

Meso-Scale Modeling of Polycrystal Deformation

DISSERTATION

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ABSTRACT

Computational material modeling of material is essential to accelerate material/process design and reduce costs in wide variety of applications. In particular, multi-scale models are gaining momentum in many fields as computers become faster, and finer structures become accessible experimentally. An effective (i.e. sufficiently accurate and fast to have practical impact) multi-scale model of dislocation-based metal plasticity may have many important applications such as metal forming.

A two-scale method to predict quantitatively the Hall-Petch effect, as well as dislocation densities and lattice curvatures throughout a polycrystal, has been developed and implemented. Based on a finite element formulation, the first scale is called a Grain-Scale Simulation (GSS) that is standard except for using novel single-crystal constitutive equations that were proposed and tested as part of this work (and which are informed from the second model scale). The GSS allows the determination of local stresses, strains, and slip magnitudes while enforcing compatibility and equilibrium throughout a polycrystal in a finite element sense.

The second scale is called here a Meso-Scale Simulation (MSS) which is novel in concept and application. It redistributes the mobile part of the dislocation density within grains consistent with the plastic strain distribution, and enforces slip transmission criteria at grain boundaries that depend on local grain and boundary properties. Stepwise

simulation at the two scales proceeds sequentially in order to predict the spatial distribution of dislocation density and the flow stress for each slip system within each grain, and each simulation point. The MSS was formulated with the minimum number of undermined or arbitrary parameters, three. Two of these are related to the shape of the strain hardening curve and the other represents the initial yield. These parameters do not invoke additional length scales.

The new model made possible the following advances:

- 1) Quantitative prediction of the Hall-Petch slopes without imposing unrealistic or unobserved dislocation configurations (pile-ups). The predicted slopes agree with experiment within a factor of 1.5.
- 2) Quantitative prediction of the spatial distribution of dislocation density on slip systems consistent with grain dislocation and dislocation-dislocation interactions. Comparisons with maximum lattice curvatures measured experimentally show agreement within 5%.
- 3) A computationally tractable meso-scale treatment of realistic numbers of dislocations, their interactions, and the relationship between their redistribution and strain. CPU times required to simulate 64 grains with 8000 elements was 6.5 hours.
- 4) A simple model and method for deploying it to treat grain boundaries as obstacles depending on local configurations: grain boundary character, grain misorientation, and slip system orientation on both sides of the boundary. The magnitude of the effect of grain boundaries on flow strength was illustrated by simulations.

DEDICATION

To my beloved wife, Jungrim and my daughter, Seohee.

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1. INTRODUCTORY NOTE

The organization of this dissertation, while appearing to be standard, needs some explanation in order to be clear in terms of attribution of the work and style of several chapters. In particular, Chapter 3 is an accepted peer-reviewed paper, and Chapter 4 will be submitted for publication in a peer-reviewed journal.

Chapter 3 is a peer-reviewed paper accepted for publication by the International Journal of Plasticity and is in press at this writing. Hojun Lim (who is submitting this dissertation to fulfill some of the requirements for the Ph.D. at the Ohio State University) is the second author on this paper. While he did not have the principal responsibility for initiating the work that appears in that paper and Chapter 3, he carried out the simulations and their comparison with experiments in order to verify the material model proposed there. In order to delineate the work for which Mr. Lim had secondary responsibility but which is essential to understanding the subsequent chapters, Chapter 3 is presented word-for-word the same as the accepted Int. J. Plasticity paper. Therefore, the background and conclusions appear and are not duplicated in Chapter 2, where the literature background is reviewed.

The need for the new model presented in Chapter 3 became apparent by the remainder of the work presented in this dissertation, for which Mr. Lim had primary responsibility. “Primary responsibility” means that he conducted the work, drew the

conclusions wrote the reports, papers, and dissertation, but had the benefit of the normal advice and assistance of Professor Robert H. Wagoner and Research Associate Dr. Ji Hoon Kim, who are co-authors on the papers. This work was collaborative with Professor Brent L. Adams and his group at the Brigham Young University in Provo, Utah. Professor Adams's group performed all orientation imaging microscopy (OIM) reported in this dissertation, including polishing and specimen preparation after mechanical deformation and stress-strain measurement. One more technical attribution is significant: an earlier and now abandoned version of the two-scale model was originally proposed and tested by Dr. Myoung-Gyu Lee (former Research Associate in the Wagoner group and now Assistant Professor, Pohang University of Science and Technology). This model is mentioned briefly in Chapter 4 and Dr. Lee will be a co-author on the paper represented by Chapter 4. With these two exceptions, Mr. Lim conducted all of the work presented in Chapter 4.

Chapter 4 forms a second paper to be submitted to the International Journal of Plasticity. In order to maintain the peer-review paper format, again the introductory part of the literature pertinent to that work appears in Chapter 4 (and is not duplicated in Chapter 2), and conclusions to the work appear as part of Chapter 4.

Chapter 5, Conclusions, simply restates the conclusions reached and reported in Chapters 3 and 4.

2. BACKGROUND

Many existing models of polycrystal metal deformation are formulated based on phenomenological approaches that address only the grain texture (i.e. the statistical orientation of crystal lattices), not the presence of grain boundaries. However, the grain size and grain boundary character are critical aspects of a material's microstructure influencing strength and ductility. For true design of materials for applications, the fundamental role of grain boundaries must be understood and predictable. The development of a more physical and predictive simulation model that accounts for microscopic aspects of the polycrystals would guide the understanding, quantification, and prediction of the role of grain size and grain boundary character on the mechanical behavior of polycrystal metals.

The principal obstacle facing a predictive model connecting two extreme length scales is the large numbers of defects involved (e.g. 10^{12} - 10^{14} dislocations/m²), or, conversely, the wide disparity of scales to be linked (10^{-10} m for a typical Burgers vector versus 10^{-2} m for a part or component, or, 10^{-5} m for the size of a typical grain in a polycrystal). This discrepancy of scales renders a direct multi-scale model of metal plasticity computationally intractable.

In the current work, a novel two-scale model is proposed to simulate large number of dislocation arrays in a tractable way to link two extreme scales and predict

quantitatively the Hall-Petch effect. The two-scale model is formulated with the aim of minimizing the number of arbitrary fitting parameters while being able to accurately predict stress-strain curves for single- and multi crystals, lattice curvatures as well as the Hall-Petch Law. In the following sections, a review of the various polycrystal plasticity models, relevant dislocation theories and the Hall-Petch Law is presented. Note also that brief, focused reviews appear at the start of Chapter 3 and Chapter 4.

2.1 Polycrystal Plasticity Models

Experimental studies in the early 1900s revealed that the plastic deformation of the metals is due to the dislocation movement through the crystal lattice and these microscopic behaviors are closely related to the macroscopic mechanical behavior of materials. Single crystal plasticity theories have been extended to the polycrystal plasticity theories that relate the macroscopic properties of polycrystalline materials to the fundamental mechanisms of single crystal deformation. In order to do this, highly simplified rules relating grain deformation to polycrystal deformation were formulated. The main interest of a polycrystal plasticity theory has been to formulate the relations between the macroscopic and microscopic quantities and to predict mechanical properties and texture evolution of the polycrystalline bodies.

Early studies on polycrystal plasticity were originated by Sachs (Sachs, 1928) and Taylor (Taylor, 1938). The Sachs model assumes uniform stress in all grains so that the equilibrium condition across the grain boundary is satisfied but the kinematical compatibility condition is neglected. On the other hand, Taylor's model satisfies the

compatibility condition by assuming uniform deformation within grains and across the grain boundaries but violates equilibrium conditions. Later, relaxed constraints approach and self consistent approaches were developed in order to provide more accurate texture predictions and agreement with the experiments (Honneff, 1978; Kocks and Canova, 1981; Van Houtte, 1981). In contrast to the fully constrained Sachs and Taylor models, relaxed constraints theory allows strain heterogeneities as the individual grains deform and become non-equiaxed. The problem with this model is that it is difficult to prescribe a generalized criterion for how to accomplish relaxation.

In order to satisfy equilibrium and compatibility conditions between the grains, a self consistent model was proposed (Kröner, 1961) and extended by Budiansky and Wu (Budiansky and Wu, 1962). In this self-consistent model, each grain is regarded as an inclusion embedded in a homogeneous, isotropic elastic body. In this way, the interaction between the grains is approximately determined using Eshelby's theory (Eshelby, 1957). Self-consistent approaches, however, involve severe assumptions in order to simplify the formulations and to reduce the computation time.

Strain gradient models have been introduced in order to reproduce measured scale size effects (Fleck et al., 1994; Fleck and Hutchinson, 1997; Gurtin, 2000, 2002). The strain gradient and its work conjugate were introduced into phenomenological constitutive models in order to simulate a length-scale mechanical response of materials. The differential strengthening of very small grains (near 1-10 μ m) can be modeled because of the elastic/constitutive length scales introduced in the models and fit to experimental data. These models, however, ignore crystal structures, grain boundary

structures, and slip systems. Therefore, while they are convenient for application to continuum mechanics problems, it is difficult to see how they can be predictive based on material microstructure. Such models generally fail to predict the Hall-Petch effect in the range of typical interest, that is, for grain sizes from 10 - 1000 μm .

Later, this model was extended by Evers (Evers et al., 2002) and Arsenlis (Arsenlis and Parks, 2002; Arsenlis et al., 2004) by taking account the evolution of dislocation densities; geometrically necessary dislocations (GNDs) and statistically stored dislocations (SSDs). Extension of strain gradient models taking crystal structure and unitary dislocation mechanisms into account has succeeded in eliminating the need for arbitrary length scales (Evers et al., 2002; Arsenlis et al., 2004). In the work of Evers et al. (Evers et al., 2002) material points are considered as aggregates of grains and each crystal is subdivided into core and its boundaries. By the intragranular incompatibilities (or heterogeneous deformation near the grain boundary region) by introducing bi-crystals concept at the grain boundaries, the geometric dislocation density is determined. By this method, the grain size dependent behavior of polycrystal material was reasonably described. However, this method includes arbitrary division of crystals into core and boundaries, which does not consider real grain structure. Also, the stress at each material point is determined by the averaged response of crystals as done with modified Taylor approximation.

On the contrary to the work by Evers et al. (Evers et al., 2002), Arsenlis et al. (Arsenlis et al., 2004) considers a more natural length scale by discretizing each grain into many finite elements in the framework of crystal plasticity. In this model, dislocation

densities are characterized by statistical and geometric parts which evolve by dislocation mechanism and divergence of dislocation fluxes, respectively. This method is promising in terms of avoiding arbitrary length scales and taking crystal structure and dislocation density into account, but is very computationally intensive because of their treatment of each component of dislocation densities as additional degree of freedom. Therefore, simulations of idealized single crystal with only simplified single slip geometry were performed to demonstrate the length scale-dependence of their constitutive models.

To improve on pure texture models, finite element analysis based on crystal plasticity (CP-FEM) has been developed (Peirce et al., 1982; Asaro, 1983; Dawson, 2000). CP-FEM considers the equilibrium and compatibility as well as interactions between neighboring grains in a finite element sense, still based on the single crystal constitutive equations. An integration of crystal plasticity into non-linear variational formulations was first proposed by Peirce et al. (Peirce et al., 1982) and Asaro (Asaro, 1983). CP-FEM models can represent detailed predictions on the texture evolution and strain distribution under realistic boundary conditions (Raabe et al., 2002). A finite element can represent many grains by adopting simple assumptions such as Taylor iso-strain (Kalidindi et al., 1992; Dawson et al., 2003), a single grain (Nakamachi et al., 2001) or a small part of one grain (Peirce et al., 1983; Sarma and Dawson, 1996).

2.2 Theories on Evolution of Dislocation Densities in Plasticity Models

An evolution of dislocation density has been studied using various experimental techniques including etch-pitting, decoration, electron microscopy, x-ray diffraction, and

more recently by TEM and electric resistivity tests. From these direct and indirect experimental measurements, various formulations were developed to describe the evolution of dislocation densities to be used in dislocation density based polycrystal plasticity models. In general, evolution of dislocation density is described with two competing processes: generation and annihilation of dislocations. Generation of dislocations is generally assumed to be originated from the Frank-Reed type sources or from the grain boundaries. Cross slip from other slip systems may also increase dislocation density for one slip system. Annihilation of dislocation is described with the recovery process, such mechanisms as pairing of dislocation segments with opposite Burgers vectors which cancel each other (Li, 1963a; Essmann and Mughrabi, 1979), tangling process between dislocations moving on two different slip planes (Li, 1963a), cross-slip of screw dislocations (Estrin and Mecking, 1984) or climb of edge dislocations (Mecking et al., 1986; Roters et al., 2000), respectively. Detailed mechanism for dislocation annihilation is less well understood compared to generation mechanisms of dislocations and in some cases, it is neglected at temperatures below $0.5T_m$ (Domkin et al., 2003).

Later works (Kocks, 1976; Bergström and Hallen, 1982; Roters et al., 2000; Zerilli, 2004) distinguished dislocations from mobile and immobile and proposed that only immobile dislocations affect flow stress of the material. Therefore, evolution of immobile dislocation density has been mainly focused and developed based on immobilization and remobilization rate of mobile dislocations. In general, mobile dislocation density is assumed to be much smaller than immobile dislocation density

(Bergström, 1970; Bergström and Hallen, 1982). TEM observations showed that mobile dislocations are predominantly generated at the cell walls and move towards the opposite walls where they become immobilized by formation of dislocation locks and dislocation dipoles in cell walls (Roters et al., 2000; Ma and Roters, 2004). It has been proposed that remobilizing a stopped dislocation decrease immobile dislocation density (Zerilli, 2004) but an annihilation of dislocation occurs at a rate negligible in comparison to immobilization and remobilization of dislocations (Roberts and Bergström, 1973).

The first generation of describing dislocation generation is based on well-known Orowan's model (Orowan, 1940) that the dislocation density can be calculated to attain the plastic shear strains. Orowan's simple model is extended to describe the increase of immobile dislocation density as follows (Essmann and Mughrabi, 1979):

$$d\rho^{(+)} = \frac{1}{bL} d\gamma \quad (2.1)$$

where L denotes the active slip distance before the immobilization. Above equation can be further developed by assuming L is proportional to the average spacing between obstacle dislocations, and hence, inversely proportional to the square root of total dislocation density as follows (Kocks, 1976):

$$d\rho^{(+)} = k_1 \sqrt{\rho} d\gamma \quad (2.2)$$

k_1 in the above equation is associated with the athermal storage of moving dislocations which become immobilized after having traveled a distance proportional to the average spacing between the dislocations.

Dislocation annihilation term is associated with dynamic recovery and generally assumed to follow the first order kinetics, i.e. to be linear with the density of forest dislocations as follows (Kocks, 1976; Essmann and Mughrabi, 1979; Estrin and Mecking, 1984; Estrin, 1998):

$$d\rho^{(-)} = k_2\rho d\gamma \quad (2.3)$$

k_2 can be understood as an annihilation rate or the strain- independent probability for remobilization of immobile dislocations (Bergström and Hallen, 1982).

Whether change of dislocation density is derived using generation-annihilation or immobilization-remobilization processes, evolution of dislocation density is most generally represented as follows (Kocks, 1976; Estrin and Mecking, 1984):

$$d\rho = (k_1\sqrt{\rho} - k_2\rho) d\gamma \quad (2.4)$$

Some recent works describe dislocation dynamics in two separate phases: in dense dislocation wall and cell interior with more than one mechanism (Prinz and Argon, 1984; Nix et al., 1985; Gottstein and Argon, 1987; Mughrabi, 1987; Haasen, 1989; Ma and Roters, 2004; Hirth, 2006). For example, formulation of dislocation dipoles in dense dislocation walls, thermally activated climb of edge dislocations and interaction between mobile and immobile dislocations on the same system are considered (Ma and Roters, 2004). Initial models (Prinz and Argon, 1984; Nix et al., 1985; Gottstein and Argon, 1987; Mughrabi, 1987; Haasen, 1989) failed to account for all experimental features and not sufficient experiments were conducted to check models at large strains (Zehetbauer, 1993). On the other hand, latter models succeeded to predict mechanical behaviors of

FCC and BCC materials successfully but intensive fitting is required (Ma and Roters, 2004; Ma et al., 2006).

2.3 Hall- Petch Law

The well-known Hall-Petch relationship has been proposed by Hall (Hall, 1951) and Petch (Petch, 1953) from their separate works arriving at essentially the same conclusion that the yield stress of the material is proportional to $D^{-1/2}$.

$$\sigma_y = \sigma_0 + k_y D^{-1/2} \quad (2.5)$$

Here, σ_y and D are the yield stress and the mean grain size of the material, while σ_0 and k_y are the material constants usually referred to as frictional stress and the Hall-Petch slope, respectively. Empirically determined σ_0 and k_y have been the subject of much investigation and their physical significance has been difficult to rationalize.

In general, the frictional stress, σ_0 , is understood as the stress to move mobile dislocations in the absence of grain boundaries. σ_0 can be explained in terms of sum of solute strengthening plus hardening due to the initial dislocation density (Chia et al., 2005) or can be considered as an internal back stress. It has been shown that σ_0 depends strongly on temperature (Rao et al., 1975; Chia et al., 2005), strain (Jago and Hansen, 1986; Chia et al., 2005) and alloy content (Norström, 1977; Kako et al., 2002), whereas σ_0 is virtually unaffected by the grain size (Jago and Hansen, 1986) and presence of the second phase particles (Anand and Gurland, 1976; Chang and Preban, 1985).

Hall- Petch slope, k_y , represents the strength of grain boundaries as a barrier to slip that is related to the strength of dislocation locking by impurity atoms (Evans, 1963). k_y depends on grain boundary structure (Wyrzykowski and Grabski, 1986), solute (Floreen and Westbrook, 1969; Norström, 1977; Varin and Kurzydowski, 1988; Kako et al., 2002) and second phase particle concentration (Chang and Preban, 1985) but has less dependence on strain (Lloyd and Court, 2003; Chia et al., 2005) and temperature (Gray et al., 1999; Chia et al., 2005). Other factors influencing Hall-Petch slope are grain shapes (Kuhlmeyer, 1979) and presence of interfaces such as in two phase lamellar alloy.

