
\]

(2.8)
where $c$ can range between 0.3 to 0.5, $G$ is the shear modulus, and $b$ is the magnitude of the Burger’s vector. The obstacle density $\rho^{(\alpha)}_o$ on slip system $\alpha$, depends on the density of the stored dislocations $\rho^{(s)}$ on every slip system. The slip-system interactions of these stored dislocations can be quantified through a set of interaction coefficients $i^{(\alpha s)}$ (Franciosi and Zaoui, 1982) as,

$$\rho^{(\alpha)}_o = \frac{12}{\sum_{s=1}^{12} i^{(\alpha s)} (\rho^{(s)}_{SSD} + \rho^{(s)}_{GND})}, \quad (2.9)$$

where

$$\rho^{(\alpha)}_{GND} = |\rho^{(\alpha)}_{G, e}| + |\rho^{(\alpha)}_{G, s}|. \quad (2.10)$$

$\rho^{(\alpha)}_{G, e}$ are edge GND densities, and $\rho^{(\alpha)}_{G, s}$ are the screw GND densities. Since GNDs’ polarity has no effect on their role as short-range barriers, their absolute values have been used in Eq. (2.10).

The back-stress tensor $\tilde{\sigma}_b$ is determined from the long-range stresses, $\tau^{(\alpha)}_{lr}$, on every slip system, as

$$\tilde{\sigma}_{b_{ij}} = -\sum_{\alpha=1}^{12} \tau^{(\alpha)}_{lr} P_{ij}^{(\alpha)}. \quad (2.11)$$

$\tau^{(\alpha)}_{lr}$ is obtained from the spatial distribution of GND’s, using a method proposed by Evers et al. (2003). It is assumed that $\tau^{(\alpha)}_{lr}$ can be decomposed into $\tau^{(\alpha)}_{lr-e}$ and $\tau^{(\alpha)}_{lr-s}$ that are developed by GND’s of edge and screw type, respectively. Determination of each of these contributions is based on stress concentration near the individual edge and screw
dislocations (Cottrell, 1961). Integrating these equations over a circular domain with radius \( R \), while assuming the GND densities can vary linearly in space results in

\[
\tau_{lr-e}^{(a)} = \frac{GbR^2}{8(1-\nu)} \left( \nabla \rho_{GND}^{(a)} \cdot \delta^{(a)} \right),
\]

\[
\tau_{lr-s}^{(a)} = \frac{GbR^2}{4} \left[ \left( \nabla \rho_{GND}^{(a)} \cdot \tilde{t}^{(a)} \right) + \left( \nabla \rho_{GND}^{(a')} \cdot \tilde{t}^{(a')} \right) \right],
\]

where \( \tilde{t}^{(a)} \) is the transverse axis of slip system \( \alpha \), and \( \alpha' \) is the slip system co-linear with slip system \( \alpha \). Co-linear systems have the same slip direction but are on different slip planes.

When the crystallographic slip-rates are obtained, the global stress rate tensor \( \sigma_{ij}^{\nabla} \) can then be obtained as a co-rotational stress rate tensor as

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

where \( L_{ijkl} \) is the elastic moduli

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

and \( \lambda \) and \( \mu \) are the Lame’ elastic constants and \( \delta_{ij} \) is the Kronecker delta.

### 2.2 MICROSTRUCTURAL EVOLUTION LAWS FOR STATISTICALLY STORED DISLOCATIONS (SSD)

In general, the SSD evolution equations account, in an average sense, for the generation, immobilization, recovery and annihilation of dislocations. One-variable models (for example, Kocks, 1976) are solely based on the density of statistically stored
dislocations. These models are used to predict a linear decrease of the strain-hardening rate with stress. Two-variable models distinguish between mobile and immobile dislocations (see, for example, Zikry and Kao, 1996). These models can better describe behavior at large inelastic strains. These models, however, only assume a homogeneous distribution of SSD’s, and hence formulations are needed for the representation of cell-type microstructures, which are commonly observed in deformed metals. In this section, the flow-kinetics and microstructural evolution equations are formulated for a cell-type microstructure resembling the heterogeneous distribution of SSD’s, based on a modification of the microstructural model originally proposed by Nix et al. (1985) and the composite model of Mughrabi (1987) and Estrin et al. (1998).

### 2.2.1 HETEROGENEOUS MICROSTRUCTURE: DISLOCATION CELLS

In a heterogeneous distribution of SSDs, a microstructure consists of high-density regions of cell-walls with a local density of $\rho_w$ separated by low-density cell-interiors with a local density of $\rho_c$. A consequence of having such a cell-type microstructure is the emergence of internal micro-stresses. As a result of internal micro-stresses, plastic strain mismatches form between the cell-interiors and the cell-walls. Assuming that the total strain rate is the same in the cell-walls and cell-interiors, and that it has to be equal to the overall slip system strain rate $\dot{\gamma}^{(\alpha)}$ results in

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}^{(\alpha)}_w + \frac{\tau^{(\alpha)}_w}{G} = \dot{\gamma}^{(\alpha)}_c + \frac{\tau^{(\alpha)}_c}{G},$$

(2.16)
where $\dot{\gamma}_w^{(\alpha)}$ are slip-rates corresponding to the cell-walls and $\dot{\gamma}_c^{(\alpha)}$ are the slip-rates corresponding to the cell-interiors on slip system $\alpha$, and $\dot{\tau}_w^{(\alpha)}/G$ and $\dot{\tau}_c^{(\alpha)}/G$ are the local elastic strain-rates corresponding to the cell-walls and the cell-interiors.

It is assumed that the local crystallographic slip-rates for the cell-walls and the cell-interiors are of the same form as Eq. (2.5),

$$
\frac{\dot{\gamma}_w^{(\alpha)}}{\dot{\gamma}_0} = \left( \frac{\tau_c^{(\alpha)}}{\hat{\tau}_c} \right)^{\frac{1}{m}} \exp \left( -\frac{\Delta F}{kT} \left( 1 - \frac{\tau_c^{(\alpha)}}{\hat{\tau}_c} \right) \right) \text{sign}(\tau_c^{(\alpha)}), \tag{2.17-a}
$$

$$
\frac{\dot{\gamma}_c^{(\alpha)}}{\dot{\gamma}_0} = \left( \frac{\tau_w^{(\alpha)}}{\hat{\tau}_w} \right)^{\frac{1}{m}} \exp \left( -\frac{\Delta F}{kT} \left( 1 - \frac{\tau_w^{(\alpha)}}{\hat{\tau}_w} \right) \right) \text{sign}(\tau_w^{(\alpha)}), \tag{2.17-b}
$$

where $\tau_c^{(\alpha)}$ is the cell interior resolved shear stress, and $\tau_w^{(\alpha)}$ is the cell wall resolved shear stress. Overall stress equilibrium requires a balance between the overall slip system resolved shear stress $\tau_{\text{eff}}^{(\alpha)}$ and its local components as

$$
\tau_{\text{eff}}^{(\alpha)} = f_c^{(\alpha)} \tau_c^{(\alpha)} + (1 - f_c^{(\alpha)}) \tau_w^{(\alpha)}, \tag{2.18}
$$

where $f_c^{(\alpha)}$ is the average volume fraction of the cell interiors for slip system $\alpha$, and $f_w^{(\alpha)}$ is the volume fraction of the cell-walls. Since the volume fractions must sum to unity, they can be recast in terms of an average dislocation cell size $\delta_c^{(\alpha)}$ and cell wall thickness $\delta_w^{(\alpha)}$ as

$$
f_w^{(\alpha)} = \frac{\delta_w^{(\alpha)}}{\delta_w^{(\alpha)} + \delta_c^{(\alpha)}}, \quad f_c^{(\alpha)} = \frac{\delta_c^{(\alpha)}}{\delta_w^{(\alpha)} + \delta_c^{(\alpha)}} \tag{2.19a-b}
$$
The flow-stress parts of the local slip resistances \( \tau_c^{(\alpha)} \) and \( \tau_w^{(\alpha)} \) can have the general form of Eq. (2.7) as follows

\[
f(\rho_{co}^{(\alpha)}) = c b G \sqrt{\rho_{co}^{(\alpha)}} \quad f(\rho_{wo}^{(\alpha)}) = c b G \sqrt{\rho_{wo}^{(\alpha)}}, \tag{2.20a-b}
\]

where \( \rho_{co}^{(\alpha)} \) and \( \rho_{wo}^{(\alpha)} \) are the obstacle densities for the cell-interior and cell-wall regions of any slip system \( \alpha \). The density of obstacles at each region of a slip system depends on the density of stored dislocations \( \rho_c^{(\alpha)} \) and \( \rho_w^{(\alpha)} \) at corresponding regions of all slip systems and how they interact with each other, as

\[
\rho_{co}^{(\alpha)} = \sum_{s=1}^{12} i^{\alpha_s} (\rho_c^{(s)}) \quad \rho_{wo}^{(\alpha)} = \sum_{s=1}^{12} i^{\alpha_s} (\rho_w^{(s)}) \tag{2.21a-b}
\]

\( \rho_c^{(\alpha)} \) and \( \rho_w^{(\alpha)} \) are defined using appropriate evolution equations, which describe their underlying fundamental dislocation processes. They then are related to the slip system average density of SSD’s as

\[
\rho_{SSD}^{(\alpha)} = f_c^{(\alpha)} \rho_c^{(\alpha)} + (1 - f_c^{(\alpha)}) \rho_w^{(\alpha)}. \tag{2.22}
\]

### 2.2.2 STRUCTURAL EVOLUTION IN THE CELL-INTERIOR

The overall rate of change of the SSD density in the cell-interior can be stated as the sum of storage and recovery rates. Therefore, the net rate of change of dislocation density on every slip system can be written as a positive storage rate and a negative recovery rate as

\[
(\dot{\rho}_c^{(\alpha)}) = (\dot{\rho}_c^{(\alpha)})^+ + (\dot{\rho}_c^{(\alpha)})^- \tag{2.23}
\]
The mean free path \( L_c^{(\alpha)} \) for the mobile dislocations on slip system \( \alpha \), is determined by the number of stored dislocations on other systems

\[
L_c^{(\alpha)} = \frac{C}{\sqrt{\sum_{s=1}^{12} h_s^{\alpha_s} \rho_c^{(\alpha)}}},
\]  