Hall-Petch slope for various materials are listed in Table 2.1. In general, FCC and HCP metals have relatively lower k_y compared to BCC metals. For FCC materials, k_y is generally below $0.3 \text{ MN/m}^{3/2}$ while BCC materials generally have values close to 1. It should be noted that k_y computed for ultimate tensile strength have slopes approximately 30% higher than ones for yield strength. Apparently, smaller grain sizes (i.e. more grain boundaries) contribute to strain hardening as well as initial yield.

	Material	Hall-Petch Slope (MN/m ^{3/2})	References
BCC	Fe-3% Si	1.08	(Hull, 1975)
	Fe-3% Si	0.82	(Abson and Jonas, 1970)
	Mild Steel (yield point)	0.74	(Meyers and Chawla, 1998)
	Mild Steel ($\epsilon_p = 0.1$)	0.39	(Meyers and Chawla, 1998)
	Mild Steel (Fe-0.03% C)	0.51	(Abson and Jonas, 1970)
	UFGF/CH Steel	0.065	(Zhao et al., 2006)
	IF Steel	0.143	(Tsuji et al., 2001)
	Spheroidized Steel	0.412-0.581	(Anand and Gurland, 1976)
	Carbon Steels (0.03%)	0.81	(Chang and Preban, 1985)
	Carbon Steels (0.07%)	0.88	(Chang and Preban, 1985)
	Carbon Steels (0.17%)	1.21	(Chang and Preban, 1985)
	Carbon Steels (0.23%)	1.58	(Chang and Preban, 1985)
FCC	Copper ($\epsilon_p = 0.005$)	0.11	(Meyers and Chawla, 1998)
	Nickel 99.99% (Annealed)	0.3	(Suits and Chalmers, 1961)
	Ni – 1.2 % Al	0.19 – 0.88	(Nembach, 1990)
	Cu – 3.2% Sn ($\epsilon_p = 0$)	0.19	(Meyers and Chawla, 1998)
	Cu – 30% Sn ($\epsilon_p = 0$)	0.31	(Meyers and Chawla, 1998)
	Aluminum	0.11	(Abson and Jonas, 1970)
	Aluminum ($\epsilon_p = 0.005$)	0.07	(Meyers and Chawla, 1998)
	Al – 4.5% Cu	0.19 – 0.47	(Zoqui and Robert, 1998)
	Silver ($\epsilon_p = 0.005$)	0.07	(Meyers and Chawla, 1998)
	Silver ($\epsilon_p = 0.20$)	0.16	(Meyers and Chawla, 1998)
	310 Austenitic Steel	0.24	(Grabski and Wyrzykowski, 1980)
HCP	Zinc ($\epsilon_p = 0.005$)	0.22	(Meyers and Chawla, 1998)
	Magnesium ($\epsilon_p = 0.002$)	0.28	(Meyers and Chawla, 1998)
	Titanium (yield point)	0.40	(Meyers and Chawla, 1998)

Table 2.1: Hall-Petch slopes for various materials

Although numerous experimental observations in polycrystalline metals support the Hall-Petch law, deviations from $d^{-1/2}$ dependence and better experimental fits were reported by using exponents other than $-1/2$ (Baldwin, 1958; Christman, 1993). However, most of fitted exponents other than $-1/2$ seem to have no clear supporting physical

explanations and exponents ranging from $-1/3$ to -1 may not deviate much in the normal grain size range (Kocks, 1959).

The validity of the Hall-Petch Law is most frequently questioned for deviation from the linear plot of the experimental data at both large and small grain sizes (Anand and Gurland, 1976). Some suggests deviation from the Hall-Petch Law originates from extrinsic factors such as microcracks, inclusions, holes or surface defects that may act as stress concentration generators. However, various experimental results for different materials over a broad range of grain sizes (4~200 μm for Armco iron; 0.3~10 μm for AISI 1010; 0.1~130 μm for nickel) clearly showed that the plot of yield stress versus $D^{-1/2}$ is not linear. These results indicate that the linear behavior is an approximation applicable only over a limited range of grain sizes, typically around $10^{-1} \sim 10^3 \mu\text{m}$.

Recent work on nano-scale revealed that evident deviation from the Hall-Petch relation was observed at small grain size, less than 100 nm. At nano-scale, grain size strengthening has less effect and even a reverse Hall-Petch relation was observed (Chokshi et al., 1989; Liu et al., 1993) where the strength decreased with decreasing grain size. For instance, critical size from a positive to negative Hall-Petch slope is reported to be 3.4 nm for iron (Nieh and Wadsworth, 1991). Mechanism behind this softening is still a matter of controversy, but this behavior is most frequently explained by the change of deformation mechanism (Schiotz and Jacobsen, 1998), Coble creep (Chokshi et al., 1989), effect of discrete dislocations (Pande et al., 1993) and unique properties of nanocrystalline materials such as a large porosity. For example, Schiotz and Jacobsen (Schiotz and Jacobsen, 2003) showed that in the case when grains are in the range of

10~20 nm, the plastic deformation is no longer dominated by dislocation motion but by atomic sliding of grain boundaries. This sliding effect would tend to dominate because of the larger ratio of grain boundary to crystal lattice and leads to observed softening of a material.

Nevertheless, in a normal grain size regime ($D > 1\mu\text{m}$), conventional grain size hardening is relatively well obeyed and various models have been proposed to explain this empirically observed Hall-Petch law. Existing models can be classified into three broad categories. The three main models are 1) the dislocation pileup model, 2) the dislocation density model and 3) the composite model.

The first generation of theories describing the Hall-Petch Law is based on the idea of a dislocation pileup (Hall, 1951; Petch, 1953; Cottrell, 1958; Li and Liu, 1967; Hirth and Lothe, 1969; Armstrong, 1970; Conrad, 2004). In this pileup model, grain boundaries are assumed to act as a barrier to the dislocation motion and mobile dislocations transmit through grain boundaries when the stress at the head of the pileup exceeds the critical obstacle stress, τ_{obs} . The pileup length, l , is given by (Chou, 1967)

$$l = \frac{\mu b n}{\pi k \tau_{applied}} \quad (2.6)$$

where n is the number of dislocations in the pileup, $\tau_{applied}$ is the applied shear stress, μ is the shear modulus and b is the Burgers vector. k represents the characteristics of dislocations where $k = 1$ for screw dislocations and $k = 1 - \nu$ for edge dislocations. The tip stress at the head of the pileup is given by $\tau_{tip} = n\tau_{applied}$ (Hirth and Lothe, 1969) and accounting for the friction stress, σ_0 , and orientation factor, M , leads to

$$\sigma = \sigma_0 + M \left(\frac{\mu b \tau_{obs}}{\pi k} \right)^{1/2} D^{-1/2} \quad (2.7)$$

The pileup model reproduces the form of Hall-Petch law readily from a simple assumption that grain boundaries act as an obstacle to dislocation motion. Despite this simplicity, conventional pileup model has been questioned for various reasons. As listed in Table 2.2, calculated Hall-Petch slope using equation (2.7) is about an order smaller than measured values (using the obstacle strength of 5 times the yield stress (Shen et al., 1986)). In contrast to what the pileup model predicts, dislocation pileups across the whole diameter of large grains have not been clearly observed, particularly at large strains (Saada, 2005). At large strains, dislocation sources at the interior of grains may become more active so that dislocation pileup may have less effect (Narutani and Takamura, 1991). Some experimental investigations of FCC alloys showed that the dislocation pileups disappear at the hardening transition between stage I and stage II (Feaugas and Haddou, 1999, 2003).

	Material	Measured k_y	Calculated k_y
FCC	Al	0.11	0.02
	Cu	0.15	0.01~0.10
	Ni	0.30	0.08~0.16
HCP	Mg	0.28	0.02~0.03
	Ti	0.40	0.05~0.08
BCC	Fe	0.74	0.06~0.08

Table 2.2: Measured and calculated Hall-Petch slope using the dislocation pileup model

(Unit: $\text{MN/m}^{3/2}$).

The pileup of dislocation has been seldom observed in pure metals with high stacking fault energy (Li and Chou, 1970) since cross-slip can occur easily near the grain boundary. Hence, these metals are expected to have a relatively low Hall-Petch slope. However, BCC metals tend to have higher Hall-Petch slope despite higher stacking fault energy compared to FCC metals. This cannot be readily explained in terms of the pileup model.

Also, equation (2.6) is only applicable when the number of dislocations in the pileup is large enough that their distributions can be described by a continuous density function. At smaller length scales, the effect of discrete dislocations has to be taken into account (Fang and Friedman, 2007). In addition, grain boundary structure should be introduced in the pileup models through appropriate expressions of grain boundary obstacle strength.

The dislocation density model, or the work hardening model, is based on an assumption that flow stress is proportional to the square root of dislocation density (Conrad, 1961, 1970, 2004; Li, 1963a; Ashby, 1970; Chia et al., 2005). The flow stress is given by

$$\sigma = M\alpha\mu b\sqrt{\rho} \quad (2.8)$$

where M is the average Taylor factor and α is a constant. Hall-Petch relation can be readily derived from dislocation density model by assuming dislocation density is inversely proportional to the grain size. Inversely proportional relation between the dislocation density and the grain size is supported by TEM observations (Keh, 1961;

Conrad et al., 1968; Evans and Rawlings, 1969; Chia et al., 2005) and electrical resistivity tests (Narutani and Takamura, 1991).

It has been proposed that the grain boundaries act as a dislocation source and these emitted dislocations increase forest dislocation density and the overall flow stress (Mott, 1946; Li, 1962). TEM observations have shown that dislocations are emitted from the ledges (Mascanzoni and Buzzichelli, 1970; Murr, 1981) and Li (Li, 1961, 1963b) proposed correlation between k_y and the density of grain boundary source, e.g. k_y is proportional to square root of ledge density. However, various experimental observations contradict to Li's model. For instance, it has been reported that the pure nickel showed linear relation between k_y and ledge densities (Venkatesh and Murr, 1978) or no clear correlation has been established between k_y and the density of ledges (Bernstein and Rath, 1973). Also, discrete dislocation simulations showed that source density and location have a negligible effect on the Hall-Petch relation (Biner and Morris, 2003).

Ashby (Ashby, 1970) proposed two types of dislocations: the statistically stored dislocations (SSD) and the geometrically necessary dislocations (GND). SSDs correspond to the dislocations accumulated during a general, uniform deformation that is randomly distributed over the entire grain while GNDs are the dislocations necessary to avoid overlaps or voids near the grain boundaries during a local, non-uniform deformation (Thompson et al., 1973). Statistically stored dislocation density (ρ_s) and geometrically necessary dislocation density (ρ_G) are expressed as (Cottrell, 1953; Ashby, 1970):

$$\rho_s = \frac{C_1 \varepsilon}{b \lambda_s} \quad (2.9)$$

$$\rho_G = \frac{C_2 \varepsilon}{b D}$$

where C_1 and C_2 are constants, λ_s is the average slip length, D is the grain size and b is the Burgers vector. The flow stress is then represented as follows:

$$\sigma(\varepsilon) = \sigma_0 + \alpha \mu \sqrt{\varepsilon} \sqrt{\frac{C'_1}{\lambda_s} + \frac{C'_2}{D}} \quad (2.10)$$

Equation (2.10) shows similar form of $D^{-1/2}$ dependence on the flow stress and implies that the flow stress is increased by the reduction of the slip length and increase in GND density necessary to maintain the material continuity across the grain boundaries (Conrad, 1961, 1970). It should be noted that equation (2.10) reduces to Hall-Petch Law if $\lambda_s = D$. The major difference between pileup model and dislocation density model is the consideration of the dislocation arrangement and the effect of grain size on the total dislocation density (Conrad, 2004). The dislocation density model predicts higher dislocation density near the grain boundaries in terms of GNDs.

Another approach to describe the Hall-Petch Law is the composite model where each grain is described as a composite material with the grain interior and the grain boundary region which have different material properties (Kocks, 1970; Hirth, 1972; Meyers and Ashworth, 1982). Using a simple law of mixture between two different materials, overall flow stress is expressed as:

$$\sigma_f = f \sigma_f^{GB} + (1 - f) \sigma_f^{BULK} \quad (2.11)$$

where σ_f^{GB} and σ_f^{BULK} are the flow stresses of the grain boundary and bulk regions respectively, and f is the volume fraction of the grain boundary.

An assumption that the grain boundary region forms a hardened layer can be understood in terms of dislocation pileups, concentration of GNDs near the grain boundaries (Thompson et al., 1973) or elastic anisotropy of adjacent grains that establishes stress concentration forming a work hardened layer (Meyers and Ashworth, 1982). Also the differing properties are presumed to arise from elastic and plastic incompatibilities that promote multiple slip and increased entanglements. Since polycrystalline material with smaller grain size has a relatively larger amount of grain boundary regions, fine grained materials are expected to have higher yield stress. Equation (2.11) can be further developed into an expression that explains the relation between the flow stress and grain size by assuming idealized spherical grain (Meyers and Ashworth, 1982):

$$\sigma_f = \sigma_f^{bulk} + 8(\sigma_f^{GB} - \sigma_f^{bulk})D^{-1} - 16(\sigma_f^{GB} - \sigma_f^{bulk})^2 D^{-2} \quad (2.12)$$

where t is the thickness of a grain boundary layer. Assuming constant t and neglecting the D^{-2} term, the above equation implies that the flow stress is inversely proportional to the grain size. The composite model is consistent with previous models in the sense that more dislocations are accumulated near the grain boundary and would induce higher local flow stress. However, it is difficult to explain $D^{-1/2}$ dependence, and arbitrary assumptions about the thickness and properties of grain boundary layer are required. Therefore, while the composite model is an attractive general picture that is very likely a correct overview of the behavior, it lacks predictive capability based on microstructure.

Although these models succeeded to reproduce the form of the Hall-Petch Law based on simplifying assumptions, none of them seem to capture all the important mechanisms near the grain boundaries. All models mentioned above lack connection to the structure or orientation of the grain boundary, the actual slip systems, or the grain misorientation, all of which are known to affect slip transmission at grain boundaries (Shen et al., 1986; Wagoner et al., 1998). Therefore, it is difficult to conclude that the actual mechanism will rigorously follow one of the proposed models but the actual behavior near the grain boundary is likely to show mechanisms proposed by different models and affected by the grain boundary structure, actual slip systems and grain orientations. Hence, an integrated model that would encompass the effect of dislocation interactions and grain boundary characteristics accurately describe and predict the Hall-Petch relationship.

3. SINGLE CRYSTAL CONSTITUTIVE EQUATIONS

Note: Chapter 3 is presented in the format of a peer-reviewed paper that is accepted for publication by the International Journal of Plasticity and is in press at this writing (Lee et al., 2009).

3.1 Abstract

Single-crystal constitutive equations based on dislocation density (SCCE-D) were developed from Orowan's strengthening equation and simple geometric relationships of the operating slip systems. The flow resistance on a slip plane was computed using the Burger's vector, line direction, and density of the dislocations on all other slip planes, with no adjustable parameters. That is, the latent/ self-hardening matrix was determined by the crystallography of the slip systems alone. The multiplication of dislocations on each slip system incorporated standard 3-parameter dislocation-density evolution equations applied to each slip system independently; this is the only phenomenological aspect of the SCCE-D model. In contrast, the most widely used single-crystal constitutive equations for texture analysis (SCCE-T) feature 4 or more adjustable parameters that are usually back-fit from a polycrystal flow curve. In order to compare the accuracy of the two approaches to reproduce single-crystal behavior, tensile tests of single crystals oriented for single slip were simulated using crystal-plasticity finite element modeling.

Best-fit parameters (3 for SCCE-D, 4 for SCCE-T) were determined using either multiple or single-slip stress-strain curves for copper and iron from the literature. Both approaches reproduced the data used for fitting accurately. Tensile tests of copper and iron single crystals oriented to favor the remaining combinations of slip systems were then simulated using each model (i.e. multiple slip cases for equations fit to single slip, and vice versa). In spite of fewer fit parameters, the SCCE-D predicted the flow stresses with a standard deviation of 14 MPa, less than one half that for the SCCE-T conventional equations: 31 MPa. Polycrystalline texture simulations were conducted to compare predictions of the two models. The predicted polycrystal flow curves differed considerably, but the differences in texture evolution were insensitive to the type of constitutive equations. The SCCE-D method provides an improved representation of single-crystal plastic response with fewer adjustable parameters, better accuracy, and better predictivity than the constitutive equations most widely used for texture analysis (SCCE-T).

3.2 Introduction

Modern “texture analysis” routinely predicts the plastic anisotropy and texture evolution of polycrystals during large deformation, particularly for FCC crystal structures. Such calculations make use of single-crystal constitutive equations based on slip systems and statistical grain orientation information. The procedure does not consider specific neighboring grain interactions or the presence of grain boundaries, as illustrated in Figure 3.1. The linkage among grains in texture analyses is based on numerical

convenience, assuming that all grains exhibit identical strains (Taylor, 1938), or stresses (Sachs, 1928), or combinations of stress and strain components (Canova, 1985). Such models enforce some aspects of inter-grain equilibrium or compatibility, but not both (Parks, 1990). An alternative formulation treats a single grain as an inclusion within a homogenized medium (Kröner, 1961; Molinari, 1987).

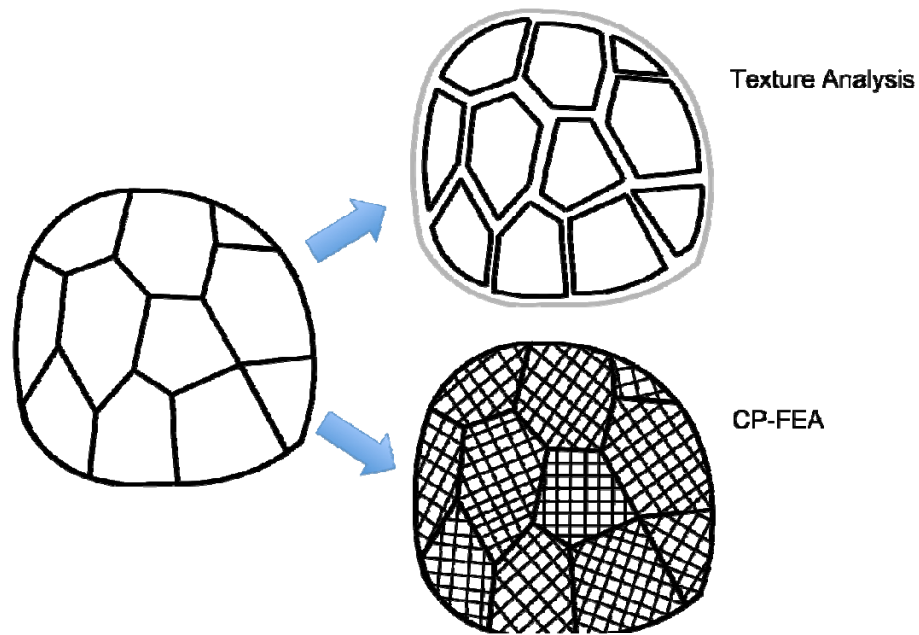


Figure 3.1: Schematic view of typical texture analysis and crystal plasticity-finite element analysis (CP-FEA). Texture analysis imposes highly-simplified inter-grain rules while CP-FEA imposes compatibility and equilibrium in a finite element sense.

Crystal-plasticity finite element analysis (CP-FEA) (Peirce, 1982; Asaro, 1983; Dawson, 2000) enforces inter-grain equilibrium and compatibility in a finite element sense (with many elements in a single grain), thus treating the interactions among

neighboring grains more realistically (Raabe, 2002), Figure 3.1, but with large penalties in computation time. Recent applications of CP-FEA have been extended to the deformation of single, bi- and polycrystals (Zaefferer, 2003; Ma, 2006; Zaafarani, 2006; Raabe, 2007), incorporating size dependence through strain gradient terms (Abu Al-Rub, 2005) and nanoindentation simulations (Wang, 2004; Liu, 2005; Liu, 2008). These methods are too CPU-intensive for use with large grain assemblies (i.e. typical polycrystals) or for treating applied deformation boundary-value problems. Modifications to improve the efficiency of the calculations limit the accuracy by, for example, applying iso-strain conditions within a grain (Kalidindi, 1992; Dawson, 2003) or having each finite element represent a single grain (Nakamachi, 2001).

Polycrystal simulations, whether of the texture type or CP-FEA type, use single crystal plasticity constitutive models based on slip system activity. Typical formulations are either elastic-plastic rate-independent (Mandel, 1965; Hill, 1966, 1972; Rice, 1971; Asaro and Rice, 1977; Anand and Kothari, 1996; Marin and Dawson, 1998) or viscoplastic (Peirce et al., 1982; Asaro and Needleman, 1985). This viscoplastic approach has recently been referred to in the literature as “PAN” (e.g. (Alcalá et al., 2008; Patil et al., 2008; Thakare et al., 2009)), named for “Peirce, Asaro, Needleman” (Peirce et al., 1982; Asaro and Needleman, 1985). The PAN approach uses an arbitrary small strain-rate sensitivity index to avoid numerical non-uniqueness. The most commonly used PAN formulation relies on a power-law equation relating shear stress to shear strain rate on each slip system (Asaro and Needleman, 1985) with the slip system

resistance evolving with total slip on each slip system according to latent and self-hardening (Mandel, 1965; Hill, 1966).

The adjustable parameters in the single-crystal constitutive equations used for texture analysis are almost universally determined by back-fitting them to mechanical test results (i.e. uniaxial tension or compression) of macroscopic polycrystals that are simulated using the same technique for which the constitutive equations are destined. Such a procedure guarantees that the macroscopic tests used to fit the parameters are reproduced accurately by the simulations, *but not that the single-crystal constitutive equations represent true single-crystal behavior*. Simulations of problems based on such an approach have proven useful for a range of strain, strain rates, and temperatures (Mathur and Dawson, 1989; Bronkhorst et al., 1992; Beaudoin et al., 1994; Kumar and Dawson, 1998; Nemat-Nasser et al., 1998). However, there is evidence that single-crystal plasticity models fitted in this way do not always represent single-crystal behavior properly (Becker and Panchanadeeswaran, 1995; Kumar and Yang, 1999; Arsenlis and Parks, 2002). If the presence and characterization of grain boundaries (and grain shape, size, misorientation, etc.) influences the relationship between single-crystal and polycrystal deformation characteristics, the standard back-fitting procedure evidently would not yield a correct description of single-crystal behavior. Instead, the single-crystal constitutive equations embed undetermined aspects of the inter-grain interactions and thus, may not represent single crystal behavior but rather some amalgam of single and polycrystal aspects. One of the purposes of the current work is to determine whether the predominant formulation of single-crystal constitutive equations used for a wide range of

successful texture calculations (“SCCE-T”) captures single crystal behavior properly, particularly single slip vs. multiple slip. The answer to that question bears on the question of whether inter-grain interactions are incorporated in an unknown way into the SCCE-T’s fit to macroscopic observations.

Note: “SCCE-T” refers in this paper to a set of choices within the broader PAN framework. It is SCCE-T that is used with wide success in texture calculations appearing in the literature. SCCE-T is a subset of PAN, the latter of which has greater flexibility with a commensurate number of additional adjustable parameters. As a particular example, the majority of successful texture calculations use a fixed value, 1.4, describing the ratio of latent hardening to self hardening that agrees with experience at the macro/ texture level. SCCE-T, in addition to having the validation of wide testing over more than 20 years, has only one additional parameter compared with the constitutive model proposed here. Thus, comparisons between the two are meaningful. Summaries of the constitutive forms considered in this paper are presented later.

Alternate developments to represent single-crystal behavior based on dislocation densities have appeared. Models of this type typically exhibit considerable complexity and large numbers of undetermined parameters. Models based on statistical aspects of dislocation densities represented as internal state variables (Ortiz et al., 1999; Arsenlis and Parks, 2002) captured the orientation-dependent flow behavior of FCC single crystals. Developments for FCC and BCC single crystals make use of Orowan’s equation (Orowan, 1940) and have incorporated many physical complexities, including

dislocation velocities, activation energies, and dislocation walls (Roters et al., 2000). In order to reproduce the compression of aluminum single crystals at elevated temperature, 8 fit parameters and 2 activation energies were required to predict stress strain curves for a range of strain rates and temperatures in one study (Ma and Roters, 2004).

In the current work, a dislocation-based single crystal constitutive equation (“SCCE-D”) is newly formulated with 3 undetermined parameters corresponding to a standard equation representing the evolution of dislocation density. The form is similar to standard corresponding texture-type equations, except that the dislocation density for each slip system and its evolution is used explicitly rather than implicitly via slip system strength and its evolution with total slip (Ortiz and Popov, 1982; Brown et al., 1989; Kalidindi et al., 1992; Kuchnicki et al., 2006; Wang et al., 2007). Use of physical dislocation densities allows application of Orowan’s strengthening model (Orowan, 1948) to determine the cross-hardening effects without undetermined parameters (see also (Bassani and Wu, 1991) and (Liu et al., 2008)). Such cross-hardening effects depend on the geometry of the crystal lattice type, not on undetermined parameters.

Tests of SCCE-D are made for single-crystal and polycrystal deformation and the results are compared with corresponding ones using standard SCCE-T. We emphasize that we have selected the SCCE-T for comparison with the new model because it dominates successful texture calculations presented in the literature. As such, it represents an informal “consensus” of what has been found to work. None of the other variants within the PAN formalism approach the breadth of experience or acceptance in the community. The question to be answered is whether the SCCE-T formulation that

finds broad success for polycrystal simulations represents single-crystal behavior properly, and if not, whether a less-adjustable/ more predictive formulation can improve on the single-crystal representation. A secondary question is how such an alternative formulation would affect macroscopic texture calculations.

3.3 Crystal Plasticity based on Single Crystal Constitutive Equations

The kinematics for either SCCE-T or SCCE-D are based on well-established developments (Lee, 1969; Rice, 1971; Hill and Rice, 1972; Asaro and Rice, 1977; Peirce et al., 1982). The total deformation gradient is decomposed into elastic and plastic parts (Lee, 1969):

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^p \quad (3.1)$$

where $\mathbf{F}^e$ corresponds to elastic distortion of lattice, and $\mathbf{F}^p$ defines the slip by the dislocation motion in the unrotated configuration (Mandel, 1965).

The plastic velocity gradient in the unrotated (or intermediate) configuration is:

$$\bar{\mathbf{L}}^p = \dot{\mathbf{F}}^p \mathbf{F}^{p-1} \quad (3.2)$$

The evolution of the plastic deformation can be expressed as the sum of all crystallographic slip rates, $\dot{\gamma}^\alpha$ (Rice, 1971),

$$\bar{\mathbf{L}}^p = \sum_{\alpha=1}^n \dot{\gamma}^\alpha \mathbf{s}_0^\alpha \otimes \mathbf{n}_0^\alpha \quad (3.3)$$

where $\mathbf{s}_0^\alpha$ and $\mathbf{n}_0^\alpha$ are the vectors representing slip direction and slip plane normal of the slip system α , respectively and n is total number of slip systems.

3.3.1 Common Elements of SCCE-T and SCCE-D

For a rate-dependent crystal plasticity model, the plastic shear rate of each slip system α is typically expressed as a power law function of the resolved shear stress τ^α as (Hutchinson, 1976; Peirce et al., 1982):

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left(\frac{\tau^\alpha}{g^\alpha} \right)^{\frac{1}{m}} \text{sign}(\tau^\alpha) \quad (3.4)$$

where $\dot{\gamma}_0$ is reference shear rate, g^α is the slip resistance (or flow stress) of the slip system α and m is the rate sensitivity exponent. The initial flow stress is generally assumed to be the same, i.e. g_0 , for all slip systems. Reference shearing rate and rate sensitivity, 0.001 s^{-1} and 0.012 respectively, are adopted from the literature (Bronkhorst et al., 1992; Kalidindi et al., 1992).

To complete the constitutive equations, the second Piola-Kirchhoff stress is defined as follows, and is related elastically to the strain:

$$\mathbf{S} = \mathbf{C}^e : \mathbf{E} = \det(\mathbf{F}^e) \mathbf{F}^{e-1} \boldsymbol{\sigma} \mathbf{F}^{e-T} \quad (3.5)$$

where $\mathbf{E} = \frac{1}{2}(\mathbf{F}^{eT} \mathbf{F}^e - \mathbf{I})$ is the Lagrangian strain tensor, $\boldsymbol{\sigma}$ is the Cauchy stress, and $\mathbf{C}^e$ is the fourth order elastic constant matrix.

The resolved shear stress of slip system α in equation (3.4) is approximately,

$$\tau^\alpha = \mathbf{S} : \mathbf{P}_0^\alpha \equiv \mathbf{S} : (\mathbf{s}_0^\alpha \otimes \mathbf{n}_0^\alpha) \quad \text{or} \quad \tau^\alpha = \mathbf{S}_{ij} \mathbf{P}_{0ij}^\alpha \equiv \mathbf{S}_{ij} : (\mathbf{s}_{0i}^\alpha \mathbf{n}_{0j}^\alpha) \quad (3.6)$$

The slip resistance (equivalent to a critical resolved shear stress (CRSS) for a rate-independent elastic-plastic law) of slip system α , g^α evolves as the slip (or gliding) of dislocations on the slip system occurs. The governing rule of the evolution of slip resistance (hardening) is a critical aspect of the constitutive framework and causes the SCCE-T and SCCE-D approaches to diverge, as described in the following sections.

3.3.2 Single-Crystal Constitutive Equations developed for Texture models (SCCE-T)

Texture analyses predominantly utilize phenomenological models for the evolution of flow stress on a slip system α as related to the slip increment on all slip systems β as follows (Asaro, 1983):

$$\dot{g}^\alpha = \sum_{\beta} h_{\alpha\beta} \dot{\gamma}^\alpha \quad (3.7)$$

where $h_{\alpha\beta}$ are hardening coefficients. Most texture analyses have adopted the following form for the hardening coefficient matrix (Hutchinson, 1970; Asaro, 1979; Peirce et al., 1982):

$$h_{\alpha\beta} = h_{\beta} (q_{\text{lat}} + (q_{\text{self}} - q_{\text{lat}}) \delta_{\alpha\beta}) \quad (3.8)$$

where $\delta_{\alpha\beta}$ is the Kronecker delta and q_{self} and q_{lat} determine the self and latent hardening, respectively. The hardening matrix contains two distinct values: diagonal terms (q_{self}) for the self-hardening and off-diagonal terms (q_{lat}) for the latent hardening. Experimental observations (Kocks, 1970) suggested that the range $1 \leq q_{\text{lat}} / q_{\text{self}} \leq 1.4$ applies for FCC single crystals, and $q_{\text{lat}} / q_{\text{self}} = 1.4$ is typically used in texture analyses of FCC

polycrystals (Peirce et al., 1982; Asaro and Needleman, 1985; Mathur and Dawson, 1989; Kalidindi et al., 1992).

The form of $\mathbf{h}_\beta$ in equation (3.8) has been proposed to properly represent the stress-strain behavior of polycrystals. Here, the widely-used form proposed by Brown et al. (Brown et al., 1989) is adopted:

$$\mathbf{h}_\beta = \mathbf{h}_0 \left(\mathbf{1} - \frac{g^\beta}{g_s} \right)^a \quad (3.9)$$

where h_0 is the initial hardening rate, g_s is the saturated flow stress and a is the hardening exponent. The initial hardness g_0 is typically fitted to reproduce the macroscopic yield stress. Equations (3.7)-(3.9) have been shown to predict the stress-strain response and evolution of texture for simple deformation of FCC polycrystals (Mathur and Dawson, 1989; Kalidindi et al., 1992). When the parameters are back-fitted to stress-strain responses of polycrystals, there are 4 arbitrary parameters to be fit from macroscopic polycrystal stress-strain curves to complete equations (3.7)-(3.9): h_0 , g_s , g_0 and a in equations (3.4), (3.8) and (3.9). These undetermined parameters, h_0 , g_s , g_0 , and a are typically set from the stress strain curve for a polycrystal tensile test.

3.3.3 Single-Crystal Constitutive Equations based on the Dislocation density model (SCCE-D)

In the SCCE-D derived here, the hardening is expressed in terms of the interaction of mobile dislocations with corresponding forest dislocations that act as point obstacles, Figure 3.2. These interactions are evaluated using Orowan's strengthening model

assuming that forest dislocations are hard pins with respect to intersecting mobile dislocation. That is, the intersection points become immobile and the mobile dislocation must bypass by looping around the obstacle rather than cutting through it. In fact, dislocation intersections are known to be hard pins in most metals at low homologous temperatures (Hirth and Lothe, 1969).

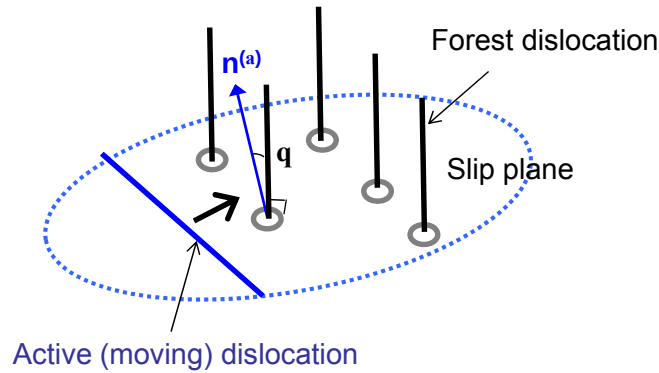


Figure 3.2: Interaction between a moving dislocation on an active slip system and corresponding forest dislocation array.

In Orowan's model (Orowan, 1948), if the applied stress is large enough, dislocations loop around an obstacle and will overcome and bypass it, leaving dislocation loops behind. The critical stress (σ^c) necessary to bow out a dislocation on a slip system α to a radius r is calculated by considering the equilibrium with the line tension of the dislocation, T :

$$\sigma^c \cdot b = \frac{T}{r} \quad (3.10)$$

where b is the Burger's vector. The dislocation is considered to have a line tension equal to its self-energy per unit length and is approximated (Weertman, 1992) as follows:

$$T \approx \frac{1}{2} \mu b^2 \quad (3.11)$$

where μ is shear modulus. Combining equations (3.10) and (3.11), we express the critical bypass stress as

$$g^\alpha = \frac{\mu b}{2r} = \frac{\mu b}{l} \quad (3.12)$$

where the critical radius of curvature is set equal to half of the inter-pin spacing. Equation (3.12) is the well-known relationship for Orowan's bypass mechanism. If the applied stress exceeds the bypass stress, dislocations bypass the obstacle, allowing long-range plastic straining, and loops are formed around each obstacle. Now we assume that the obstacles are forest dislocations, that is dislocations lying on other slip systems that pierce the slip plane of the α slip system. Since the obstacle spacing distance l , in equation (3.12) depends on the density of forest dislocations, equation (3.12) can be rewritten as:

$$g^\alpha = \mu b \sqrt{\rho_f} \quad (3.13)$$

where ρ_f is the density of dislocations that penetrate the slip plane of slip system α .