(2.24)

where \( C \) is a material constant and \( h_s^{\alpha_s} \) quantifies the mutual immobilization effects of slip systems. The plastic strain increment of cell interiors on each slip system can be stated in terms of the increment in their stored dislocation density as

\[
d\gamma_c^{(\alpha)} = b L_c^{(\alpha)} d\rho_c^{(\alpha)},
\]  

(2.25)

where \( b \) is the Burger’s vector magnitude. Therefore, the storage rate can be written as

\[
(\dot{\rho}_c^{(\alpha)})^+ = \left| \gamma_c^{(\alpha)} \right| \frac{1}{b L_c^{(\alpha)}}.
\]  

(2.26)

In cross-slip, two screw dislocations of length \( L_{sc} \) and opposite directions are recovered. Assuming that the stored dislocations in cell-interiors have a screw type, the number of potential sites for cross-slip process can approximately be stated as \( \rho_c^{(\alpha)}/w \), where \( w \) is taken as the length of a potential site. Assuming that the attempt frequency of this process to be \( \nu_0 \), and that the probability of each successful attempt to be \( P_{cs} \), the dynamic recovery rate by cross-slip in the cell-interior can then be stated as

\[
(\dot{\rho}_c^{(\alpha)})^- = -\frac{\rho_c^{(\alpha)}}{w} 2L_{sc}\nu_0 P_{cs}.
\]  

(2.27)

Since \( L_{sc}^{(\alpha)} \) is proportional to the average spacing of screw dislocations in the cell interior on slip system \( \alpha \), \( L_{sc}^{(\alpha)} \propto (1/\sqrt{\rho_c^{(\alpha)}}) \), the recovery rate can be restated as
\[(\dot{\rho}_{c}^{(\alpha)})^- = -A\sqrt{\rho_c^{(\alpha)}} P_{cs}.\]  

(2.28)

The probability term is determined for each slip system as the result of two competing forward and backward processes as

\[P_{cs}^{(\alpha)} = \exp(-\frac{w_f^{(\alpha)}}{kT}) - \exp(-\frac{w_b}{kT}),\]  

(2.29)

where \(w_f\) is the forward activation energy

\[w_f^{(\alpha)} = w_{cs}(1 - \frac{T_c^{(\alpha)}}{G}),\]  

(2.30)

where \(w_{cs}\) is the activation enthalpy of cross-slip, and \(w_b\) is the backward activation energy, which in here, is assumed to be equal to the activation enthalpy of cross-slip \(w_{cs}\).

### 2.2.3 STRUCTURAL EVOLUTION IN THE CELL-WALL

The net rate of change in the density of dislocations stored in the cell-walls on each slip system is equal to the sum of storage and recovery rates as

\[(\dot{\rho}_w^{(\alpha)}) = (\dot{\rho}_w^{(\alpha)})^+ + (\dot{\rho}_w^{(\alpha)})^- .\]  

(2.31)

Assuming that edge dislocations become stored in the cell walls as mobile screw dislocations glide in the cell-interiors, the resultant increment of slip in cell-walls on system \(\alpha\) can be determined by knowing the density of mobile screw dislocations \(\rho_{c,m}^{(\alpha)}\) in cell-interiors and the average distance traveled by them \(d\gamma_w^{(\alpha)}\)

\[d\gamma_w^{(\alpha)} = b \rho_{c,m}^{(\alpha)} dr^{(\alpha)}.\]  

(2.32)
It can be further assumed that as a screw dislocation moves a distance $dr$ in a cell, an edge dislocation of length $2dr$ is deposited into the cell walls. Hence, the total line length of edge dislocations formed into a unit area of wall during a plastic strain increment of $d\gamma_c$ is $2dr\rho_{c,m}$. Substituting for $dr$ in Eq. (2.32), the dislocation density increment in the cell-walls becomes

$$
(\dot{\rho}_w^{(\alpha)})^+ = \left| \frac{j^{(\alpha)}_c}{b\delta_w} \right| \frac{2}{b\delta_w}, \tag{2.33}
$$

where $\delta_w$ is cell-wall thickness.

The recovery within the cell wall is assumed to occur by diffusion controlled climb and the annihilation of oppositely signed edge dislocations. This recovery rate can be stated as

$$
(\dot{\rho}_w^{(\alpha)})^- = -\rho_w^{(\alpha)} D_L \frac{G b^3}{kT}, \tag{2.34}
$$

where $D_L$ is lattice diffusivity.

### 2.3 Density of Geometrically Necessary Dislocations (GND)

In the plastic deformation of crystalline materials, the mismatch of slip at the boundaries of the grains or intragranular regions can result in gradients of plastic strain, which in turn result in the storage of the GND’s at geometrically necessary boundaries, which are required for the compatible deformations of different parts of the grains (see, for example, Hughes and Hansen, 1997).
The GND density is determined from the gradient of the crystallographic slip. Furthermore, the type and sign of GND’s can also be known from crystalline orientations.

Plastic strain gradient along slip direction $\tilde{s}^{(\alpha)}$ of slip system $\alpha$, can result in GND’s of edge type with density of $\rho_{G,e}$ to form on the slip system $\alpha$ as

$$\rho_{G,e}^{(\alpha)} = -\frac{1}{b} \left( \nabla \gamma^{(\alpha)} \cdot \tilde{s}^{(\alpha)} \right), \quad (2.35)$$

The plastic strain gradient along the transverse direction $\tilde{t}^{(\alpha)}$ is defined as $\tilde{s}^{(\alpha)} \times \tilde{n}^{(\alpha)}$, where $\tilde{n}^{(\alpha)}$ is slip system’s normal direction. This gradient can result in GND’s of screw type with density of $\rho_{G,s}$ to form on the slip system $\alpha$ as

$$\rho_{G,s}^{(\alpha)} = \frac{1}{b} \left[ \left( \nabla \gamma^{(\alpha)} \cdot \tilde{t}^{(\alpha)} \right) + \left( \nabla \gamma^{(\alpha')} \cdot \tilde{t}^{(\alpha')} \right) \right], \quad (2.36)$$

where $\alpha'$ is the co-linear system of slip system $\alpha$. Since screw dislocations are assumed to be free to cross-slip between co-linear systems, their density on each slip system is determined from both of the planes they can glide on. The plastic strain gradient in the normal direction $\tilde{n}^{(\alpha)}$ does not contribute to GND’s (Ashby 1970).

2.4 DENSITY OF GRAIN BOUNDARY DISLOCATIONS (GBD)

GBs are planar defects, where gliding dislocations can be impeded due to lattice discontinuity. A general GB usually contains several sets of edge and screw dislocations. Low-angle boundaries (misorientation less than 10 - 15°) can normally be considered as an array of dislocations. As misorientations across the GBs exceed the limit below which
boundaries are considered to be low-angle, the spacing between misfit dislocations becomes so small that individual misfit dislocations can no longer be physically identified, and the GB becomes a random high-angle GB.

In contrast, high-angle GBs contain large areas of poor fit while low-angle boundaries contain large areas of good fit separated by misfit dislocations. However, there are certain high-angle GBs with particular misorientation and boundary planes, which allow the fitting of atoms across the boundary. In this section, a formulation is presented, which approximately accounts for the density of GB misfit dislocations (Evers et al. 2004). Exact determination of the grain boundary dislocation densities, needs to be dealt with in a more precise manner.

Based on the best geometrical match between the slip systems of two adjacent grains, each slip system of one grain can be paired with a slip system of the other grain. Using the symmetries of an fcc lattice, there are twelve possible configurations. The best match is the one that causes the least amount of grain boundary dislocation (GBD) density.

As is shown in Fig. 2.1, magnitude of the resolved Burger’s vector $b^{GB}$ of a slip system $(\mathbf{\tilde{s}}, \mathbf{\tilde{n}})$ at the GB interface is

$$b^{GB} = \frac{b}{\cos(\alpha_2)}$$  \hspace{1cm} (2.37)
Taking $\tilde{n}_{gb}$ as the unit vector normal to the GB plane, $\alpha_1$ and $\alpha_2$ are then supplementary angles. Therefore $\cos(\alpha_2) = -\cos(\alpha_1)$. On the other hand $\cos(\alpha_1)$ is known from the inner product of $\tilde{n}$ and $\tilde{n}_{gb}$. Therefore, $b^{GB}$ can be restated as

$$b^{GB} = -\frac{b}{\tilde{n} \cdot \tilde{n}_{gb}} = \frac{b}{|\tilde{n} \cdot \tilde{n}_{gb}|}.$$  \hspace{1cm} (2.38)

As Fig. 2.2 illustrates, the misfit length $h$ between a slip system of grain 1 and its corresponding system in grain 2, is related to the magnitude of their resolved Burger’s vectors as

$$\frac{1}{\tilde{h}} = \frac{1}{b^{GB}_{A1}} - \frac{1}{b^{GB}_{A2}},$$  \hspace{1cm} (2.39)

Figure 2.1. Projection of the Burger’s vector of a slip system on the grain boundary plain
where the subscript $A_1$ indicates slip system $A$ in grain 1 and $\hat{A}_2$ is its pair in grain 2.

Figure 2.2. Misfit length between corresponding slip systems of two neighboring grains

With $h$ representing the spacing between the misfit dislocations at the GB, for slip systems $A_1$ and $\hat{A}_2$, the density of the misfit dislocations is

\[
\left| \rho_{A_1-\hat{A}_2}^{\text{GB}} \right| = \frac{1}{h^2} = \left( \frac{1}{b_{A_1}^{\text{GB}}} - \frac{1}{b_{\hat{A}_2}^{\text{GB}}} \right)^2. \tag{2.40}
\]

Using Eq. (2.38), Eq. (2.40) can be restated as
\[ \rho_{\Delta_1 \rightarrow \Delta_2}^{GB} = \left( \frac{||\tilde{n}_{A1} \cdot \tilde{n}_{gb}|| - ||\tilde{n}_{\Delta_2} \cdot \tilde{n}_{gb}||}{b^2} \right)^2. \] (2.41)
CHAPTER 3

COMPUTATIONAL AND MICROSTRUCTURALLY-BASED
FINITE-ELEMENT METHODOLOGIES

In this chapter, a brief outline of the microstructurally-based nonlinear finite-element method (FEM) that is used to solve the dislocation-density multiple-slip crystalline plasticity is presented. Specialized preprocessing tools were also used and developed to generate physically-based grain shapes and distributions that are based on Voronoi tessellation and polygons. These preprocessing tools also included schemes for the generation of grain orientations and GB misorientations by the random distribution of Euler angles.

3.1 MICROSTRUCTURALLY-BASED FEM TECHNIQUES

The FEM method that is used here is based on the modification of the method developed by Zikry (1994) for multiple-slip dislocation-density crystal plasticity. The deformation-rate tensor \( D \) and the plastic part of it \( D^p \) are needed to update the material stress state. An implicit finite-element method is used to obtain the total deformation-rate tensor. Nodal displacements are obtained by the quasi-Newton BFGS method. The B-bar method is used to overcome any spurious modes associated with incompressible deformations. By knowing the nodal displacements, the deformation gradient tensor \( F \)
that maps the undeformed configuration of an element to its deformed configuration is derived in two dimensions as

\[
F = \begin{bmatrix}
\frac{\partial x'}{\partial x} & \frac{\partial x'}{\partial y} \\
\frac{\partial y'}{\partial x} & \frac{\partial y'}{\partial y}
\end{bmatrix},
\]  

(3.1)

where \( x' \) and \( y' \) are the coordinates of the deformed state for finite inelastic deformations (Fig. 3.1).

**Figure 3.1. Reference and deformed states of an element**

In this investigation, planar deformations will be investigated, and hence four nodded quadrilateral elements will be used. For bilinear shape functions, the partial derivatives in global coordinates at the integration points from the nodal values are

\[
\frac{\partial x'}{\partial x} = P_1 x'_1 + P_2 x'_2 + P_3 x'_3 + P_4 x'_4,
\]

(3.2-a)
\[
\frac{\partial x'}{\partial y} = Q_1 x_1' + Q_2 x_2' + Q_3 x_3' + Q_4 x_4'.
\] (3.2-b)

From Eq. (2.1), the velocity gradient tensor is

\[
L = \dot{F} F^{-1}.
\] (3.3)

Fig. 3.2 illustrates the sequential steps that are needed for calculating the velocity gradient tensor. Assuming that \( A \) represents the initial undeformed configuration and \( A' \) represents the deformed state for which the stress state is known, and also that \( A'' \) is the new deformed state for which the stress state is not known, the velocity gradient tensor that describes the transition from \( A' \) to \( A'' \) can be obtained as

\[
L_{A'A''} = \frac{1}{dt} \left( F_{AA''} - F_{AA'} \right) F_{AA'}^{-1}.
\] (3.4)

Once the velocity gradient tensor is obtained, the derivation of the total deformation-rate tensor and the total spin tensor can be updated. At this point the stress state at integration point can be updated and consequently the nodal forces will be updated.

Figure 3.2. Schematic of velocity gradient tensor calculation
For the inelastic components, the microstructure pertaining to the dislocation-density based formulation has to be updated. For the density of the SSDs, the governing ordinary differential equations of evolution are solved using a fifth-order Runge-Kutta method, and the density of the GNDs is determined from the gradient of the crystallographic shear slip.

The elements are also automatically flagged in the code in such a way that the GB elements are distinguished from the grain interior elements. Since, the crystal lattice may not be continuous across the GB, then the gradient formulation for the GNDs is not applied at the GB region.

To determine the GBD densities, the set of the twelve slip systems in every GB element is matched with the slip systems of its neighboring element in twelve different ways. The desired configuration is the one that results in the least amount of dislocation density. For every boundary element, at each increment, all the twelve possible configurations are analyzed and twelve densities are calculated, from which the smallest one is taken as the density at the GB.

The sequence of steps that are taken to update the inelastic components and dislocation-densities is outlined in Fig. 3.3.
Figure 3.3. Formulation steps and sequence
3.2 GENERATION OF GRAIN SHAPES AND GRAIN DISTRIBUTIONS

Voronoi tessellation was used to generate two-dimensional grains. Starting with a set of initial points that are randomly distributed over the domain of the sample, Voronoi tessellation (see, for example, Aboav, 1970; Weyer et al., 2002) assigns a polygon to each initial point. Each polygon then represents a grain. Voronoi tessellation is done using the built-in Voronoi function of MATLAB (The MathWorks Inc., MATLAB documentation set). The coordinates of the vertices of the resulted polygons are then input to a code that calculates the coordinates of the boundary points based on the dimensions of the sample (Fig. 3.4).

Refined mesh regions are needed in the GB region to be able to model processes, such as GBD evolution. Therefore, an algorithm was implemented to represent a boundary region on each side of every boundary line with a specified width (Fig. 3.5). The vertices of each polygon are projected by a distance along the bisectors of their corresponding angles. An inner polygon is then created from these projected vertices. The area between the inner and outer polygons is the boundary region, which can be meshed with any desirable level of refinement. More importantly, the refinement can be done just along the normal to the boundary, which can then restrict mesh refinement to the desired GB regions.

The crystallographic orientation of each randomly oriented grain is represented by the Euler angles $\phi_1, \Phi, \phi_2$ (see, for example, Hill and Havner, 1982).
Figure 3.4. A polycrystal sample generated by Voronoi tessellation with randomly distributed initial points

Figure 3.5. An enhanced polycrystal model with grain boundaries added to the Voronoi tessellation
CHAPTER 4

ROLLING COMPRESSION AND GRAIN SUBDIVISION IN SINGLE CRYSTALS: MODELING AND EXPERIMENTAL VALIDATION

A detailed understanding and characterization of grain subdivision at different scales is needed to delineate how different microstructural entities, such as dislocation-cells and walls, their densities and crystallography evolve for an unstable orientation. In this chapter, the crystal plasticity formulation is used in a specialized finite-element analysis to investigate the grain subdivision in a cube oriented aluminum single crystal under rolling compression with strains of up to 30%. At the macroscopic scale (length scales of approximately 100 µm or greater), grain subdivision is characterized by deformation bands consisting of wide matrix bands (MBs), which are separated by narrow transition bands (TBs). MBs have alternate positive and negative rotations, while TBs maintain their initial orientation to maintain lattice continuity. At the microscopic scale, grain subdivision is characterized by dislocation-cells separated by cell-walls and cellblocks, which are surrounded by high-angle dislocation boundaries. A shear amplitude imbalance is used to initiate deformation banding, and comparisons are made with experimental observations and measurements. A detailed presentation is given in Rezvanian et al. (2006).
4.1 CUBE ORIENTATION AND SHEAR-STRAIN AMPLITUDE

In a single crystal with a cube orientation (Euler angles $\varphi_1 = 0, \Phi = \Phi_1$ and $\varphi_2 = 0$), if the slip resistance is the same for all slip-systems, it can be shown that there are four active slip systems with the same magnitude of slip. Furthermore, the plastic spin can also be shown to be zero. However, experimental observations (see, for example, Wert et al. (1997)) have shown that under rolling, single crystals with a cube orientation split into deformation bands, which alternatively rotate mainly about the transverse direction (TD) (Fig. 4.2). Wert et al. (1997) suggested that a shear-strain imbalance between the four potentially active slip-systems was the main mechanism that resulted in this rotation. As noted by Wert et al. (1997), if a shear imbalance is imposed between the four active slip-systems, the overall strain tensor remains unchanged, but a lattice rotation about the TD is attained. Assuming that the four slip-systems are denoted b1 ((1 1 1) [0 1 1]), d1 ((1 1 1) [0 1 1]), a3 ((1 1 1) [0 1 1]) and d3 ((1 1 1) [1 0 1]) the imbalance can be imposed as

$$\gamma^{(-a_3)} = \gamma^{(-c_3)} = \gamma_0 + d\gamma$$

$$\gamma^{(-b_1)} = \gamma^{(-d_1)} = \gamma_0 - d\gamma.$$  \hspace{1cm} (4.1)

Then the plastic deformation rate tensor can be recast as

$$D_{ij}^p = P_{ij}^{(a_3)}(\gamma_0^{(a_3)} + d\gamma) + P_{ij}^{(b_1)}(\gamma_0^{(b_1)} - d\gamma) + P_{ij}^{(c_3)}(\gamma_0^{(c_3)} + d\gamma) + P_{ij}^{(d_1)}(\gamma_0^{(d_1)} - d\gamma)$$

$$= P_{ij}^{(a_3)}\gamma_0^{(a_3)} + P_{ij}^{(b_1)}\gamma_0^{(b_1)} + P_{ij}^{(c_3)}\gamma_0^{(c_3)} + P_{ij}^{(d_1)}\gamma_0^{(d_1)}. \hspace{1cm} (4.2)$$

The spin tensor then becomes

$$W_{\gamma/\gamma_e} = W_{\gamma/\gamma_e}^{(a_3)}(\gamma^{(a_3)} + d\gamma) + W_{\gamma/\gamma_e}^{(b_1)}(\gamma^{(b_1)} - d\gamma) + W_{\gamma/\gamma_e}^{(c_3)}(\gamma^{(c_3)} + d\gamma) + W_{\gamma/\gamma_e}^{(d_1)}(\gamma^{(d_1)} - d\gamma). \hspace{1cm} (4.3)$$

From these equations, it can be seen that the sign and the magnitude of the lattice rotation is a function of sign and magnitude of the shear imbalance. Macroscopic transverse shear
strain’s profile of change along the normal direction which is resulted from the combined effect of geometry and surface friction during rolling, has been found to be similar to the pattern by which lattice rotation around TD changes (see, for example, Liu and Hansen, 1998). In order to be able to model the shear imbalance, it is assumed in this formulation that the macroscopic transverse shear strain $\varepsilon_{yz}$ can affect the slip resistance of the slip-systems so that under equal resolved shear stresses they show unequal amount of plastic slips

$$\hat{\tau} = (1 + (n^{(\alpha)} \cdot j) \varepsilon_{yz}) \tau_y + f(\rho),$$

(4.4)

Where $j$ is the unit vector in the rolling direction and $n^{(\alpha)}$ is the unit vector normal to the slip plane of the slip system $\alpha$. The sign of the shear imbalance depends on the relative position of the slip system and the rolling direction. The modified slip-resistance will impose an imbalance between the two sets of co-directional slip systems.