For the flow stress derived in equation (3.13) assumes that all of the forest dislocation lines are assumed to be parallel to the α slip plane normal. For an arbitrary angle, θ , between the two directions, as shown in Figure 3.2, the effective forest dislocation density $\bar{\rho}_f$ is as follows:

$$\bar{\rho}_f = \rho_f \cos \theta = \rho_f \cdot (\mathbf{n}^a \cdot \xi_f) \quad (3.14)$$

where $\mathbf{n}^a$ and ξ_f are the slip plane normal of the moving dislocation being considered and the line direction of the corresponding forest dislocation, respectively. The effective forest dislocation density, $\bar{\rho}_f$ is maximized when $\theta = 0^\circ$ and vanishes if $\theta = 90^\circ$, i.e. if the mobile and forest dislocations are coplanar. Therefore, the flow stress can be represented as:

$$g^a = \mu b \sqrt{\rho_f \cdot (\mathbf{n}^a \cdot \xi_f)} \quad (3.15)$$

Equation (3.15) includes the assumption that all forest dislocations are parallel to each other. To generalize to an array of forest dislocations, the interactions are summed over each type of dislocations/ slip system (Franciosi and Zaoui, 1982). If there are n different slip systems, the equation (3.15) becomes:

$$g^a = \mu b \sqrt{\sum_{\beta=1}^n \mathbf{h}_{a\beta} \rho_\beta} \quad (3.16)$$

where $\mathbf{h}_{a\beta} = \mathbf{n}^a \cdot \xi^\beta$ is given by the geometries of edge dislocations for each slip system, with no undetermined parameters.

To complete the SCCE-D development, a widely-used dislocation density evolution equation based on slip systems is adopted (Kocks, 1976).

$$\dot{\rho}^a = \frac{1}{b} \left(\frac{\sqrt{\sum_{\beta} \rho^\beta}}{k_a} - k_b \rho^a \right) \cdot |\dot{\gamma}^a| \quad (3.17)$$

where k_a and k_b are material parameters for the generation and annihilation terms of dislocations, respectively. The final SCCE-D defined by equations (3.16) and (3.17) has three parameters to be determined, each of them related to dislocation density and its evolution: k_a , k_b and ρ_0 . In order to compare the accuracy and usefulness of SCCE-T and SCCE-D as described above, the adjustable parameters were fit to reproduce the measured stress-strain response of single crystals oriented for either multiple or single slip. The resulting material models were then used with finite element modeling to predict the stress-strain response for tensile tests oriented for the activation of other combinations of slip systems. The predicted responses were then compared with corresponding experimental results from the literature.

3.4 CP-FEM Implementation

The two single-crystal constitutive equations described in the previous section were implemented into the commercial finite element program ABAQUS/Standard via the user material subroutine, UMAT (Hibbit, 2005). A single eight-noded continuum element (C3D8) was utilized to simulate the tensile tests of single crystals. The tensile direction was aligned with one of the element axes and the two faces of the cube element were initially perpendicular to the loading axis. During the deformation, the two faces remain parallel to each other and perpendicular to the loading axis, simulating the deformation mode imposed by a stiff tensile machine. Crystallographic slip was considered on the 12 equivalent $\{111\} \langle 110 \rangle$ slip systems for FCC copper and 12 $\{110\} \langle 111 \rangle$ and 12 $\{112\} \langle 111 \rangle$ slip systems for BCC iron.

The tensile stress-strain responses for oriented single crystals have been measured. For FCC copper single crystals, 4 tensile axis orientations are available (Takeuchi, 1975; Arsenlis and Parks, 2002): $\langle 123 \rangle$, $\langle 112 \rangle$, $\langle 100 \rangle$, and $\langle 111 \rangle$. The $\langle 123 \rangle$ tensile axis is oriented for single slip while $\langle 112 \rangle$, $\langle 111 \rangle$ and $\langle 100 \rangle$ tensile axes are oriented for multiple slip, with 2, 6 and 8 equally favored slip systems respectively. For BCC iron single crystals, 3 tensile axis orientations are available (Keh, 1965): $\langle 348 \rangle$, $\langle 110 \rangle$, and $\langle 100 \rangle$. The $\langle 348 \rangle$ tensile axis is oriented for single slip while the $\langle 110 \rangle$ and $\langle 100 \rangle$ tensile axes are orientated for multiple slip, with 2 and 4 equally favored slip systems respectively.

3.5 Prediction of Single Crystal Stress-strain Response

SCCE-T and SCCE-D models were fit by comparing FE simulations of single-crystal tensile tests oriented along directions with most equivalent slip systems, $[001]$, with corresponding experimental stress-strain curves from the literature. The best-fit parameters, Table 3.1, were determined using the procedure described below. The stress-strain responses for other orientations of tensile axis were then predicted using the resulting constitutive equations. For SCCE-T, h_0 affects the initial hardening rate, g_s determines the final saturated value of stress, g_0 determines initial yield and a affects the shape of the stress-strain curve (Kalidindi et al., 1992). For SCCE-D, ρ_0 corresponds to g_0 for SCCE-T, which determines the yield stress while k_a and k_b affect the shape of the flow curve.

Best fit parameters		SCCE-T					SCCE-D			Std. Error of Fit (MPa)
Fit direction		g_0 (MPa)	g_s (MPa)	h_0 (MPa)	a		ρ_0 (mm ⁻¹)	k_a	k_b	
Cu	[001]	1	89	255	1	0.67	10^3	22	33.5b	0.64
	[-123]	1	58	37	-0.75	2.10	10	51	3b	1.65
Fe	[001]	18	81	141	0.25	0.41	2.5×10^5	59	4b	0.77
	[-348]	18	58	17	-1.25	0.29	2.5×10^5	156	0.5b	1.89

Fit procedure parameters									
Data range	*	0-300	0-300	-3-3		*	1-200	0-50b	
Increment 1	-	10	10	1		-	10	10b	
Increment 2	-	1	1	0.25		-	1	0.5b	

*Obtained by simple trial and error, b: Burgers vector (=0.257 nm)

Table 3.1: Best fit parameters and range of parameters for fitting SCCCE-T and SCCE-D

In order to determine the set of parameters with minimum standard error of fit, g_0 for SCCE-T and ρ_0 for SCCE-D were first obtained from the observed yield stress by simple trial and error. Then, a 3-D “box” containing an assumed range of all possible combinations of parameters was constructed, along with equally-spaced interior points. Using SCCE-T as an example, 6727 equally-spaced interior points (i.e. $31 \times 31 \times 7$) representing 6727 choices of constitutive parameters was considered with ranges and increments as defined in Table 3.1: Best fit parameters and range of parameters for fitting SCCCE-T and SCCE-D (Increment 1). The following steps were then followed:

1. For each of the 6727 choices, a finite element analysis was performed and a standard deviation of stress from the simulation and experiments was determined up to a strain of 0.1. The set of parameters representing the minimum standard deviation was identified for further refinement.
2. The behavior of the standard deviation moving along any parametric axis was examined. For all the cases considered here, the standard deviation increased monotonically in all such directions moving away from the minimum standard deviation set identified in Step 1.
3. Starting from the set of parameters identified in Step 1, a smaller set of increments (Increment 2 in Table 3.1) was used to define 3969 ($21 \times 21 \times 9$) new sets of parameters throughout a range that includes the original cells adjacent to the location of the minimum standard deviation. Step 1 was again carried out using these choices, and the minimum standard deviation was thus refined. Again, the standard deviation was

verified to increase monotonically from this set of values moving away from it along any parametric axis.

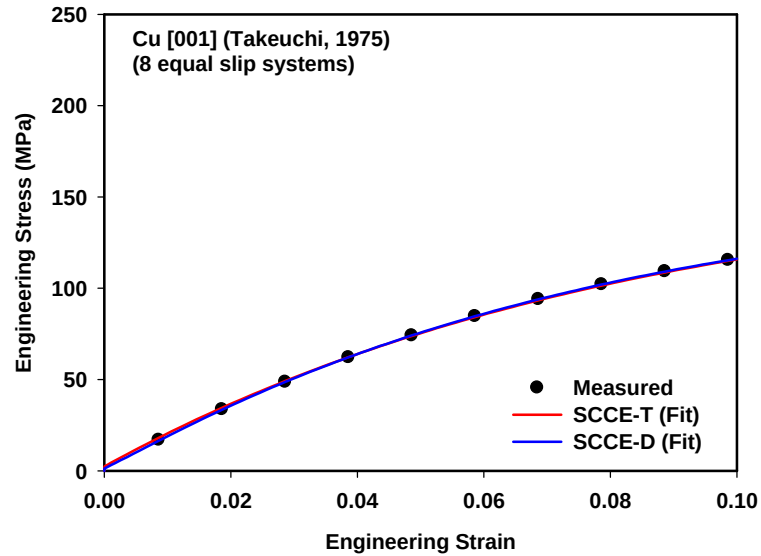
In this way, a unique set of best-fit constitutive parameters was determined and confidence in its uniqueness established. Anisotropic elasticity constants and shear modulus for copper and iron single crystals are used in all finite element simulations are shown in Table 3.2.

	C_{11}	C_{12}	C_{44}	Shear Modulus (μ)
Cu	170	124	75	48
Fe	242	150	112	80

Table 3.2: Anisotropic elasticity constants for single crystal copper (Simmons and Wang, 1971) and iron (Hirth and Lothe, 1969) (Unit: GPa).

Predicted and measured stress-strain curves are compared in Figure 3.3 and Figure 3.4 for copper and iron single crystals, respectively. Figure 3.3 (a) and Figure 3.4 (a) show the accuracy of SCCE-T and SCCE-D fitted curves as compared to the [001] experimental data used to fit them. The two approaches fitted the multiple-slip [001] tensile data with approximately the same accuracy (Table 3.1). Figure 3.3 (b)-(d) and Figure 3.4 (b)-(c) compare the predictions of SCCE-T and SCCE-D models (based on [001] tensile data) with experimental results for other tensile test directions. The fitting parameters for SCCE-T do not adequately represent the stress-strain response of single crystals, especially for single slip. The likely source of error for SCCE-T is the self/latent hardening ratio, $q_{\text{lat}}/q_{\text{self}} = 1.4$, which corresponds to significant self-hardening. In

contrast, the measured hardening rate of the stress-strain curve oriented for single slip is very low, implying negligible self-hardening.*



(a)

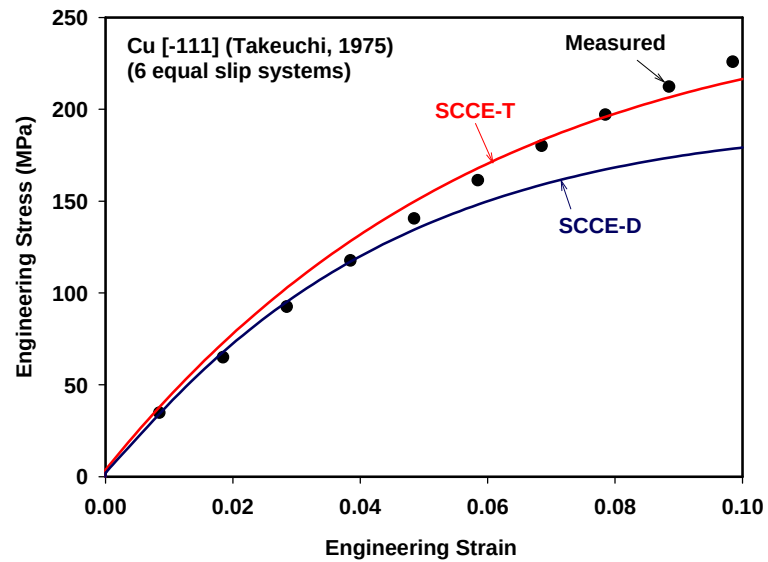
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Figure 3.3: Comparison of stress-strain curves from SCCE-T and SCCE-D constitutive models and measurements from the literature (Takeuchi, 1975) for copper single crystals with tensile axes in the following orientations: (a) [001] (b) [-111] (c) [-112] (d) [-123].

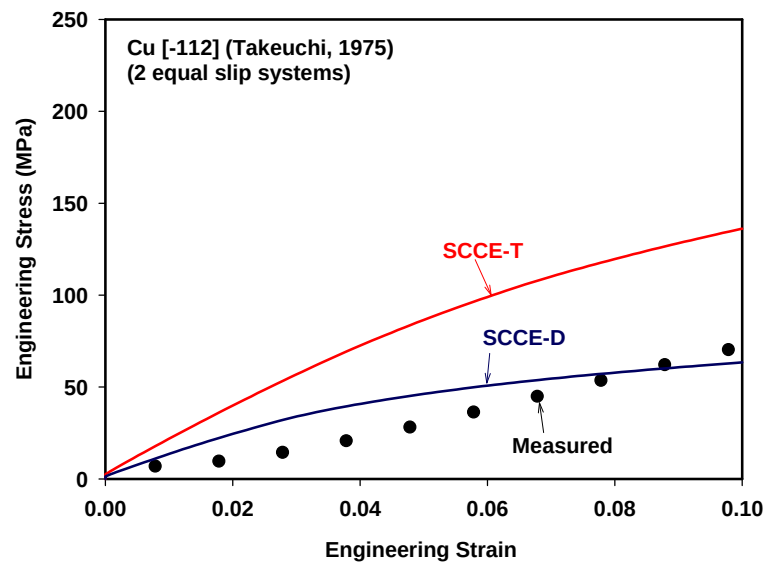
The parameters for the SCCE-T and SCCE-D constitutive models have been fitted to the [001] tensile test results, as shown in part (a).

* There is some hardening in single slip orientations even without self hardening because of the rotation of the crystallographic direction relative to the tensile axis toward a less favorable slip orientations (Anand, 1996)

Figure 3.3 continued



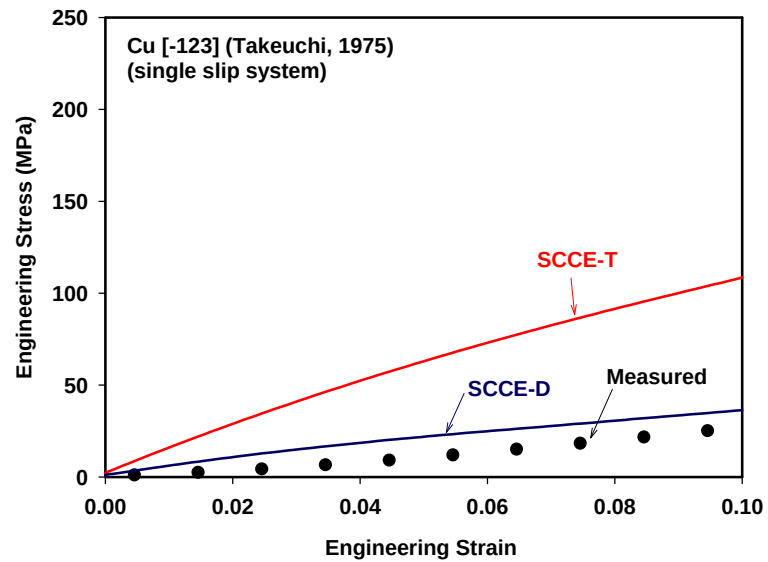
(b)



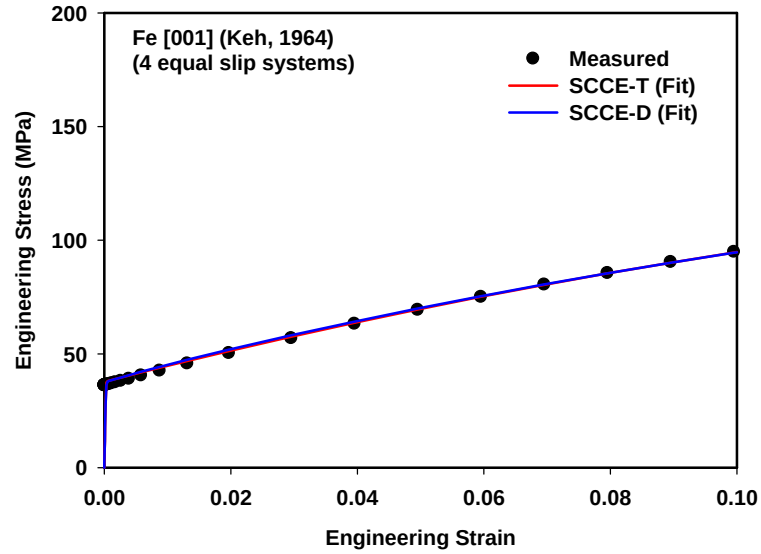
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Figure 3.3 continued



(d)

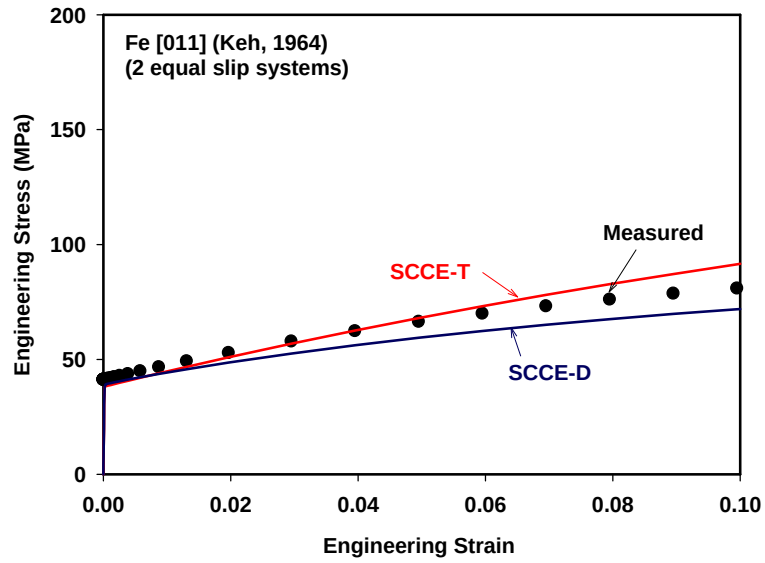


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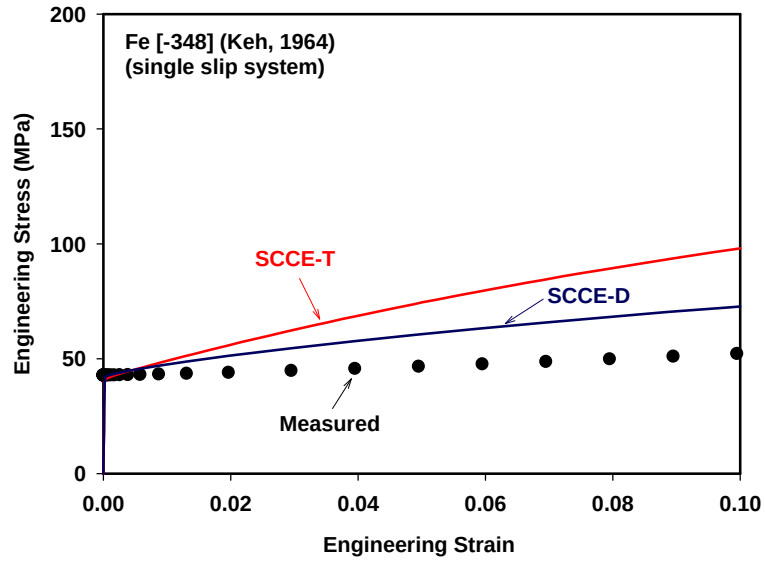
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Figure 3.4: Comparison of stress-strain curves from SCCE-T and SCCE-D constitutive models and measurements from the literature (Keh, 1965) for iron single crystals with tensile axes in the following orientations: (a) [001] (b) [011] (c) [-348]. The parameters for the SCCE-T and SCCE-D constitutive models have been fitted to the [001] tensile test results, as shown in part (a).