### 4.2 RESULTS AND DISCUSSION

The multiple-slip crystalline formulation, the computational approach, and the interrelated evolution equations pertaining to cell-interior and cell-wall dislocation densities and dislocation-cell size were applied to investigate how deformation bands evolve in an Aluminum single crystal subjected to rolling.

In rolling (see, for example, Lee and Duggan, 1991), the imposed deformation geometry and the surface friction are the main factors that cause texture inhomogeneity both at the surface and through the thickness of a rolled grain. It can be shown that by
adding a shear component to the strain tensor, texture evolves as \( \gamma_g \), which is the ratio of the shear strain to the compression strain approaches 0.5. A simplified geometrical model of the rolling process is shown in Fig. 4.1, where \( r \) is the reduction, \( d \) is the specimen thickness, and \( L \) is the contact length.

To model the rolling process, the displacement of each node is determined based on the relative position of the roller. As the plate passes through the rollers, the top nodes, in the finite element model, displace downwards from their original position (Fig. 4.2, level 1), to the final displaced position (Fig. 4.2, level 3). The final displaced position corresponds to the desired final reduction and the transition level (Fig. 4.2, level 2) corresponds to the contact surface.

Using this scheme, the virtual roller is modeled by imposing a time-delayed nodal displacement. As shown in Fig. 4.3(b), after the first node \( n_1 \) is displaced, it takes a time period of \( T_d = m \times dt \) for the second node \( n_2 \) to be displaced. The time it takes for each node to reach the final displaced position is \( T_n = n \times dt \). \( T_n \) is determined based on the imposed strain-rate and the amount of reduction needed at each path

\[
\dot{\varepsilon} = r / T_n. \tag{4.5}
\]

From Fig. 4.3(d) it is seen that \( T_n \) is a multiple of \( T_d \), \( T_n = k \times T_d \). Fig. 4.3(d) also shows that \( k \) is known from the contact length and the length of the finite elements, \( dx \)

\[
L = k \times dx. \tag{4.6}
\]

The contact length is \( L = d / (2\gamma_g) \). Therefore the desired time delay is obtained as a function of contact length, length of finite elements and \( T_n \). Obviously, reduction of the time delay will result in an increase in the number of elements (Table 4.1). So, it is
important to reach a trade-off between the accuracy and the computational effort. Different simulations were run to determine a convergent mesh size of 1960 quadrilateral elements. The material properties that are used are representative of aluminum (Table 4.2).

The modeling of the subdivision of a cube oriented single crystal under rolling into matrix bands, which rotate around the TD and transition bands, which connect the matrix bands, is one of the major objectives of this analysis. Fig. 4.4(a) shows the variation of the average rotation angle over the half thickness of the model after a 30% reduction. One matrix band and a transition zone have developed over the top half of the specimen under rolling. A comparison is made with the experimental measurements of Liu and Hansen (1998) shown in Fig. 4.4(b) in which four matrix bands and three transition bands have formed across the full thickness. There is good agreement between the experimental values and the computational predictions. As seen from these results, the lattice rotation is high in the matrix band and decreases toward the center of the transition band. Contours of lattice rotation at reductions of 10, 20 and 30% are shown in Fig. 4.5. As these results indicate, the lattice rotations are lowest at the bottom and highest at the top of the deformed geometry.

The trend of the rotation variation through the thickness is seen to be the same, although the number of bands is different for the predicted values. Both results show a counter-clockwise rotation at the first matrix band M1. This grain break-up by lattice rotation around TD is in agreement with experimental observations (Liu and Hansen, 1998).
Experimental observations (Liu and Hansen, 1998) have shown that there is a large difference between the microstructure of a matrix band and a transition band. Matrix bands break into cellblocks whereas transition bands consist of a non-uniform cell structure. The difference is due to the size of the dislocation cells and the morphology of dislocation boundaries in the two regions, and these differences can be more pronounced at large strains. Ridha and Hutchinson (1982) observed a cell size difference in their early work on rolled copper. They observed relatively large cells in a region of the rolled sample, which had remained in a perfect cube orientation and more narrow cells in other regions. Liu and Hansen (1998) reported observing an average cell size in the central region of transition bands about twice the average size of the cells in the matrix bands after 50% reduction of a rolled aluminum. As seen in Figs. 4.6(a) and (b), the stored dislocation density decreases as the cell size increases, which is in agreement with these experimental observations. Contours of normalized cell-interior dislocation density at reductions of 10, 20 and 30% are shown in Fig. 4.7.

It has also been suggested that the dislocation glide ratio affects dislocation cell size changes and boundary morphology differences in both the matrix and transition bands. Liu and Hansen (1998) have reported an equal amount of slip system activity on the two sets of co-directional slip systems at the center of a transition band, while in the matrix band one co-directional set dominates. Therefore, in a matrix band, there are two slip systems with one Burgers vector, whereas in a transition band, there are four slip systems with two types of Burgers vector. The existence of two types of Burgers vector results in the formation of equiaxed dislocation cells in the transition bands, while the existence of one Burgers vector in the matrix bands results in the formation of extended
dislocation boundaries that encompass cell blocks. Fig. 4.8 shows the ratio of the slip-rate on slip system a sub 3 to b sub 1, with two different Burgers vectors. It is clearly seen that at the center of the transition band, the ratio of slip-rates on the two systems is very close to unity, which is indicative of the existence of different Burgers vectors. In the matrix band, slip-system a sub 3 is the dominant slip-system, and shows approximately 25% more activity than slip-system b sub 1 at values corresponding to a 30% reduction. The contours of slip-rate of these two slip systems are shown in Fig. 4.9 at reductions of 10, 20 and 30%.

4.3 CONCLUSIONS

A dislocation density based crystal plasticity formulation and a finite-element computational method were used to investigate grain subdivision into inhomogeneous bands in a cube oriented aluminum single crystal under large rolling strains. Evolution equations related to the densities and dimensions of dislocation-cells and walls have been formulated and coupled to a multiple-slip crystal plasticity formulation. The effects of shear strain imbalances due to transverse shear strains was examined by modifying slip-system threshold resistances.

The computational analyses clearly show that inhomogeneous deformation bands that are comprised of two MBs separated by a TB initiated and evolved across the thickness of the aluminum crystal. The lattice rotation in the MBs was as high as 4 degrees at 30% reduction due to rolling. A slip system analysis showed there was a combination of four active slip systems with equal activity in the TB, while in the MBs
there were two dominant slip systems. These different combinations of active slip systems result in microstructures of different morphology. The TBs were shown to consist of a microstructure of dislocation cells, and the MBs were shown to have a cell-block structure with narrower dislocation cells. The dislocation cell size profile along the normal direction increased as the interior dislocation-densities decreased. These predictions were in good agreement with experimental measurements and observations related to TB and MB formation and evolution in cube-oriented single crystals subjected to large strain rolling. The present analysis underscores how different interrelated microstructural characteristics, such as dislocation cell size, dislocation densities at cell interiors, and threshold stresses can be coupled to crystalline behavior to physically represent inhomogeneous deformation bands in cube-oriented single crystals that theoretically should only undergo homogenous deformations.
Table 4.1 Required time delays associated with the number of elements

<table>
<thead>
<tr>
<th>No. of elements</th>
<th>20</th>
<th>25</th>
<th>10</th>
<th>250</th>
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<td>32</td>
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<td></td>
</tr>
<tr>
<td>40</td>
<td>50</td>
<td>20</td>
<td>1000</td>
<td></td>
</tr>
<tr>
<td>56</td>
<td>70</td>
<td>28</td>
<td>1960</td>
<td></td>
</tr>
<tr>
<td>64</td>
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<td></td>
</tr>
<tr>
<td>80</td>
<td>100</td>
<td>40</td>
<td>4000</td>
<td></td>
</tr>
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Table 4.2 Material properties and constitutive parameters for pure aluminum

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elastic modulus</td>
<td>E</td>
</tr>
<tr>
<td>Shear modulus</td>
<td>G</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>ν</td>
</tr>
<tr>
<td>Density</td>
<td>ρ</td>
</tr>
<tr>
<td>Yield stress</td>
<td>$\sigma_y$</td>
</tr>
<tr>
<td>Strain rate sensitivity parameter</td>
<td>m</td>
</tr>
<tr>
<td>Burger’s vector magnitude</td>
<td>b</td>
</tr>
<tr>
<td>Initial cell-interior dislocation density</td>
<td>(\rho_{c,initial})</td>
</tr>
<tr>
<td>Initial cell-wall dislocation density</td>
<td>(\rho_{w,initial})</td>
</tr>
</tbody>
</table>
Figure 4.1. Rolling geometry

Figure 4.2. Rolling geometry and schematic finite element mesh
Figure 4.3. Nodal displacements at the surface resembling roller movement
Figure 4.4 Average TD rotations as a function of distance from the top surface at 30% reduction. (a) Simulation (ND/RD=(001)[010]); (b) Experimental measurements by Liu and Hansen (1998), (ND/RD=(001)[100])
Figure 4.5. Contours of lattice rotation around transverse axis at different reduction levels. (a) 0 to 10%; (b) 10% ;(c) 10 to 20%; (d) 20; (e) 20 to 30%; (f) 30%
Figure 4.6. (a) Relative magnitude of average total stored dislocation density as a function of distance from the top surface at 30% reduction; (b) Relative size of average dislocation cells as a function of distance from the top surface at 30% reduction.
Figure 4.7. Contours of relative total stored dislocation density (m/m³) at different reduction levels. (a) 0 to 10%; (b) 10%; (c) 10 to 20%; (d) 20%; (e) 20 to 30%; (f) 30%. Initial value of dislocation density is assumed to be 1e11
Figure 4.8. Ratio of average slip-rate on slip system $(111)[0\bar{1}1]$ to the average slip-rate on $(\bar{1}\bar{1}1)[011]$ as a function of distance from the top surface at the third pass of roller from 20% to 30% reduction.
Figure 4.9. Contours of slip-rates on slip systems (111)[011] on the left and (TT1)[011] on the right at different reduction levels. (a and d) first pass; (b and e) second pass; (c and f) third pass.
CHAPTER 5

THE EVOLUTION AND INTERACTION OF STATISTICALLY STORED DISLOCATIONS IN F.C.C. POLYCRYSTALLINE AGGREGATES

Grain shapes and their effects on inelastic deformations are among the key factors that need to be addressed to better understand the localized behavior in polycrystalline aggregates. As noted earlier, generating random geometries can be used to approximate the actual geometry of the grains in polycrystals. This is naturally more realistic than approximating the actual geometry by uniform geometrical shapes. Furthermore, in certain circumstances, it may prove to be superior to approximating shapes from SEM and TEM images, since then the actual shapes would also have to be averaged to account for the microstructural representation of an entire sample.

In this chapter, Voronoi tessellation is used to generate a polycrystalline aggregate with physically realistic grain shapes. A dislocation density based multiple-slip crystal plasticity formulation that considers only the evolution of SSDs will be coupled to specialized finite-element analysis. This formulation is then used to study the inelastic deformation of a polycrystalline aggregate with randomly distributed low and high-angle GBs. The GBDs due to lattice misorientations across the GBs and GNDs due to plastic strain gradients are not incorporated in the formulation, in order to understand how the evolution of SSDs affects the microstructural response. The coupled effects of GNDs and GBDs will be fully investigated in Chapters 6-8.
5.1 POLYCRYSTAL MODEL

A 50-grain polycrystal sample of 500 by 500 microns is generated using Voronoi tessellation with random initiation points. The model is meshed with 1803 quadrilateral elements, based on a convergence analysis. The geometry, loading and boundary conditions are shown in Fig. 5.1. The material properties of the grains are representative of copper (a f.c.c material). The material properties and the parameters used in the crystal plasticity formulation are given in Table 5.1. The grains initial orientations are equally proportioned between the three regions of the inverse pole figure as shown in Fig. 5.2. Within each region, grains are randomly oriented in such a way that causes a combination of random low and high-angle GB misorientations (Fig. 5.3). In Table 5.2, the slip systems’ numbering and their corresponding slip planes and slip directions are shown. A 3-D schematic of slip planes and directions is shown in Fig. 5.4.

5.2 RESULTS AND DISCUSSION

Under the applied quasi-static tensile loading, the deformation in the aggregate is dominated by three slip systems 9, 10, and 12 as seen in Fig. 5.5 at a nominal strain of 20%. It is seen that the accumulated crystallographic shear slips have a localized high values, with a maximum of 1.44, at the region where necking has occurred due to the random texture and grain shape, which results in the geometrical softening of the material (Ashmawi and Zikry, 2003). However, the sheared region is limited to a small region and not developed to form a larger sheared strip across a number of grains. This can show
that inelastic intergranular and intragranular deformations are constrained due to slip incompatibilities between the grains.

Contours of dislocation density in dislocation cell interiors and cell walls and dislocation cell size are shown in Figs. 5.6, 5.7, and 5.8 at a nominal strain of 20%. A comparison of the distribution of dislocation densities of the cell-interiors and walls, and dislocation cell size with the distribution of the accumulated plastic slips (Fig. 5.5) shows a very similar pattern, which is an indication that dislocation cell and wall formation are strongly dependent on the plastic slip. It can also be seen that dislocation cell size is inversely proportional to the density of cell interior dislocations that is due to the proportional distribution of the stress between dislocation cells and walls.

The contours of shear slip rates, which are scaled by the reference slip rate (Table 5.1), are shown in Fig. 5.9 for nominal strains of 10% and 20%. A comparison between these two nominal strains indicates that maximum shear strains occur at different locations in the aggregate, which is an indication of the slip hardening and reorientation changes that occur as the microstructure evolves.

The contours of the normalized (normalized by the static yield stress, Table 5.1) resolved shear stresses corresponding to the active slip systems are shown in Fig. 5.10 for a nominal strain of 20%. The distribution of the resolved shear stress on each slip system changes from grain to grain based on the slip system orientations.

The contours of the normalized slip resistance (normalized by the static yield stress, Table 5.1) at a nominal strain of 20% are shown in Fig. 5.11. In comparison with the resolved shear stress contours, a more uniform distribution is seen for the slip
resistance, which is due to the interaction of the stored dislocation densities on each slip system with other slip systems (c.f. Eq. (2.9)).

The lattice rotations (Fig. 5.12), at a nominal strain of 20% indicate the grain subdivision phenomena, as seen by the intragranular regions that have rotated in opposite directions or with different magnitudes. Some localized high intragranular rotations are seen that are due to the combined effects of the random grain shapes and the texture.

The total accumulated shear slip contour is shown in Fig. 5.13 at a nominal strain of 20%. Here more accumulation is seen in a sheared strip at the bottom right corner that is most likely due to the random texture, grain shape, and geometrical softening effects. The necking at the right end of the band causes the global unloading of the stress-strain curve, which is due to geometrical softening (Fig. 5.16).

The contour of the normal stress (normalized by the yield stress) is shown in Fig. 5.14 at a nominal strain of 20%. The intragranular stress distribution is seen to be very homogeneous with no localization at the GBs. The strain-hardened region at the place of necking shows the highest level of normal stress. The contour of the lateral stress (normalized by the yield stress) in Fig. 5.15 for a nominal strain of 20% shows the same pattern. The overall stress-strain curve is shown in Fig. 5.16. The strain hardening is due to the interaction of the SSDs with mobile dislocations. The global unloading is due to the necking that occurs because of the random texture and grain shapes and geometrical softening.
5.3 CONCLUSIONS

The developed dislocation density based multiple-slip crystal plasticity formulation that considers a heterogeneous distribution of SSDs has been coupled to specialized finite-element analysis for polycrystalline aggregates with physically realistic grain shapes. This formulation was then used to analyze the inelastic deformation of a polycrystalline aggregate with randomly distributed low and high-angle GBs. The heterogeneous representation of the SSDs provided an understanding of the dislocation microstructure as a function of the plastic slip. Physically realistic grain shapes, texture evolution, and geometrical softening resulted in localized phenomena to initiate in some grains. However, the growth of these localized patterns and modes is inhibited that is a strong indication that GB strength can play an essential role in the growth of localized modes by providing a medium for propagation of intragranular heterogeneous deformations. This will be investigated in detail in the forthcoming chapters.
Table 5.1. Material properties and constitutive parameters for pure copper

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Value</th>
<th>Unit</th>
<th>Used in Eq.</th>
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</thead>
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<td>Young’s modulus</td>
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<td>GPa</td>
<td></td>
</tr>
<tr>
<td>Yield stress</td>
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<td>MPa</td>
<td>Eq. (2.7)</td>
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<td></td>
<td></td>
</tr>
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<td>GPa</td>
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<td>m</td>
<td></td>
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<td></td>
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<tr>
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<td>Eq. (2.8,20-a,20-b)</td>
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<tr>
<td>Attempt frequency of cross-slip</td>
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<td>Eq. (2.27)</td>
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<tr>
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<td>m</td>
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<tr>
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<td>Interaction coefficient $\alpha_2$</td>
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<td>0.61</td>
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<td>Eq. (2.9,21-a,21-b)</td>
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<tr>
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<td>Eq. (2.24)</td>
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<td>J</td>
<td>Eq. (2.5,17-a,17-b)</td>
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<td>GND long-range effect radius</td>
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<td>$3 \times 10^{-6}$</td>
<td>m</td>
<td>Eq. (2.12,13)</td>
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Table 5.2. Slip systems numbering and corresponding slip planes and directions

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<tr>
<th>Slip system number</th>
<th>Slip plane unit normal $\mathbf{n}$</th>
<th>Slip direction unit normal $\mathbf{s}$</th>
<th>Schmid &amp; Boas notation</th>
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<td>1</td>
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<td>$\frac{1}{\sqrt{2}} [\overline{1}01]$</td>
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<td>$\frac{1}{\sqrt{2}} [\overline{1}10]$</td>
<td>B5</td>
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<tr>
<td>3</td>
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<td>$\frac{1}{\sqrt{2}} [0\overline{1}1]$</td>
<td>B2</td>
</tr>
<tr>
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<td>$\frac{1}{\sqrt{2}} [011]$</td>
<td>C1</td>
</tr>
<tr>
<td>5</td>
<td>$\frac{1}{\sqrt{3}} (\overline{1}\overline{1}1)$</td>
<td>$\frac{1}{\sqrt{2}} [\overline{1}01]$</td>
<td>C5</td>
</tr>
<tr>
<td>6</td>
<td>$\frac{1}{\sqrt{3}} (\overline{1}\overline{1}1)$</td>
<td>$\frac{1}{\sqrt{2}} [011]$</td>
<td>C3</td>
</tr>
<tr>
<td>7</td>
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<td>$\frac{1}{\sqrt{2}} [101]$</td>
<td>A3</td>
</tr>
<tr>
<td>8</td>
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<td>$\frac{1}{\sqrt{2}} [110]$</td>
<td>A6</td>
</tr>
<tr>
<td>9</td>
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<td>$\frac{1}{\sqrt{2}} [0\overline{1}1]$</td>
<td>A2</td>
</tr>
<tr>
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<td>$\frac{1}{\sqrt{2}} [011]$</td>
<td>D1</td>
</tr>
<tr>
<td>11</td>
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<td>$\frac{1}{\sqrt{2}} [110]$</td>
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<td>12</td>
<td>$\frac{1}{\sqrt{3}} (1\overline{1}1)$</td>
<td>$\frac{1}{\sqrt{2}} [\overline{1}01]$</td>
<td>D4</td>
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Figure 5.1. 50-grain aggregate’s geometry, grain numbering, loading and boundary conditions
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Figure 5.3. Initial GB misorientations and distributions. -- shows GB misorientations less than 15°, --- shows GB misorientations between 15° and 25°, ----- shows GB misorientations greater than 25°
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Figure 5.5. (continued)
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CHAPTER 6

GEOMETRICALLY NECESSARY DISLOCATION AND GEOMETRICAL BOUNDARY DISLOCATION DENSITIES AND MICROSTRUCTURAL EVOLUTION IN F.C.C. POLYCRYSTALLINE AGGREGATES

As noted earlier, polycrystalline aggregates can subdivide into smaller microstructural constituents. At the smallest scale there are dislocation cells, and at the larger scale, GNBs can form cell-blocks that enclose the dislocation cells. This subdivision is mainly due to anisotropic crystallographic texture that leads to intercrystalline inhomogeneities. Since deformations should be compatible at the GBs, at least for athermal deformations when there is no GB sliding, intragranular deformation inhomogeneities can arise that eventually result in gradients of the plastic slip. This in turn results in intragranular texture to develop that leads to intragranular lattice misorientations. GNBs are then needed to preserve the lattice continuity. These GNDs also act as obstacles to mobile dislocations, and therefore increase the strain hardening of the material.