Figure 3.4 continued



(b)



(c)

The SCCE-D model agrees better with measurements in spite of having less number of arbitrary parameters. The standard deviations between the measured and

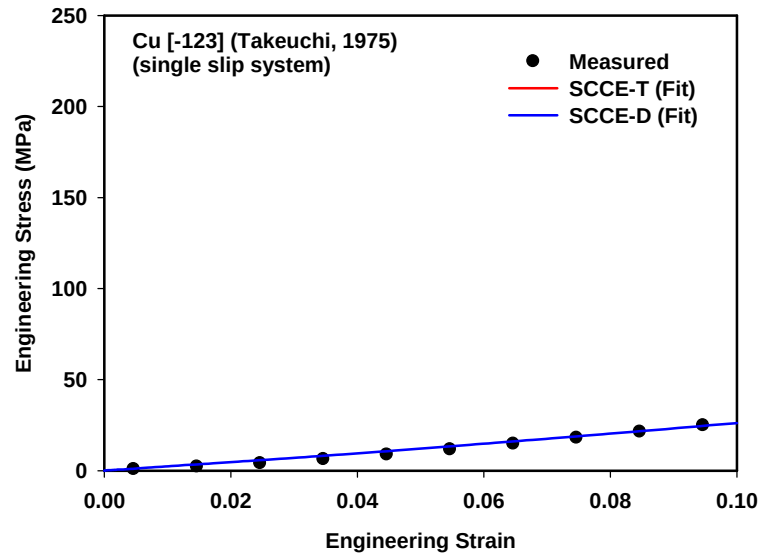
predicted results are listed in Table 3.3. The average standard deviation of measurements to the SCCE-D prediction is 14 MPa while that for the SCCE-T prediction is 31 MPa.

	Fit direction	Tensile axis direction	SCCE-T	SCCE-D
Cu	[001]	[111]	8 (6%)	23 (16%)
		[-112]	54 (150%)	13 (35%)
		[-123]	58 (451%)	10 (79%)
Fe	[001]	[011]	5 (8%)	7 (11%)
		[-348]	31 (66%)	15 (31%)
Avg. (Multiple slip fit)			31 (136%)	14 (34%)
Cu	[-123]	[001]	62 (82%)	38 (50%)
		[111]	113 (78%)	79 (55%)
		[-112]	19 (54%)	7 (20%)
Fe	[-348]	[001]	30 (42%)	23 (32%)
		[011]	24 (36%)	20 (30%)
Avg. (Single slip fit)			50 (58%)	33 (37%)

¹error percentage (%) = standard deviation/averaged flow stress×100

Table 3.3: Standard deviations and error percentage¹ between predicted and measured stress-strain curves.

To check whether the above conclusions are unique to fitting to multiple slip tensile experiments, we refitted the equations to single slip data, with the results shown in Table 3.3 and Figure 3.5 and Figure 3.6. The average standard deviation for the SCCE-T model is 50 MPa while that for the SCCE-D model is 33 MPa. The difference in the fit parameters and the standard deviations show that the new approach does not predict perfectly the differences between single slip and multiple slip, but SCCE-D is significantly better, with fewer adjustable parameters, than the standard SCCE-T.

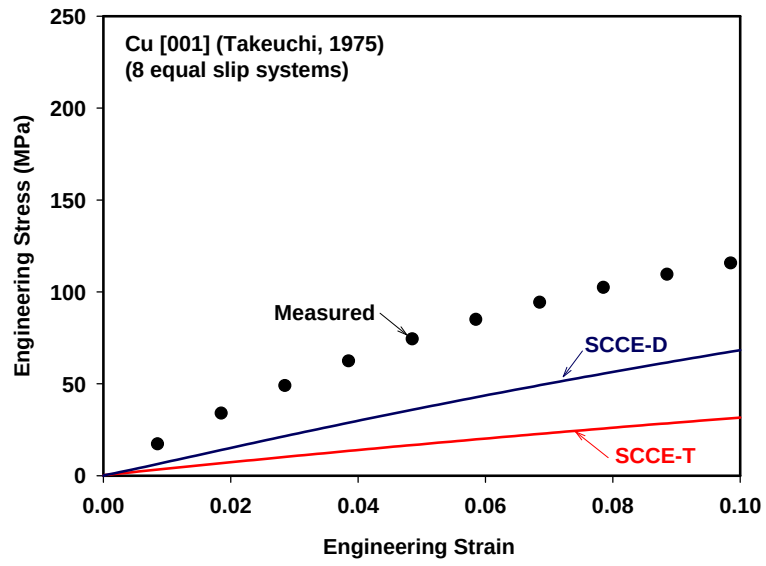


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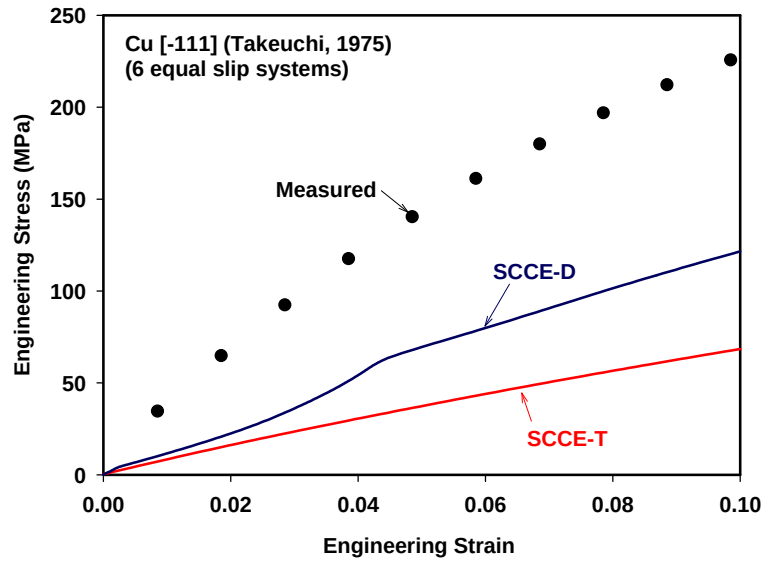
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Figure 3.5: Comparison of stress-strain curves from SCCE-T and SCCE-D constitutive models and measurements from the literature (Takeuchi, 1975) for copper single crystals with tensile axes in the following orientations: (a) $[-123]$ (b) $[-112]$ (c) $[-111]$ (d) $[001]$. The parameters for the SCCE-T and SCCE-D constitutive models have been fitted to the $[-123]$ tensile test results, as shown in part (a).

Figure 3.5 continued



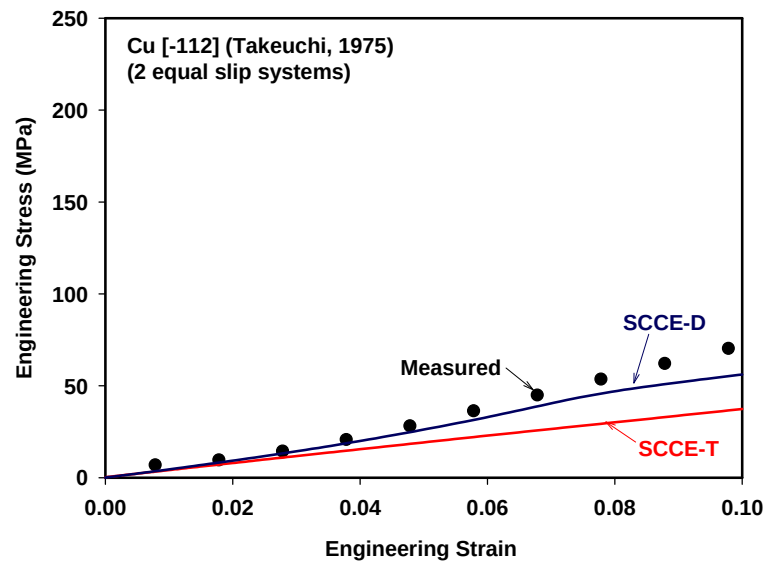
(b)



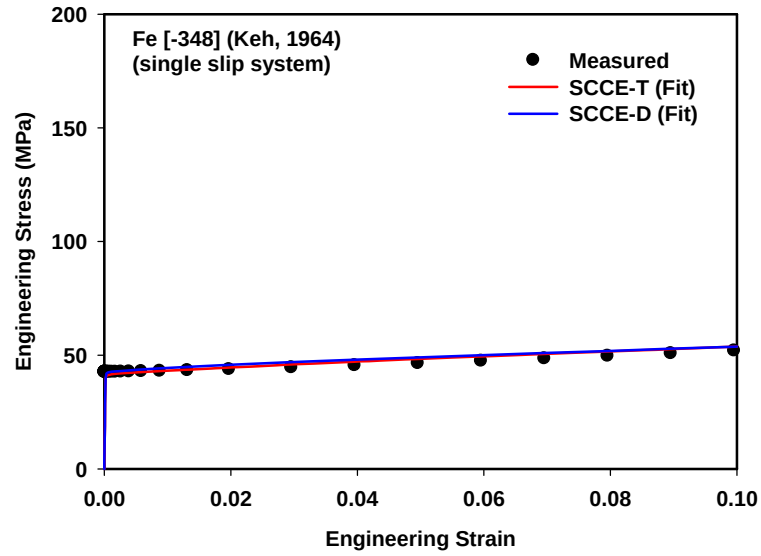
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Figure 3.5 continued



(d)

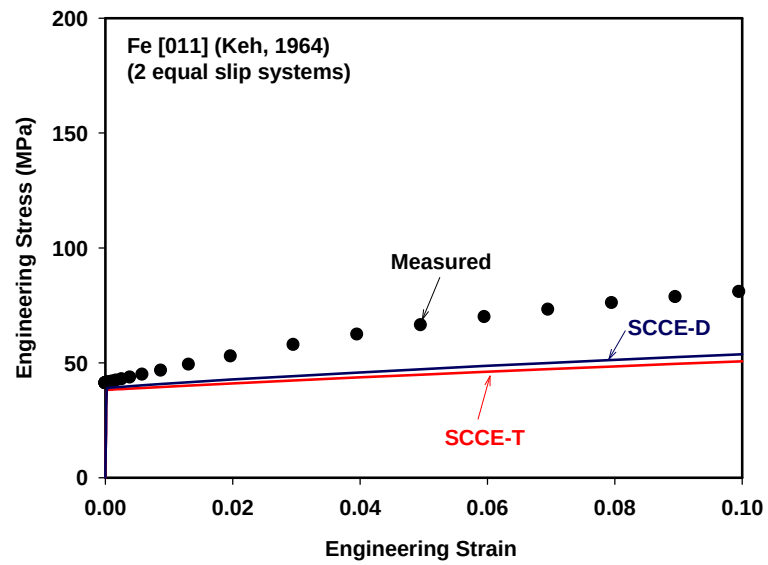


(a)

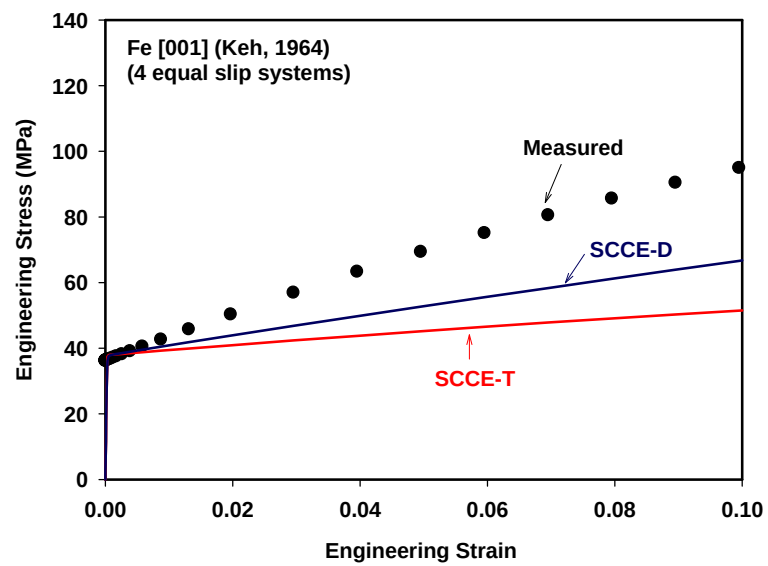
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Figure 3.6: Comparison of stress-strain curves from SCCE-T and SCCE-D constitutive models and measurements from the literature (Keh, 1965) for iron single crystals with tensile axes in the following orientations: (a) $[-348]$ (b) $[011]$ (c) $[001]$. The parameters for the SCCE-T and SCCE-D constitutive models have been fitted to the $[-348]$ tensile test results, as shown in part (a).

Figure 3.6 continued



(b)



(c)

3.6 Prediction of stress-strain response and texture evolution in polycrystals

Uniaxial compression and tension tests of polycrystalline copper and iron were simulated using SCCE-T and SCCE-D models to examine their role on the predicted stress-strain response and texture evolution of polycrystals. Material properties shown in Table 3.1 for the [001] fit were used, along with an FE mesh with a total of 1,000 (10×10×10) 3-dimensional solid elements, each representing a single grain. An isotropic texture was generated by assigning a random orientation to every element in the form of Bunge's Euler angles. The initial mesh and random crystal orientation as described by equal-area pole figures are shown in Figure 3.7.

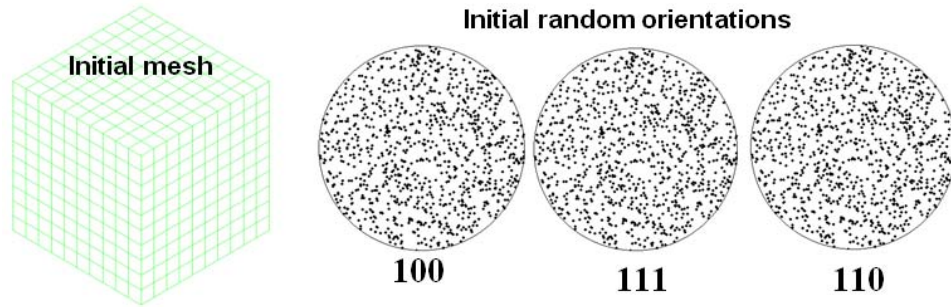
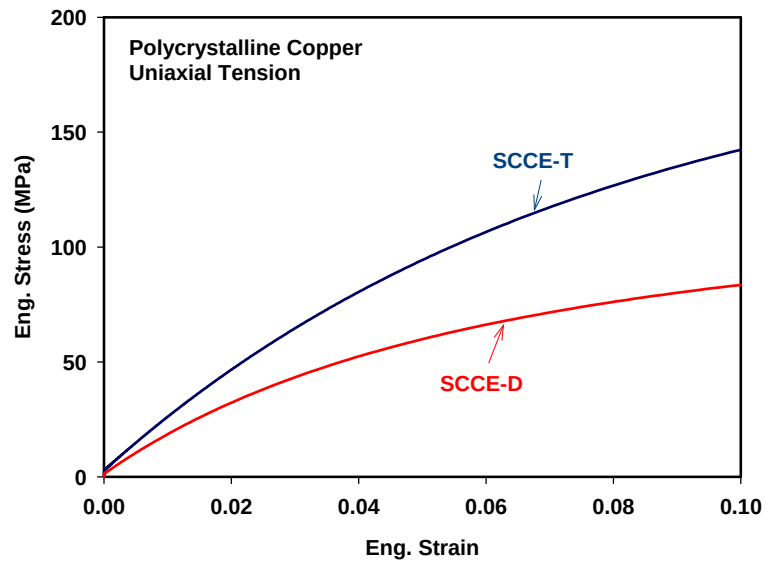
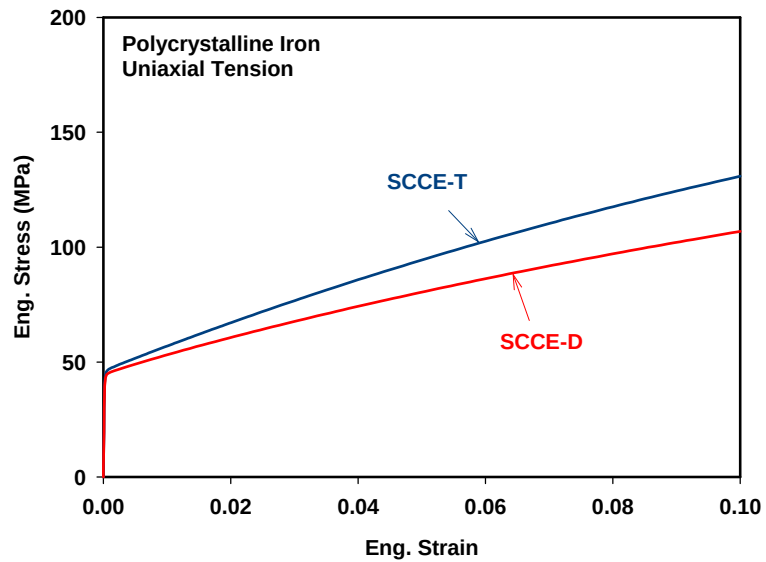


Figure 3.7: Initial mesh and pole figures for the initial random orientations used for the finite element simulations.