Experimental analysis of the correlation between the slip pattern and the microstructure (Liu et al., 1998; Hansen et al., 2001) has indicated that some grain orientations (Fig. 1.1, region II) develop GNBs that contain Burger’s vectors, which belong to one slip plane. These GNBs are commonly denoted (Hansen and Juul Jensen, 1999) as crystallographic boundaries, and they form when two co-planar active slip systems account for a large fraction of the slip. Whereas, some other grain orientations
(Fig. 1.1, region III) result in the formation of GNBs with Burger’s vectors belonging to two active slip planes. These GNBs are denoted as non-crystallographic boundaries. It has been further observed (see, for example, Liu et al., 1998) that the crystallographic boundaries have a mixed tilt and twist characteristic, while the non-crystallographic boundaries have predominantly tilt characteristic. Crystallographic boundaries can then consist of both types of GNDs, namely edge and screw types, and non-crystallographic boundaries are mostly comprised of GNDs of edge type.

At the GBs, misfit dislocations form to accommodate the intergranular lattice misorientations. The high density of dislocations at the GBs, makes them more resistant to slip than the grain bulk interiors, which subsequently causes a highly heterogeneous pattern of stress distribution to develop. These GB dislocations also serve as obstacles to mobile dislocations, and thereby increase the aggregate’s strain hardening response.

Hence, in this chapter, the GB and GNB dislocation-density effects are investigated by accounting for their evolution in the same aggregate and with the same distribution of random low and high-angle GBs as that was used in Chapter 5. In that analysis, only SSDs were considered, therefore based on this study, we will be able to understand how the interrelated effects of SSDs, GBDs, and GNDs affect microstructural behavior.

6.1 RESULTS AND DISCUSSION

The geometry of the 50-grain aggregate and the loading conditions are the same as Chapter 5. Under the applied quasi-static tensile loading, the deformation in the
aggregate is dominated by three slip systems 9, 10, and 12 as seen in Fig. 6.1 at a nominal strain of 20%. Two of these, slip systems 10 and 12 are coplanar. The GNDs of edge type are shown in Fig. 6.2 and the GNDs of screw type are shown in Fig. 6.3. These results indicate that where non-coplanar systems 9 and 10 or 9 and 12, have considerable GND densities of edge type, the GND densities of screw type are at a lower level. This is consistent with the experimental observations of Liu et al. (1998) that indicate when Burger’s vectors of the GNBs belong to two slip planes, the corresponding GNDs are edge dislocations, and therefore the microstructure at these locations consists of mainly non-crystallographic GNBs.

Furthermore, it is also seen that at regions where the two co-planar systems 10 and 12 account for the most GND density accumulations of edge type, a GND density of screw type of approximately the same magnitude is present. This is also in agreement with the slip system analysis of the experimental results of Liu et al. (1998) that indicate when Burger’s vectors of the GNBs belong to two co-planar systems, the corresponding GNDs have a mix character of edge and screw dislocations. Hence, the microstructure at these regions consists mainly of crystallographic GNBs.

Contours of dislocation density in dislocation cell interiors and cell walls are shown in Figs. 6.4 and 6.5 at a nominal strain of 20%. A comparison of the distribution of dislocation densities of the cell-interiors and walls with the distribution of the accumulated plastic slips (Fig. 6.1) shows a very similar pattern, which is another indication that dislocation cell and wall formation are strongly dependent on the plastic slip.
The dislocation cell size contours of Fig. 6.6 have smaller dislocation cells in the grain interiors than in the GB regions, which is consistent with the composition of the grains in which the GBs are less plastically deformable (see, for example, Randle et al., 1996). It is further observed that when the GNBs are crystallographic, the smallest dimensions of dislocation cells belong to the coplanar slip systems, and when the GNBs are non-crystallographic, the smallest dimensions belong to non-coplanar slip systems.

In Fig. 6.7, the GBD density contours are shown for a nominal strain of 20%. Based on Eq. 2.41, coplanar slip systems should have the same amount of GBD densities. Therefore, only one contour is presented for each slip plane. A comparison of the GBD density contours with the distribution of GB misorientation angles in Fig. 5.3 shows that high GB misorientations do not necessarily mean a high misfit dislocation density on all slip systems at the GB. This occurs, because even a high misorientation angle GB can result in a good fit between two slip planes. In Fig. 6.8, the change in the normalized total GBD density content (normalized by its maximum value) is shown for the total deformation history. This decreasing trend indicates that the compatible deformation of the grains results in a reorientation at the GBs, in such a way that the average misorientation between neighboring grains is lowered. From an energy perspective, lower GBD densities translate into lower energy levels, which clearly indicate that the microstructure is evolving to a stable configuration.

The contours of shear slip rates, which are scaled by the reference slip rate (Table 5.1), are shown in Fig. 6.9 for nominal strains of 10% and 20%. A comparison between these two nominal strains indicates that maximum shear strains occur at different
locations in the aggregate, which is an indication of the slip hardening and reorientation changes that occur as the microstructure evolves.

The contours of the normalized (normalized by the static yield stress, Table 5.1) resolved shear stress magnitude corresponding to the active slip systems are shown in Fig. 6.10 for a nominal strain of 20%. The distribution of the resolved shear stress on each slip system changes from grain to grain based on the slip system orientations. The high resolved shear stresses at the GBs are due to the enhanced strength of these regions that occurs due to the GBDs.

The contours of the normalized slip resistance (normalized by the static yield stress, Table 5.1) at a nominal strain of 20% are shown in Fig. 6.11. In comparison with the resolved shear stress contours, a more uniform distribution is seen for the slip resistance, which is due to the interaction of the stored dislocation densities on each slip system with other slip systems (Eq. (2.9)).

The lattice rotations (Fig. 6.12), at a nominal strain of 20% clearly indicate the grain subdivision phenomena, as seen by the intragranular regions that have rotated in opposite directions or with different magnitudes. The localized high rotations are the result of the combined effects of the texture, grain shapes, and GB misorientations. The high lattice rotation gradients correspond to regions of high GND (Figs. 6.2-3), which is consistent with the role of GNDs in preserving the lattice continuity (Hughes, 2001).

The total accumulated shear slip contour is shown in Fig. 6.13 at a nominal strain of 20%. The sheared strip at the bottom right corner is most likely due to random texture and grain shapes. The necking at the right end of the band causes the global unloading of the stress-strain curve (Fig. 6.16).
The contour of the normal stress (normalized by the yield stress) is shown in Fig. 6.14(a) at a nominal strain of 20%. Due to the random grain shapes, texture and GB distributions and misorientations, the stresses have accumulated in particular GB regions. Furthermore, it can be seen that high stress gradients occur at some triple junctions (Fig. 6.14(b)), which can indicate the potential for crack initiation.

The contour of the lateral stress (normalized by the yield stress) is shown in Fig. 6.15 at a nominal strain of 20%. The lateral stresses are heterogeneously distributed at intergranular and intragranular regions. The overall stress-strain curve is shown in Fig. 6.16 for the two different formulations. As clearly seen, if the effects of the GNDs and GBDs would not have been coupled with the SSDs, the average response would have been significantly different.

6.2 CONCLUSIONS

A unified dislocation density based multiple-slip crystal plasticity formulation that integrates SSDs, GNDs, and GBDs in one framework has been developed and coupled to specialized finite-element analysis for polycrystalline aggregates with physically realistic grain shapes. This formulation was then used to analyze the inelastic deformation of a polycrystalline aggregate with randomly distributed low and high-angle GBs. Grain subdivision was tracked at different scales. The evolution of the GNDs was used to predict and understand how crystallographic and non-crystallographic microstructures relate to intragranular and intergranular deformation patterns. Furthermore, a clear understanding of how GB strength changes due to microstructural
evolution was obtained. The combined effects of physically realistic grain shapes, random texture, and GB misorientations and distributions, led to the formation of highly heterogeneous stress distributions. High stress gradients were seen at GB locations, such as triple junctions, which indicate the likelihood of crack initiation. It would not have been possible to predict the behavior of the heterogenous microstructural mechanisms without accounting for the interrelated effects of SSDs, GNDs, and GNBs.
Figure 6.1. (a) - (l) Contours of shear slip magnitude on slip systems 1 to 12 at 20% nominal tension
Figure 6.1. (continued)
Figure 6.2. (a) - (c) Contours of density \((1/\text{m}^2)\) of GNDs of edge type on slip systems 9, 10 and 12 at 20% nominal tension.
Figure 6.3. (a) - (c) Contours of density (1/m$^2$) of GNDs of screw type on slip systems 9, 10 and 12 at 20% nominal tension
Figure 6.4. (a) - (c) Contours of density (1/m$^2$) of stored dislocations in cell interiors on slip systems 9, 10 and 12 at 20% nominal tension
Figure 6.5. (a) - (c) Contours of density (1/m$^2$) of stored dislocations in cell walls on slip systems 9, 10 and 12 at 20% nominal tension
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Figure 6.10. (a) - (c) Contours of normalized resolved shear stress magnitude on slip systems 9, 10 and 12 at 20% nominal tension
Figure 6.11. (a) - (c) Contours of normalized slip resistance on slip systems 9, 10 and 12 at 20% nominal tension
Figure 6.12. (a) - (b) Contours of positive and negative lattice rotations (deg.), at 20% nominal tension

Figure 6.13. Contour of total accumulated shear slip at 20% nominal tension
Figure 6.14. (a) Contour of stress in normal direction $\sigma_{zz}$ normalized by the yield stress at 20% nominal tension (b) A triple junction

Figure 6.15. (a) – (b) Contours of stress in horizontal direction $\sigma_{yy}$ normalized by the yield stress at 20% nominal tension
Figure 6.16. Overall stress-strain behavior (Normalized by the yield stress)
CHAPTER 7
AGGREGATE AND GRAIN SIZE-SCALE EFFECTS IN F.C.C. POLYCRYSTALLINE MATERIALS

Size-scale dependent behavior is observed in many cases involving inelastic deformation of crystalline materials, and generally characterized by a stronger response as the grain size decreases (see, for example, Valiev et al., 1993). In nanocrystalline materials, the increased strength is mainly due to the increased surface to volume ratio that signifies the high frequency of GB surfaces. However, even in a fixed surface to volume ratio, changing the GB orientations and distributions, can result in a change in the dislocation density content of the GBs, which can then affect the deformation behavior and strength of the aggregate. In addition to the GB effect, the plastic slip gradient is scale dependent, and decreases in specimen size, results in larger plastic slip gradients. Since the GNDs are directly proportional to the plastic slip gradients, then a smaller size can result in higher GND densities that can subsequently result material’s strain-hardening and strength behavior. Hence, in this chapter, the size-scale dependent behavior is investigated. For this purpose, the crystalline aggregate of Chapter 6 is scaled down to a smaller size.

7.1 RESULTS AND DISCUSSION

The geometry of the 50-grain aggregate is generated by scaling the same aggregate that was used in Chapter 6, and decreasing the specimen dimension by one-
half. Hence, the scaled specimen dimensions are 250 by 250 microns and this results in the average grain size to decrease to one-fourth. The loading conditions are the same as Chapter 6. Under the applied quasi-static tensile loading, the deformation in the aggregate is dominated by three slip systems 9, 10 and 12 as seen in Fig. 7.1 at a nominal strain of 20%. The crystallographic slips are seen to be equal to those of the larger aggregate, because of the similarity of the collective grain deformations with the larger sized aggregate. The GNDs of edge type are shown in Fig. 7.2 and the GNDs of screw type are shown in Fig. 7.3. A comparison with the GND density contours of Chapter 6 shows a marked increase in the density of the GNDs for the smaller aggregate. For a scale factor of 0.5, the slip gradients are expected to increase by a factor of two, and since the GND densities are proportional to the slip gradients, the same increase is expected. In Table 7.1, the maximum GND densities for the two aggregate sizes are shown. As the results indicate, the GND densities are inversely proportional with the aggregate size. Furthermore, the distributions of crystallographic and non-crystallographic GNBs have the same pattern of the large aggregate.

The contours of dislocation density in dislocation cell interiors and cell walls are shown in Figs. 7.4 and 7.5 at a nominal strain of 20%. Since the dislocation cell and wall formation are dependent on the plastic slip, the aggregate size does not make a change in their densities. A comparison with the SSD densities of Chapter 6 verifies this point.

The dislocation cell size contours of Fig. 7.6 are also similar to those of Chapter 6 at a nominal strain of 20%. However, the cell-blocks are expected to be smaller due to the higher density of the GNDs.
The GBD density contours are shown in Fig. 7.7 for a nominal strain of 20%. Although the total number of the GB misfit dislocations is a function of the aggregate size, but their density is independent of it. A comparison of the GBD density contours of the two aggregate sizes shows this.

The contours of shear slip rates, which are scaled by the reference slip rate (Table 5.1), are shown in Fig. 7.8 for nominal strains of 10% and 20%. Like shear slips, shear slip rates are also the same in scaled aggregates under same strains. Since the slip resistance increases in a smaller aggregate due to the increased interactions of the GNDs with mobile dislocations, the resolved shear stresses will also increase so that the slip rates remain unchanged. The contours of the normalized (normalized by the static yield stress, Table 5.1) resolved shear stress magnitude shown in Fig. 7.9 for a nominal strain of 20%, show a slight increase in comparison with those in Chapter 6. The contours of the normalized slip resistance (normalized by the static yield stress, Table 5.1) at a nominal strain of 20% shown in Fig. 7.10 also show an increase in comparison with the larger aggregate size.

The lattice rotations (Fig. 7.11), and the total shear slip (Fig. 7.12) contours at 20% nominal strain also show the same patterns and values as those in Chapter 6 for the larger aggregate.

The normal stress (Fig. 7.13), and the lateral stress (Fig. 7.14) contours (normalized by the yield stress) at 20% nominal strain show an increase for the small aggregate, which again is resulted by the increased slip resistance due to the increased GND densities. The overall stress-strain curve is shown in Fig. 7.15 for the two different
aggregate sizes. It is clearly consistent with the experimental observations (see, for example, Nix, 1989) of the size-scale dependent behavior that suggests stronger response for smaller size.

7.2 CONCLUSIONS

A unified dislocation density based multiple-slip crystal plasticity formulation that integrates SSDs, GNDs, and GBDs in one framework has been developed, and it has been coupled to specialized finite-element analysis of polycrystalline aggregates with physically realistic grain shapes. This formulation was then used to analyze the size-scale dependent behavior of a polycrystalline aggregate by comparing two aggregate sizes of the same grain composition and texture under the same loading conditions. The GND densities were used to understand the slip gradient effects due to changes in aggregate and grain size. The present analysis underscores that different dislocation densities in critical regions, such as GB interfaces, are directly related to the increased strength response pertaining to smaller sized aggregates and grains.
Table 7.1 Maximum GND densities for two aggregate sizes

<table>
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<tr>
<th>Slip system &amp; GND type</th>
<th>GND density for small aggregate</th>
<th>GND density for large aggregate</th>
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</thead>
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<tr>
<td>$\rho_{GND-e}^{(9)}$</td>
<td>$4.83 \times 10^{14}$</td>
<td>$2.94 \times 10^{14}$</td>
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<tr>
<td>$\rho_{GND-e}^{(10)}$</td>
<td>$2.66 \times 10^{14}$</td>
<td>$1.32 \times 10^{14}$</td>
</tr>
<tr>
<td>$\rho_{GND-e}^{(12)}$</td>
<td>$1.63 \times 10^{14}$</td>
<td>$8.61 \times 10^{13}$</td>
</tr>
<tr>
<td>$\rho_{GND-s}^{(9)}$</td>
<td>$1.03 \times 10^{14}$</td>
<td>$5.39 \times 10^{13}$</td>
</tr>
<tr>
<td>$\rho_{GND-s}^{(10)}$</td>
<td>$1.68 \times 10^{14}$</td>
<td>$7.93 \times 10^{13}$</td>
</tr>
<tr>
<td>$\rho_{GND-s}^{(12)}$</td>
<td>$1.32 \times 10^{14}$</td>
<td>$7.24 \times 10^{13}$</td>
</tr>
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</table>
Figure 7.1. (a) - (l) Contours of shear slip magnitude on slip systems 1 to 12 at 20% nominal tension
Figure 7.1. (continued)
Figure 7.2. (a) - (c) Contours of density (1/m^2) of GNDs of edge type on slip systems 9, 10 and 12 at 20% nominal tension
Figure 7.3. (a) - (c) Contours of density (1/m$^2$) of GNDs of screw type on slip systems 9, 10 and 12 at 20% nominal tension
Figure 7.4. (a) - (c) Contours of density (1/m$^2$) of stored dislocations in cell interiors on slip systems 9, 10 and 12 at 20% nominal tension
Figure 7.5. (a) - (c) Contours of density (1/m²) of stored dislocations in cell walls on slip systems 9, 10 and 12 at 20% nominal tension
Figure 7.6. (a) - (c) Contours of dislocation cell size (m.) on slip systems 9, 10 and 12 at 20% nominal tension
Figure 7.7. (a) - (d) Contours of density (1/m$^2$) of grain boundary misfit dislocations on slip systems 1, 4, 7 and 10 at 20% nominal tension
Figure 7.8. (a) - (f) Contours of normalized shear slip rate magnitude on slip systems 9, 10 and 12 at 10% and 20% nominal tensions
Figure 7.9. (a) - (c) Contours of normalized resolved shear stress magnitude on slip systems 9, 10 and 12 at 20% nominal tension
Figure 7.10. (a) - (c) Contours of normalized slip resistance on slip systems 9, 10 and 12 at 20% nominal tension
Figure 7.11. (a) - (b) Contours of positive and negative lattice rotations (deg.), at 20% nominal tension

Figure 7.12. Contour of total accumulated shear slip at 20% nominal tension
Figure 7.13. Contour of stress in normal direction $\sigma_{zz}$ normalized by the yield stress at 20% nominal tension

Figure 7.14. (a) – (b) Contours of stress in horizontal direction $\sigma_{yy}$ normalized by the yield stress at 20% nominal tension
Figure 7.15. Overall stress-strain behavior (Normalized by the yield stress)
CHAPTER 8
GRAIN BOUNDARY MISORIENTATION EFFECTS IN F.C.C. POLYCRYSTALLINE AGGREGATES

As noted earlier, the evolution of the heterogeneous microstructure is dependent on the crystallographic texture. Dislocation cells and cell-blocks with crystallographic or non-crystallographic GNBs occur mainly due to crystallographic orientations. GB misorientations and distributions are also a function of the texture of the aggregate and the shape of the grains.