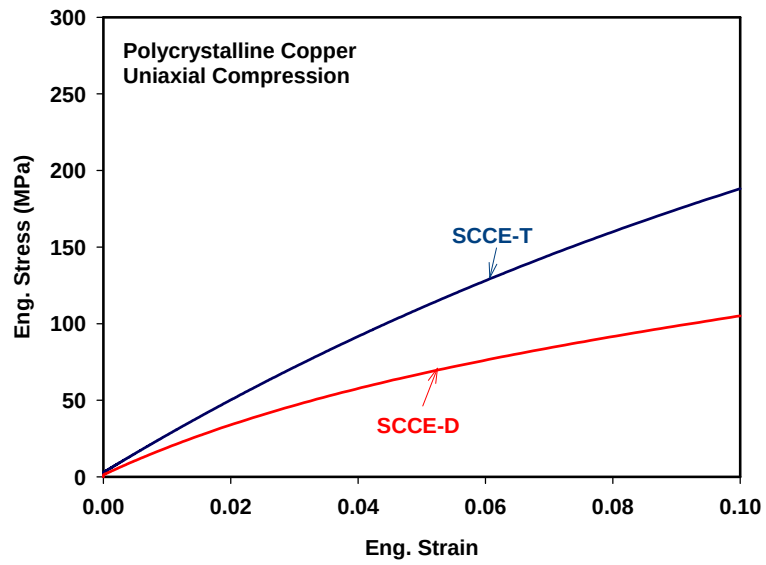


(a)

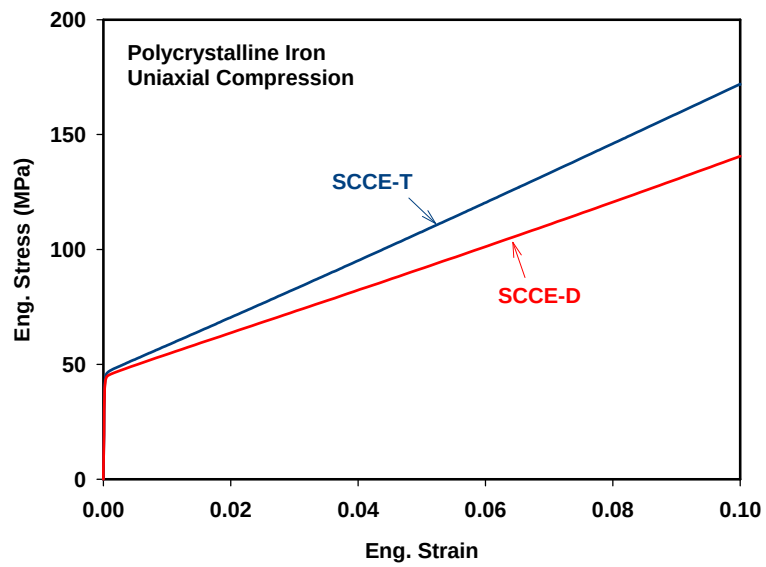


(b)

Figure 3.8: Simulated macroscopic engineering stress-strain curves for uniaxial tension for (a) polycrystal copper, and (b) polycrystal iron.



(a)



(b)

Figure 3.9: Simulated macroscopic engineering stress-strain curves for uniaxial compression for (a) polycrystal copper, and (b) polycrystal iron.

Figure 3.8 and Figure 3.9 show the simulated stress-strain curves for the SCCE-T model and the SCCE-D model for copper and iron polycrystals. The SCCE-T prediction for both copper and iron polycrystals shows higher flow stresses than SCCE-D predictions throughout the tested strain range. Recall that both constitutive models were fit to single crystals oriented for multiple slip. As Figure 3.3 and Figure 3.4 illustrate, the SCCE-T model over-predicts the single crystal tensile flow stress for single slip and cases having limited numbers of slip systems. This over-prediction is apparently important for large polycrystal arrays; that is, regions of single or limited numbers of slip systems must still be present, thereby influencing the observed macro behavior, for macroscopic applied strains up to 0.1.

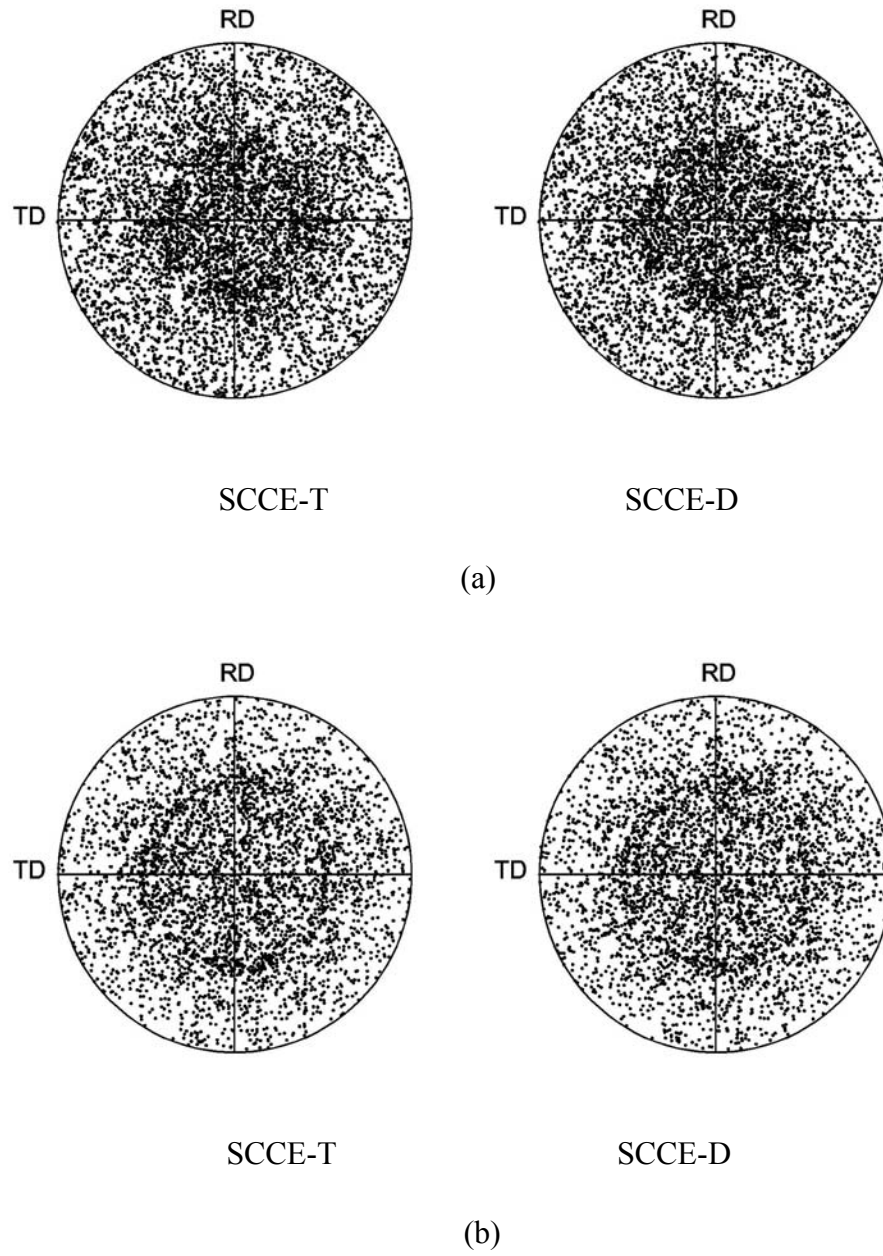
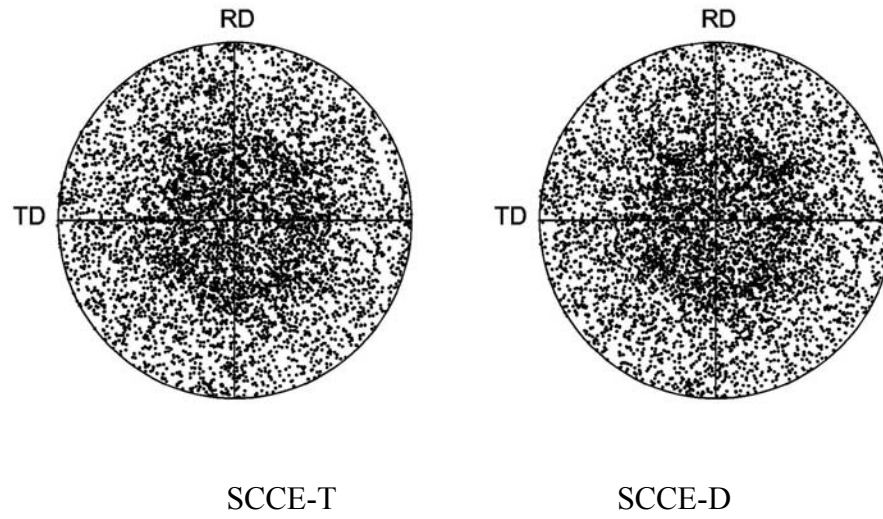
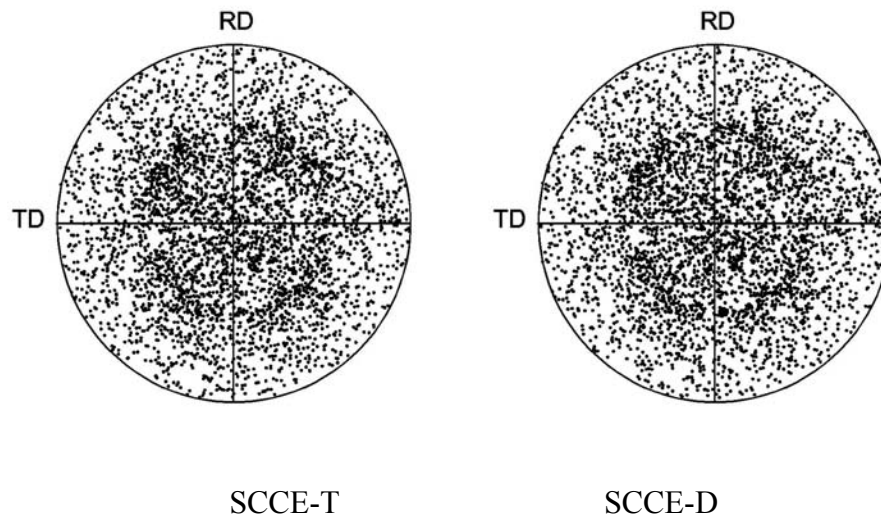


Figure 3.10: Equal area projection pole figures after 50% tension; (a) $\{110\}$ pole figure for copper, and (b) $\{111\}$ pole figure for iron.



(a)



(b)

Figure 3.11: Equal area projection pole figures after 50% compression; (a) $\{110\}$ pole figure for copper, and (b) $\{111\}$ pole figure for iron.

Figure 3.10 and Figure 3.11 shows predicted texture evolution for uniaxial tension and compression, respectively. Each pole figure is chosen to represent the major texture component in simple tension and compression for FCC and BCC, respectively. Simulated textures for both models show that the texture evolution in polycrystalline material has little sensitivity to the single crystal constitutive equations for both tension and compression.

3.7 Role of q_{lat}/q_{self} in SCCE-T

As noted above, a fixed value of $q_{lat}/q_{self}=1.4$ within the SCCE-T approach has been used with success for texture calculations in the literature and it is this implementation that has been assessed in the current work. In order to illuminate the role of q_{lat}/q_{self} in SCCE-T, a few additional fits and simulations were performed for copper single crystals. First, modified SCCE-T's were fit using alternate values of $q_{lat}/q_{self} = 1.0, 1.2, 1.4$ (standard value), $2.0, 3.0$, and 50 . The standard errors of fit for $[001]$ tension were identical (0.67 MPa) for all tested values except those for $q_{lat}/q_{self}=3.0$ and 50 which were larger (0.95 and 2.23 MPa, respectively). For fits to $[-123]$ tension, the standard error of fit for $q_{lat}/q_{self}=1.4$ was the minimum (2.1 MPa). Therefore, the best fits of SCCE-T with an arbitrarily adjustable value of q_{lat}/q_{self} gave the same “best” value as used above (and as endorsed by the literature). It should be noted that the modified SCCE-T used 5 adjustable parameters as compared with the 3 for SCCE-D, thus making the comparison increasingly biased in favor of SCCE-T.

As an extension of these tests, the various constitutive models (i.e. best-fit parameters for each choice of q_{lat}/q_{self}) were then used to simulate tension tests carried out in the direction not used for fitting. The standard deviations for [-123] tensile tests simulated using the modified SCCE-T's were 20 to 68 MPa (160-540%), as compared with 10 MPa for SCCE-D (80%). The standard deviations for [001] tensile tests simulated using the modified SCCE-T's were 45 to 64 MPa (60-85%), as compared with 38 MPa for SCCE-D (50%). Thus, even using the more flexible SCCE-T with arbitrarily adjustable q_{lat}/q_{self} (5 parameters) over a wide range of values did not match the accuracy of the fit or predictions obtained with the proposed SCCE-D (3 parameters).

3.8 Conclusions

The following conclusions apply to comparisons of new Single Crystal Constitutive Equations based on Dislocation Density (SCCE-D) and standard Single Crystal Constitutive Equations for Texture Analysis (SCCE-T):

1) SCCE-D reproduce flow curves for single slip and multi slip adequately in FCC and BCC single crystals. SCCE-D have better accuracy than SCCE-T while using smaller number of adjustable parameters. The average standard deviation predicted by SCCE-D is 14 MPa while that for the SCCE-T is 31 MPa.

2) SCCE-T, which are usually back-fitted from polycrystal flow curves, do not adequately represent orientation - dependent single crystal behavior. The discrepancy may arise from neglecting the effect of grain boundaries, grain size and relative misorientations between grains.

3) Polycrystal simulations using SCCE-T fit to multiple slip single crystal data predict higher flow stresses than SCCE-D, correlated with the high flow stresses predicted by the former for single crystals oriented for limited slip system activation. This correlation implies that there may exist significant regions of limited slip activation in polycrystals, contrary to the usual assumption.

4) Texture evolution has little sensitivity to the type of constitutive equations. Simulated textures for SCCE-T and SCCE-D for FCC and BCC polycrystals are similar, while the simulated macroscopic stress-strain responses differ.

4. TWO-SCALE MODEL

Note: Chapter 4 is presented in the format of a peer-reviewed paper that is being prepared for submission to the International Journal of Plasticity.

4.1 Abstract

Modeling of the strengthening effect of grain boundaries (Hall-Petch effect) in metallic polycrystals in a physically consistent way and without invoking arbitrary length scales is a long-standing, unsolved problem. A two-scale method to treat the interactions of large numbers of dislocations with grain boundaries predictively has been developed, implemented, and tested. At the first scale, a standard grain-scale simulation (GSS) based on a finite element formulation makes use of recently proposed single-crystal constitutive equations (“SCCE-D”) to determine local stresses, strains, and slip magnitudes. At the second scale, a novel meso-scale simulation (MSS) redistributes the mobile part of the dislocation density within grains consistent with the plastic strain, computes the associated inter-dislocation back stress, and enforces slip transmission criteria at grain boundaries. Compared with a standard finite element simulation, the two-scale model required only 5% more CPU time, making it suitable for practical material design.

Verification tests were conducted:

- 1) For suitable boundary conditions, the two-scale method reproduced expected dislocation densities in single pileups.

2) Tensile tests of iron multi-crystal specimens with 9 to 39 grains were conducted and simulated using the two-scale model and four traditional models for comparison: finite element model (GSS only) with either SCCE-D or PAN constitutive models (PAN=Peirce, Asaro, Needleman) (Peirce et al. 1982; Asaro and Needleman, 1985), and Taylor model (Taylor, 1938) with either SCCE-D or PAN constitutive models. The two-scale approach with SCCE-D predicted flow stresses 2-4 times more accurately than the other method. None of the other methods predicted the Hall-Petch.

3) Two-scale simulations of 2D and 3D arrays of regular grains predicted Hall-Petch slopes for iron of $1.2 \pm 0.3 \text{ MN/m}^{3/2}$ and $1.5 \pm 0.3 \text{ MN/m}^{3/2}$, in agreements with a measured slope of $0.9 \pm 0.1 \text{ MN/m}^{3/2}$.

4) The lattice curvature of a deformed Fe-3% Si columnar multicrystal was predicted and measured. The maximum lattice curvature (near some grain boundaries) agrees within the experimental scatter.

4.2 Introduction

Significant advances have been made in understanding the plastic behavior of metals at two extreme length scales. At the atomic/single dislocation level, molecular dynamics reveal how single dislocations move, how they are generated and annihilated in small reference volumes on the order of thousands of atoms (Kubin et al., 1992; Zbib et al., 1998; Schwarz, 1999), or in smaller volume elements to represent a single dislocation (Acharya, 2001). Such methods apply to nano-structures but are difficult to scale up to

structures of multiple-micron size, such as are encountered in the grain sizes of typical structural metals and alloys.