Hence, in this chapter, the effects of crystallographic texture and GB misorientations and distributions on the microstructure and inelastic deformation of f.c.c. polycrystalline aggregates will be investigated by considering the same aggregate composition that was used in Chapter 6, and changing the texture to represent an aggregate with GBs that have a low-angle random distribution. The GND densities and the evolution of the slip patterns are then used to predict how and why a heterogeneous microstructure forms as a function of grain shape and size and GB orientation and distribution. Therefore, based on this analysis and the previous analyses, we will develop a detailed understanding of how heterogeneous microstructures initiate and evolve.

8.1 RESULTS AND DISCUSSION

The geometry of the 50-grain aggregate and the loading conditions are the same as Chapter 5. The grain orientations are selected in such a way that 20% of the grains
correspond to region I of the inverse pole figure, 56% correspond to region II, and 24% to region III (Fig. 8.1). This texture distribution results in random low-angle GBs for the polycrystalline aggregate. Under the applied quasi-static tensile loading, the deformation in the aggregate is dominated by three slip systems 9, 10, and 12, as seen in Fig. 8.2 at a nominal strain of 20%. Two of these, slip systems 10 and 12 are coplanar. Comparing to the diverse texture and mix low and high-angle GBs of Chapter 6, the homogeneous texture along with low-angle GBs are seen to have changed the distribution of the slip in and between the active slip systems in such a way that the localized high crystallographic accumulated slips are decreased.

The GNDs of edge type are shown in Fig. 8.3 and the GNDs of screw type are shown in Fig. 8.4 at a nominal strain of 20%. From the comparison of these results with those of Chapter 6, it is seen that the frequency of the crystallographic GNBs with Burger’s vectors belonging to the coplanar slip systems and a mix tilt and twist characteristic, has significantly increased. Whereas, the frequency of the non-crystallographic GNBs with Burger’s vectors predominantly belonging to two active slip planes and a tilt characteristic, has decreased. This is consistent with experimental observations (see, for example, Huang, 1998) of the GNBs suggesting that the microstructure of the aggregates with grain orientations belonging to the region II (Fig. 8.1) predominantly consists of crystallographic GNBs. Whereas, the microstructure of the aggregates with grain orientations belonging to the region III (Fig. 8.1) mostly consists of non-crystallographic GNBs. It is also seen that the density of the GNDs have decreased in comparison to those of Chapter 6, that is due to the decreased intergranular inhomogeneities as a result of low-angle GBs.
The contours of dislocation density in dislocation cell interiors and cell walls and dislocation cell size are shown in Figs. 8.5-7 at a nominal strain of 20%. A comparison with the results of Chapter 6 shows that the localized high densities of the cell interior and cell wall dislocations have diminished significantly. This is mainly due to the homogeneous slip on active slip systems, although here the coplanar slip systems, and specifically slip system 10, are seen to have a more dominant role.

The GBD density contours are shown in Fig. 8.8 for a nominal strain of 20%. A comparison with the GBD orientations and distributions in Chapter 6 shows that although the average density of the GB misfit dislocations has decreased due to the random low-angle GBs, but the total misfit dislocation content has increased due to the misorientation distribution. This can also be seen from the change in the normalized total GBD density content (normalized by the maximum GBD density content of the aggregate with low and high-angle GBs of Chapter 6) for the total deformation history as shown in Fig. 8.9. The decreasing trend indicates that the compatible deformation of the grains results in a reorientation at the GBs, in such a way that the average misorientation between neighboring grains is lowered. From an energy perspective, lower GBD densities translate into lower energy levels, which clearly indicate that the microstructure is evolving to a stable configuration.

The contours of shear slip rates, which are scaled by the reference slip rate (Table 5.1), are shown in Fig. 8.10 for nominal strains of 10% and 20%. A comparison between these two nominal strains indicates that maximum shear strains occur at different locations in the aggregate, which is an indication of the slip hardening and reorientation changes that occur as the microstructure evolves. A comparison with the results of
Chapter 6 shows a decrease of the localized high shear slip rates in the aggregate with low-angle GBs that is due to the combined effects of the GB orientations and distributions and the texture.

The contours of the normalized (normalized by the static yield stress, Table 5.1) resolved shear stress magnitude shown in Fig. 8.11 for a nominal strain of 20%, show a more uniform distribution with a slight increase in comparison with those in Chapter 6. The contours of the normalized slip resistance (normalized by the static yield stress, Table 5.1) at a nominal strain of 20% shown in Fig. 8.12 also show more uniform distribution and an increase in comparison with the results of Chapter 6 that is due to the interactions of more homogeneously distributed SSDs, GNDs and GBDs with mobile dislocations.

The lattice rotations (Fig. 8.13) show more consistency in comparison to those of Chapter 6. A decrease of about 20 degrees is seen in negative lattice rotations that were seen in a very localized manner in the mix-angle GB aggregate. Lattice rotations are seen to be mainly in positive direction with a more homogeneous intragranular texture. This is also consistent with lower density of the GNDs that were seen in Figs. 8.3-4.

The total accumulated shear slip is shown in Fig. 8.14 at a nominal strain of 20%. The sheared strip at the bottom right corner is more diffuse than the previous aggregate with random low and high-angle GB distributions. The normal stress (normalized by the yield stress) is shown in Fig. 8.15(a) at a nominal strain of 20%. Due to the random grain shapes, texture and GB distributions and misorientations, the stresses have accumulated in particular GB regions. A comparison with the results of Chapter 6 shows a more
homogeneous intergranular and intragranular distribution of the stress. Furthermore, the stress gradients at triple junctions (Fig. 8.15(b)) have also decreased. The contour of the lateral stress (normalized by the yield stress) in Fig. 8.16 at a nominal strain of 20% shows the same pattern.

The global stress-strain curve of this aggregate is shown in Fig. 8.17 with the global stress-strain curves obtained in Chapters 5 and 6 for the aggregate with a combination of random low and high-angle GBs. It can be seen that the aggregate with random low-angle GBs has a higher stress response than the aggregate with the distribution of random low and high-angle GBs. This is mainly due to the higher density of GBDs that occurs for the random low-angle GB distribution.

### 8.2 CONCLUSIONS

A unified dislocation density based multiple-slip crystal plasticity formulation that integrates SSDs, GNDs, and GBDs in one framework has been developed, and it has been coupled to specialized finite-element analysis of polycrystalline aggregates with physically realistic grain shapes. This formulation was then used to analyze the effects of the GB orientation and distribution and the crystallographic texture on the inelastic deformation and heterogeneous microstructure of f.c.c. polycrystals by comparing two aggregates with same granular composition and different texture and GB orientation and distribution. The evolution of the GNDs was used to predict and understand how crystallographic and non-crystallographic microstructures relate to grain orientations. Furthermore, a clear understanding of how GB structure and orientation can change the
strain-hardening behavior and relieve the stress gradients in critical GB locations was obtained.
Figure 8.1. Inverse pole figure showing the initial orientations of the grains


Grain No. 2-6-12-13-19-31-32-37-40-44-45-50

Grain No. 8-11-16-17-25-26-28-46-47-48
Figure 8.2. (a) - (f) Contours of shear slip magnitude on slip systems 1 to 12 at 20% nominal tension.
(g) $\gamma^{(7)}$

(h) $\gamma^{(8)}$

(i) $\gamma^{(9)}$

(j) $\gamma^{(10)}$

(k) $\gamma^{(11)}$

(l) $\gamma^{(12)}$

Figure 8.2. (continued)
Figure 8.3. (a) - (c) Contours of density \((1/m^2)\) of GNDs of edge type on slip systems 9, 10 and 12 at 20% nominal tension
Figure 8.4. (a) - (c) Contours of density (1/m$^2$) of GNDs of screw type on slip systems 9, 10 and 12 at 20% nominal tension
Figure 8.5. (a) - (c) Contours of density (1/m²) of stored dislocations in cell interiors on slip systems 9, 10 and 12 at 20% nominal tension
Figure 8.6. (a) - (c) Contours of density (1/m$^2$) of stored dislocations in cell walls on slip systems 9, 10 and 12 at 20% nominal tension
Figure 8.7. (a) - (c) Contours of dislocation cell size (m.) on slip systems 9, 10 and 12 at 20% nominal tension
Figure 8.8. (a) - (d) Contours of density (1/m$^2$) of GB misfit dislocations on slip systems 1, 4, 7 and 10 at 20% nominal tension
Figure 8.9. Normalized total GBD density content (Normalized by the maximum total GBD density for low and high-angle GBs)
Figure 8.10. (a) - (f) Contours of normalized shear slip rate magnitude on slip systems 9, 10 and 12 at 10% and 20% nominal tensions
Figure 8.11. (a) - (c) Contours of normalized resolved shear stress magnitude on slip systems 9, 10 and 12 at 20% nominal tension
Figure 8.12. (a) - (c) Contours of normalized slip resistance on slip systems 9, 10 and 12 at 20% nominal tension
Figure 8.13. (a) - (b) Contours of positive and negative lattice rotations (deg.), at 20% nominal tension

Figure 8.14. Contour of total accumulated shear slip at 20% nominal tension
Figure 8.15. (a) Contour of stress in normal direction $\sigma_{zz}$ normalized by the yield stress at 20% nominal tension (b) A triple junction

Figure 8.16. (a) – (b) Contours of stress in horizontal direction $\sigma_{yy}$ normalized by the yield stress at 20% nominal tension
Figure 8.17. Overall stress-strain behavior (Normalized by the yield stress)
CHAPTER 9

RECOMMENDATIONS FOR FUTURE WORK

The following research areas can be pursued in the future based on the present study:

• Developing a new failure methodology, which can be coupled to the dislocation-density based crystalline formulation that is based on the creation of failure surfaces, such as cracks and microvoids, and to relate the evolution of these failure surfaces to the heterogeneous microstructure at the relevant scales;

• Developing a new three dimensional methodology that will provide an unconstrained and full-field analysis;

• An investigation of how the microstructure evolves under stress wave propagation and dynamic effects, and how this evolves over the short time durations associated with impact and high strain-rate deformations;

• A unified formulation that would account for other cubic structures, such as b.c.c. and h.c.p crystalline materials;

• The application of the current methodology to investigate alloy deformation due to underlying structures, such as martensite and pearlites, that are critical in phase transformations associated with f.c.c. alloys, such as f.c.c. and b.c.c. steel alloys.
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