At the other extreme, macroscopic texture analysis of polycrystals predicts the plastic anisotropy of textured sheets, particularly for FCC single-phase metals (Asaro and Needleman, 1985; Mathur and Dawson, 1989). As illustrated in Figure 4.1, texture analysis treats each crystal as a unitary, homogeneous body; it ignores either equilibrium or compatibility between grains or combinations of these. Such methods show no effect of grain size on the material strength, i.e. the Hall-Petch effect (Sachs, 1928; Taylor, 1934; Kröner, 1961; Hill and Rice, 1972; Asaro, 1983; Canova et al., 1985; Molinari et al., 1987; Parks and Ahzi, 1990). The texture approach neglects the roles of grain boundaries as stress concentrators, and as obstacles to, or generators of, slip. Examples of simple inter-grain interaction models are Taylor (equi-strain)(Taylor, 1934), Sachs (equi-stress) (Sachs, 1928; Parks and Ahzi, 1990), relaxed constraint (mixed stress/strain) (Canova et al., 1985), and self-consistent (grain within averaged grain) models (Kröner, 1961; Molinari et al., 1987). Continuum-based polycrystal simulations have been reported widely (Follansbee and Kocks, 1988; Mathur and Dawson, 1989; Bronkhorst et al., 1992; Beaudoin et al., 1994; Kothari and Anand, 1998; Kumar and Dawson, 1998; Nemat-Nasser et al., 1998) but do not predict polycrystalline strength, strain hardening, or the role of grain boundary character (Cuitiño and Ortiz, 1992). A computationally efficient, physically realistic method for treating the interactions of large numbers of dislocations interacting with grain boundaries has been elusive. There is some guidance at the single-dislocation level on how boundaries operate as obstacles to slip transmission (Livingston

and Chalmers, 1957; Shen et al., 1986, 1988) to induce “plastic incompatibility”, but little insight regarding the interaction of statistical numbers of dislocations. Conversely, the stresses arising from *elastic* incompatibility are readily analyzed by standard finite element models of polycrystals. The grain boundaries are modeled as welded interfaces with compatible total strains enforced across the interface. Such elastic methods have been used successfully to predict spatial distributions of active slip systems in agreement with experiment without considering the complication of slip transmission (Yao and Wagoner, 1993; Wagoner et al., 1998).

Polycrystal simulations at either atomic or grain scales tax current computer capabilities, even using today’s massively parallel machines. A multi-scale model to link large numbers of dislocations within a grain, and for hundreds of grains would be of great interest if computationally feasible. One such approach involves the modification of continuum constitutive equations via the strain gradient to simulate the role of dislocations with arbitrary length scale (Fleck and Hutchinson, 1994; Fleck et al., 1997; Gurtin, 2000, 2002). While convenient, such methods involve arbitrary length scales and do not appear to capture the essence of the physics (Needleman and van der Giessen, 2001). They ignore the crystal size and grain boundary structures as well as discrete dislocation dynamics. Other approaches divide grains into core and boundary regions, thus introducing an arbitrary length scale (Evers et al., 2002), or dislocation populations into statistical and polar populations (Arsenlis et al., 2004).

The proposed two-scale predictive technique seeks as the highest priorities: 1) introduction of no arbitrary or unknown length scales, 2) sufficient computational

efficiency to treat 100 grains or more, and 3) order-of magnitude accuracy in prediction of the Hall-Petch effect.

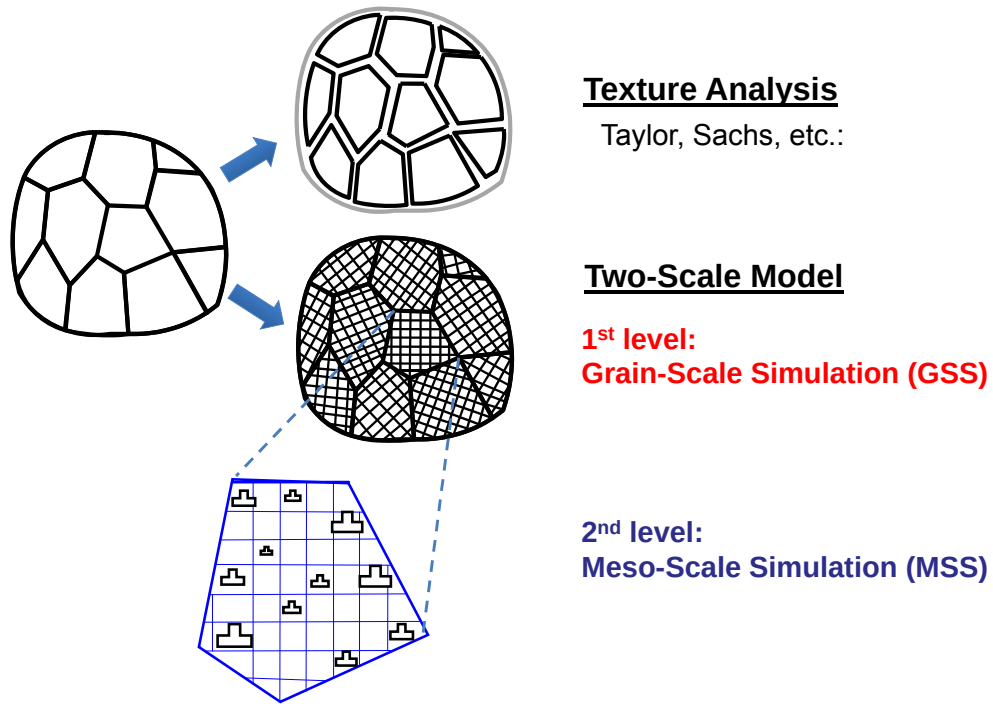


Figure 4.1: Schematic view of typical texture analysis and crystal plasticity-finite element analysis (CP-FEA) based two-scale simulation procedure.

4.3 Simulation Procedures

A two-stage simulation procedure was developed to simulate the interactions of large numbers of dislocations with grain boundaries for materials with grain sizes larger than a micron, thus avoiding nano-scale effects and the need to address individual, discrete dislocations. The intent is to be broadly predictive rather than merely descriptive;

therefore the number of undetermined, arbitrary parameters was minimized for the initial treatment presented here.

The core of the proposed method relies on a standard finite element discretization of a polycrystal with numerous elements per grain, as shown in Figure 4.1. The Grain-Scale Simulation (GSS) follows well-established developments appearing in the literature (Peirce et al., 1983; Asaro and Needleman, 1985; Beaudoin et al., 1994; Sarma and Dawson, 1996; Dawson et al., 2002; Lee et al., 2009). Mechanical equilibrium is enforced while maintaining material compatibility in a finite element sense (i.e. at the nodes). The GSS computes inhomogeneous stress, strain, and slip activity, and, as inferred from slip magnitudes using established principles, the local generation of dislocation density on each slip system in each element. (The three constants relating dislocation density to strain, i.e. strain hardening, are the only undetermined constants in the formulation. They are readily fit from a measured tensile stress-strain curve.)

The novel Meso-Scale Simulation (MSS) redistributes the mobile dislocation content for each slip system, as represented by a superdislocation at the center of each finite element. The mobile part of dislocation density is redistributed in order to accommodate the plastic strain. The redistribution of mobile dislocation content modifies the flow stress and back stress in each element according to Orowan's equation and elastic inter-dislocation interactions, respectively, which in turn alters the GSS results at the next time step. Figure 4.2 shows the flow chart of the two-scale modeling scheme.

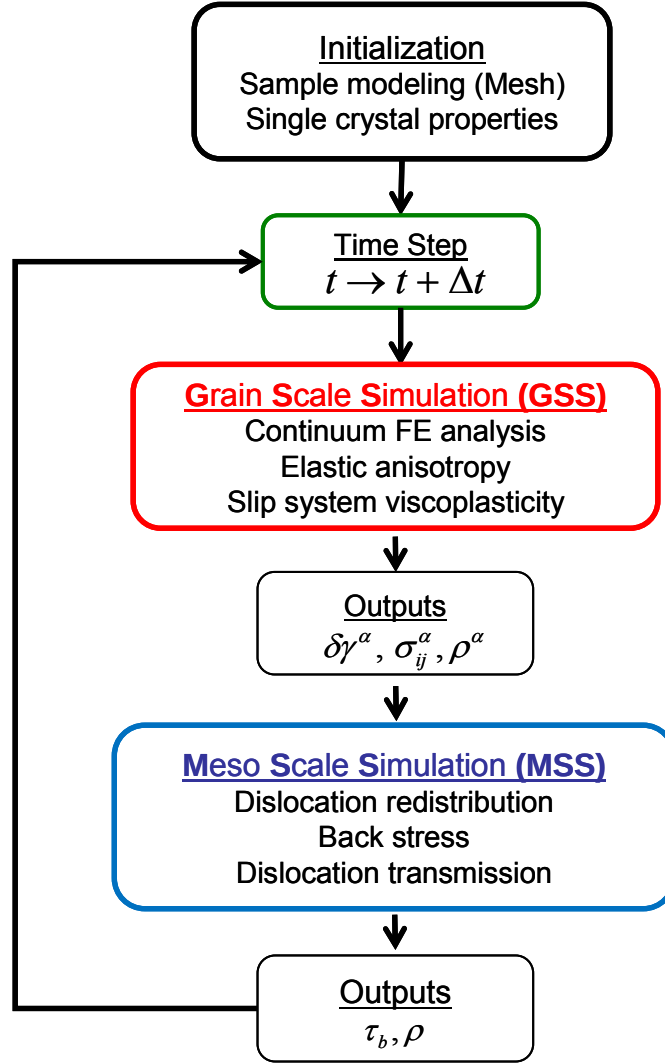


Figure 4.2: The flow chart of two-scale modeling scheme. An explicit procedure between the two scales is shown.

There are many choices among assumptions and parameters that must be made for a practical first implementation. The basic assumptions listed below were selected to minimize unknown parameters, as follows:

- 1) All plastic deformation occurs only by slip on fixed slip systems; climb, twinning, grain boundary sliding, cross-slip and other mechanisms are ignored.
- 2) The entire dislocation density has edge character such that the line direction is uniquely determined by slip plane and Burger's vector.
- 3) The dislocation density on a single slip system in a finite element can be lumped into a single superdislocation.
- 4) For purposes of computing a back stress, dislocations interact only with other dislocations within the same slip system in a single grain. These interactions are approximated using isotropic elasticity.
- 5) Elastic image effects between the dislocation content and the boundaries are ignored, except as lumped into a grain boundary obstacle stress. The obstacle stress is the sole effect arising from plastic incompatibility.

4.3.1 Grain-Scale Simulation (GSS)

The GSS procedure follows well-established continuum mechanical principles in the literature (Lee, 1969; Rice, 1971; Hill and Rice, 1972; Asaro, 1979; Peirce et al., 1982). It is based on the classical crystal plasticity framework that the total deformation gradient at a material point within a crystal is described by a multiplicative decomposition (Lee, 1969).

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^p \quad (4.1)$$

The velocity gradient, $\bar{\mathbf{L}}^p$, is represented in the intermediate configuration in terms of shear rates as follows (Rice, 1971; Asaro, 1983):

$$\bar{\mathbf{L}}^p = \dot{\mathbf{F}}^p \mathbf{F}^{p-1} = \sum_{\alpha=1}^{NS} \dot{\gamma}^{(\alpha)} \mathbf{s}_0^{(\alpha)} \otimes \mathbf{n}_0^{(\alpha)} \quad (4.2)$$

For a strain-rate-dependent crystal model, the crystalline visco-plastic shear rate of the power-law form defined on the α -th slip system may be written as (Hutchinson, 1976; Peirce et al., 1982):

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}_0 \left(\frac{\tau^{(\alpha)}}{g^{(\alpha)}} \right)^{\frac{1}{m}} \text{sign}(\tau^{(\alpha)}) \quad (4.3)$$

where $\dot{\gamma}_0$ is a reference shear rate, $\tau^{(\alpha)}$ and $g^{(\alpha)}$ are the resolved shear stress and the slip resistance of α -th slip system, respectively and m is the rate sensitivity exponent. Reference shearing rate and rate sensitivity, 0.001 s^{-1} and 0.012 respectively, were adopted from the literature (Bronkhorst et al., 1992; Kalidindi et al., 1992).

To this point, the constitutive equations mirror those used routinely for texture analysis and appearing in the literature. Those standard forms are referred to as the PAN constitutive model (Peirce, Asaro, Needleman) (Peirce et al., 1982). The evolution of $g^{(\alpha)}$ was formulated using novel single crystal constitutive equations based on dislocation density herein referred to briefly as SCCE-D (Lee et al., 2009). These constitutive equations were shown to represent single-crystal behavior accurately for both FCC and BCC metals (Lee et al., 2009). The remainder of this section outlines the development of the SCCE-D briefly, with reference to the original publication for details and testing against measured single crystal behavior and PAN model predictions (Lee et al., 2009).

The dislocation density for SCCE-D in each slip system α for each element, $\rho^{(\alpha)}$, is computed explicitly. For the first time step, a homogeneous initial dislocation density, ρ_0 , corresponding to the yield stress is adopted as using the standard relationship (Taylor, 1934):

$$\sigma_y = \alpha \mu b \sqrt{\rho_0} \quad (4.4)$$

where μ is the shear modulus, b is the Burgers vector, and the parameter α is a constant that depends on the arrangement of dislocations (Widersich, 1964; Olivares and Sevillano, 1987; Schafler et al., 2005). The parameter α has been measured and theoretically calculated for various materials and is generally reported to be in the range 0.3-0.6 (Widersich, 1964; Schoeck and Friedman, 1972; Kassner, 1990; Orlová, 2004; Schafler et al., 2005; Gubicza et al., 2009). Here, a value of $\alpha = 0.4$ was selected as a reasonable intermediate value. The slip resistance, $g^{(\alpha)}$, is expressed as follows:

$$g^{(\alpha)} = \alpha \mu b \sqrt{\sum_{\beta=1}^n h'_{\alpha\beta} \rho^{(\beta)}} \quad (4.5)$$

where $\rho^{(\beta)}$ is the dislocation density for slip system β , and $h'_{\alpha\beta} = \mathbf{n}_0^{(\alpha)} \cdot \boldsymbol{\xi}_0^{(\beta)}$ are interaction cosines where $\boldsymbol{\xi}_0^{(\beta)}$ is the dislocation line vector for slip system β . To complete the constitutive equations for a single crystal, a standard phenomenological model of dislocation evolution is adopted (Kocks, 1976).

$$\dot{\rho}^{(\alpha)} = \frac{1}{b} \left(\frac{\sqrt{\sum_{\beta}^{NS} \rho^{(\beta)}}}{k_a} - k_b \rho^{(\alpha)} \right) \cdot \left(\dot{\gamma}^{(\alpha)} \right) \quad (4.6)$$

where, k_a and k_b are material parameters representing generation and annihilation of dislocations, respectively. There are thus three fitting parameters for SCCE-D; ρ_0 , k_a and k_b , whereas the conventional PAN model requires four or more adjustable parameters.

4.3.2 Meso-Scale Simulation (MSS)

The novel MSS utilizes the slip activity and stress computed in each element from the GSS and redistributes the mobile part of dislocation densities thus changing slip resistance at the next time step in the GSS. Dislocations interact elastically with the stress field from the other dislocations and the external stress field. Thus, for n discrete dislocations interacting, n^2 interactions would need to be computed to obtain the equilibrated spatial distribution of discrete dislocations. A typical range of dislocation densities is $10^{10} - 10^{16} \text{ m}^{-2}$ (Dieter, 1976). It is the size of this problem that puts the direct treatment of individual dislocation in real materials beyond any realistic estimate computational abilities.

Discrete dislocations can be treated in a computationally more tractable way by lumping them within an element to form a superdislocation. A physical pileup of n discrete dislocations of Burgers vector $\mathbf{b}$ can be transformed mathematically into a statically equivalent one at large distances by lumping the dislocation content within a

volume element into a single “superdislocation” with Burgers vector $\mathbf{B}=n\mathbf{b}$, where n is the number of individual dislocation that were lumped. For each slip system type, the number of interacting superdislocations is equal to the number of finite elements in a grain (N_E). Using this method, the positions of each discrete dislocation is lost, but the dislocation density within a volume corresponding to the element size is obtained.

A superdislocation for the α -th slip system has strength $B^{(\alpha)}$, equal to the discrete dislocation content in that volume on that slip system, as follows:

$$B^{(\alpha)} = n^{(\alpha)}b^{(\alpha)} = \frac{\rho^{(\alpha)}V^{(\alpha)}b^{(\alpha)}}{L^{(\alpha)}} \quad (4.7)$$

where $n^{(\alpha)}$ is the number of discrete dislocations of Burgers vector $b^{(\alpha)}$ on the α -th slip system and $V^{(\alpha)}$ and $L^{(\alpha)}$ are the volume and characteristic length (in the direction parallel to dislocation line vector) of the element which are stereologically equivalent values for the slip plane orientation. The characteristic length $L^{(\alpha)}$ is determined from a line parallel to the dislocation line passing through the center of the element and terminating at the element boundaries. The boundaries of the element are readily determined using the nature of the isoparametric finite elements employed (ABAQUS element C3D8).

The elastic force per unit length operating on the i -th edge superdislocation segments caused by the stress field of j -th superdislocation with parallel Burgers vectors of magnitude B_1 and B_2 in an isotropic elastic medium is as follows (Hirth and Lothe, 1969):

$$F_{ij} = \frac{F_{glide}}{dl_i} = \frac{\mu B_i B_j}{4\pi(1-\nu)} \frac{1}{(x_2 - x_1)} \left[\frac{r_1}{r_1^2 + r_2^2} \right] [g_{11} + g_{22} - g_{12} - g_{21}] \quad (4.8)$$

where

$$g_{ij} = \frac{r_2^2}{R_{ij}} + (x_j + R_{ij}) \left(\frac{r_1^2 - r_2^2}{r_1^2 + r_2^2} \right)$$

$$R_{ij} = \sqrt{r_1^2 + r_2^2 + (y_i - x_j)^2} \quad i, j = 1, 2$$

Here, r_1 , r_2 and r_3 are components of position vector R_{ij} as shown in Figure 4.3.

Variables x_i and y_i denote relative termini of two dislocations in having line direction,

$$\hat{\xi}_i.$$

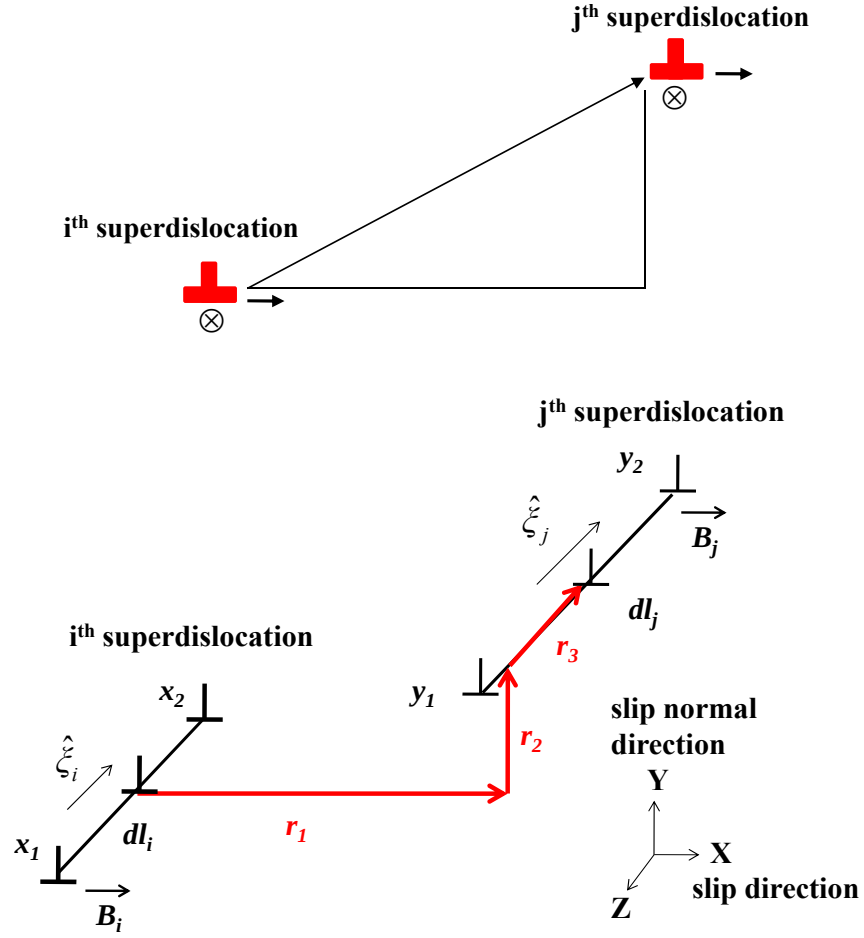


Figure 4.3: The coordinate system for expressing the interaction force of superdislocation segment j on superdislocation segment i having parallel line directions and Burgers vectors.

Grain boundaries act as barriers to dislocation motion at low temperature (Hirth and Lothe, 1969). The critical obstacle strength, τ_{obs} , can be defined as the minimum stress operating on a single dislocation near a boundary to activate transmission through or into the boundary (or to nucleate a dislocation in or on the other side of the boundary).

τ_{obs} may depend on the orientation of the grain boundary (Shen et al., 1986, 1988), the misorientation of the grains (Livingston and Chalmers, 1957; Shen et al., 1986; De Messemaeker and Van Humbeek, 2004; Anderson and Shen, 2006), the slip system geometry and stacking fault energies of the slip plane adjacent to the boundary (Anderson and Shen, 2006) .

Livingston and Chalmers (Livingston and Chalmers, 1957) first proposed a slip criterion considering a geometry of slip systems in two adjacent grains and defined slip transmissivity, N , as follows:

$$N = (e_1 \cdot e_i)(g_1 \cdot g_i) + (e_1 \cdot g_i)(g_1 \cdot e_i) \quad (4.9)$$

where e_1 and g_1 are the slip plane normal and slip direction of the pileup dislocations in the incoming plane, and e_i and g_i are the corresponding quantities in the adjacent grain.

This criterion predicts that dislocations are most easily transmitted through the grain boundary if the slip transmissivity, N , has a maximum value. This criterion, however, does not consider the orientation of the grain boundary and failed to predict the emitted slip systems (Shen et al., 1986).

Shen et al. (Shen et al., 1986) proposed series of alternative slip transmission criteria (SWC criteria) that consider grain boundary orientations, applied stress or both. In particular, SWC 2nd criterion (Shen et al., 1986) considers boundary orientation and predicted emitted slip system relatively well without involving complicated calculation of local stresses. SWC 2nd criterion is as follows:

$$N = (L_1 \cdot L_i) \times (g_1 \cdot g_i) \quad (4.10)$$

where L_1 and L_i are the intersection lines between grain boundary and slip planes and g_1 and g_i are the slip directions of incoming and emitted dislocations, respectively. The transmissivity ranges from 0 to 1 representing maximum and minimum obstacle stress, respectively.

The obstacle stress imposed by the grain boundary for a given combination of incoming and outgoing dislocations can be expressed as follows:

$$\tau_{obs} = (1 - N)\tau^* \quad (4.11)$$

where τ^* is the maximum grain boundary strength. Shen et al. (Shen et al., 1986) calculated lower-bound obstacle strength of 280-870 MPa for four grain boundaries from pileup configuration as listed in Table 4.1. τ^* can be estimated to be around 1.1 GPa, approximately 5 times the macroscopic yield stress (210MPa for bulk yield stress of annealed 304 stainless steel). For a given slip system on the incoming side of the boundary, the minimum value of τ_{obs} is chosen from the values computed for all the allowed outgoing slip systems.

Boundary	τ_{obs} (MPa)	Transmissivity (N)
1	380	0.588
2	280	0.915
3	870	0.472
4	400	0.785

Table 4.1: Measured obstacle strength for 304 stainless steel (Shen et al., 1986) and calculated transmissivity for four grain boundaries .

MSS redistributes the required number of mobile dislocations among adjacent elements to attain consistency with the plastic strain increment demanded by the GSS, through Orowan's equation (Orowan, 1940).

$$d\gamma = \rho_m b \cdot dx \quad (4.12)$$

where $d\gamma$ is the increment of plastic strain, ρ_m is the mobile dislocation density, b is the Burgers vector, and dx is the characteristic length that dislocations moved along the slip plane. In an FE sense, the net dislocation density that passes through each element required to accommodate the plastic strain increment of the element obtained from the GSS can be represented as:

$$d\rho_{pass} = \frac{1}{bl} d\gamma \quad (4.13)$$

Here, $d\rho_{pass}$ is the dislocation density that passed through the element and l is the length of the element parallel to the slip plane. In order to obtain the net mobile dislocation density in each element, the net flux of dislocation density between two elements is obtained, as illustrated in Figure 4.4:

$$d\rho_i = d\rho_i^{in} - d\rho_i^{out} \quad (4.14)$$

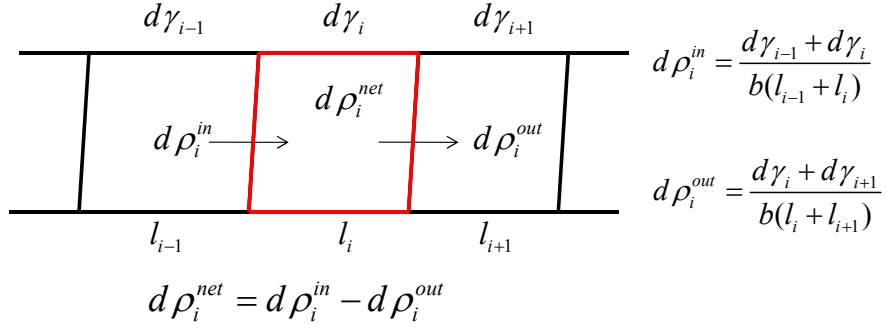


Figure 4.4: Redistribution of the mobile dislocation density from one element to adjacent elements.

After mobile dislocations are redistributed, the back stress is obtained by considering dislocation interactions within the same slip plane. In contrast to back stress formulations based on statistical models (Groma, 1997; Yefimov and Van der Giessen, 2004) or strain gradient approaches (Evers et al., 2004), the two-scale model keeps track of dislocation densities (or, equivalently, the number of dislocations) for each element and slip system so that the back stress can be obtained explicitly without involving an arbitrary length scale. The back stress on the i -th dislocation can be represented as follows:

$$\tau_i^b = \frac{1}{b_i} \sum_{\substack{j=1 \\ j \neq i}}^N F_{ij} \quad (4.15)$$

The back stress and obstacle strength imposed by the grain boundary are incorporated in the slip system constitutive response (equation (4.3)) as follows:

For non-grain boundary elements,

$$\dot{\gamma} = \dot{\gamma}_0 \left(\frac{\tau_{eff}}{g} \right)^{1/m} \text{sign}(\tau_{eff}) \quad (4.16)$$

where $\tau_{eff} = (\tau - \tau^b)$, and for grain boundary elements,

$$\tau_{eff} > \tau_{obs} \quad \dot{\gamma} = \dot{\gamma}_0 \left(\frac{\tau_{eff} - \tau'_{obs}}{g} \right)^{1/m} \text{sign}(\tau_{eff} - \tau_{obs}) \quad (4.17)$$

$$\tau_{eff} \leq \tau_{obs} \quad \dot{\gamma} = 0 \quad (4.18)$$

where $\tau'_{obs} = (1 - N)\tau^*$. Note that the obstacle stress is the stress that opposes the slip for the grain boundary elements and cannot exceed τ_{eff} . That is, it functions like a frictional stress and only attains its maximum value when dislocations are being transmitted.

4.3.3 1D stressed pileup

A simple set of parametric test is conducted using the two-scale model to see how dislocations are redistributed in 1D array of elements upon constant applied stress. Constant shear stress of 110 MPa is imposed on 1D array of elements (20 solid elements) with the dimension of $1\text{mm} \times 20\mu\text{m} \times 20\mu\text{m}$. Isotropic elasticity is used to calculate the interaction between dislocations and initial dislocation density is assumed to be zero. One end of the 1D mesh is assumed to be the grain boundary having τ^* of 375 MPa, while the other end is regarded as the free surface. For simplicity, only two slip systems are considered; one that is activated for the slip and the other that only act as forest dislocations. Constant slip resistance of 10 MPa and reference shear rate of 0.001 s^{-1} are adopted. The rate sensitivity exponent, m , is chosen to be 1 to prevent rapid increase of

the strain rate. Constant shear stress of 110 MPa to promote the accumulation of dislocations against the grain boundary is imposed until the tip stress at the head of the pileup reached the critical obstacle stress. The total number of dislocations within the specimen was 1.2×10^4 before the dislocations started to transmit through the grain boundary.

The identical problem is then solved by using two other methods: (a) analytical solution based on continuous pileup, and (b) force equilibrium model using finite element discretization into superdislocations. The analytical solution for the single pileup against an obstacle by a shear stress σ is available in Hirth and Lothe (Hirth and Lothe, 1969):

$$n(x) = \frac{2(1-\nu)\sigma}{\mu b} \left(\frac{l-x}{x} \right)^{\frac{1}{2}} \quad (4.19)$$

where μ is the shear modulus, ν is the Poisson's ratio and b is the Burger's vector, respectively. Here, $n(x)dx$ is the number of dislocations between x and $x+dx$. The pileup length, l , is obtained from equation (2.6) using the total number of dislocations obtained from the two-scale model.

Since dislocations experience a net force from other dislocations and applied stress field, equilibrium requires that the sum of forces on any dislocation is zero. Hence, using the superdislocation concept, and ignoring lattice friction stresses or other local constraints to dislocation motion, the defect equilibrium equation condition may be expressed as follows:

$$\mathbf{F}_i = \sum_j \mathbf{F}_{ij} + (\mathbf{B}_i \cdot \boldsymbol{\sigma}) \times \hat{\boldsymbol{\xi}}_i = 0 \quad (4.20)$$

where $\mathbf{F}_{ij}$ represents the elastic force per unit length operating on the i -th superdislocation caused by the stress field of j -th superdislocation (equation (4.8)) and the second term is the well-known Peach-Koehler formula (Hirth and Lothe, 1969) that represents a force exerted by the applied stress tensor on superdislocation i having Burgers vector $\mathbf{B}_i$ and line direction $\hat{\xi}_i$. Solution to equation (4.20) provides Burgers vector of the superdislocation, $\mathbf{B}_i$, located at the center of each element.

Redistribution of dislocations based on the force equilibrium between dislocations and applied stress can be generalized to an alternative MSS scheme (dislocation pileup model). This approach reproduces analytical solutions of 1D dislocation pileups and can be extended to 2D pileups as shown in Appendix A. However, this model neglects the relationship between the plastic strain and the required movement of dislocation densities to attain that strain. Predicted Hall-Petch slopes using this model were too small by a factor of ~ 30 . Detailed procedure for this approach is more fully described in Appendix A.

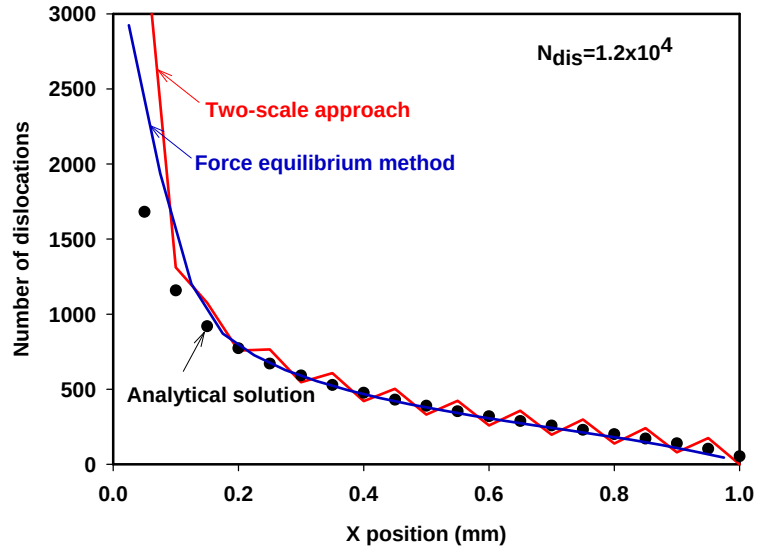


Figure 4.5: Calculated number of dislocations along the elements using the analytical solution, force equilibrium method and the two-scale approach.

Figure 4.5 compares calculated dislocation distributions using three approaches. Three models showed similar pileup profiles in this specific simplified case. It should be noted that analytical solution and force equilibrium method require only the total number of dislocations and applied stress to obtain the spatial distribution of dislocations. On the other hand, solution for the two-scale model depends on both the stress and strain of each element.

4.4 Experimental Procedures

Minimum alloy steel and Fe-3% Si tensile samples are prepared to compare the measured stress-strain response and lattice curvatures to the two-scale simulation.

Minimum alloy steel (essentially pure iron with Mn for control of hot shortness) provided by Severstal N/A has advantages that a wide range of grain sizes is obtainable, it has good ductility, and, a large Hall-Petch slope was measured as shown in Figure 4.6.

Coarse-grained Fe-3% Si tensile sample which has only single grain through the thickness is fabricated and provided by AK steel. Material parameters for single crystal constitutive equations for Fe-3% Si are reasonably well established (Wagoner et al., 1998) and has an advantage that a wide range of grain sizes, from 10 μm to 30 mm, can be readily obtained but the sample with grains larger than 2mm showed poor ductility (<7%). The chemical composition of minimum alloy steel and Fe-3% Si is listed Table 4.2.

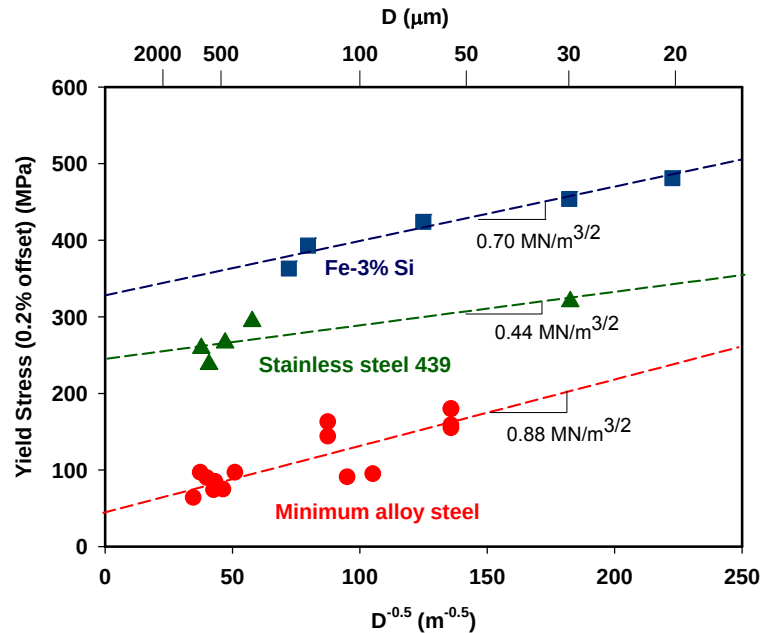


Figure 4.6: Measured Hall-Petch slope for Fe-3% Si, Stainless steel 439 and minimum alloy steel.

	Minimum alloy steel	Fe- 3% Si
C	0.001	0.004
Mn	0.13	0.09
P	0.006	0.01
S	0.005	0.025
Si	0.004	2.95
Cu	0.023	0.02
Ni	0.007	0.01
Cr	0.014	-
Mo	0.003	-
Sn	0.002	-
Al	0.038	0.03
Ti	0.001	-
N	0.003	0.015
Nb	0.001	-

Table 4.2: Chemical composition of minimum alloy steel and Fe-3% Si.

4.4.1 Minimum alloy steel tensile specimen

As provided, the initial grain size of minimum alloy steel was 60 μm . Heat treatment was carried out to obtain three other grain sizes. Grain sizes of 140 μm and 620 μm was obtained by the heat treatment at 1000 $^{\circ}\text{C}$ and 1250 $^{\circ}\text{C}$ for 5 hours in a vacuum furnace, respectively. The largest grain size of 1350 μm was obtained by strain annealing (Keh, 1961); initially heat treated at 1000 $^{\circ}\text{C}$ for an hour in a vacuum furnace, strained to 2.5% and then reheated at 1250 $^{\circ}\text{C}$ for 10 hours. Strain annealed samples were water-jet machined to obtain six multi-crystal tensile samples having 9 to 39 grains in the reduced section. Three different specimen sizes were fabricated: as shown in Figure 4.7, the first two specimen types have reduced section width of 1mm and 2mm with the original sample thickness of 2.1 mm. The specimen type III has the same sample dimensions as

type II but rolled in the cold press to obtain the thickness of 0.4 mm (19% of original thickness).

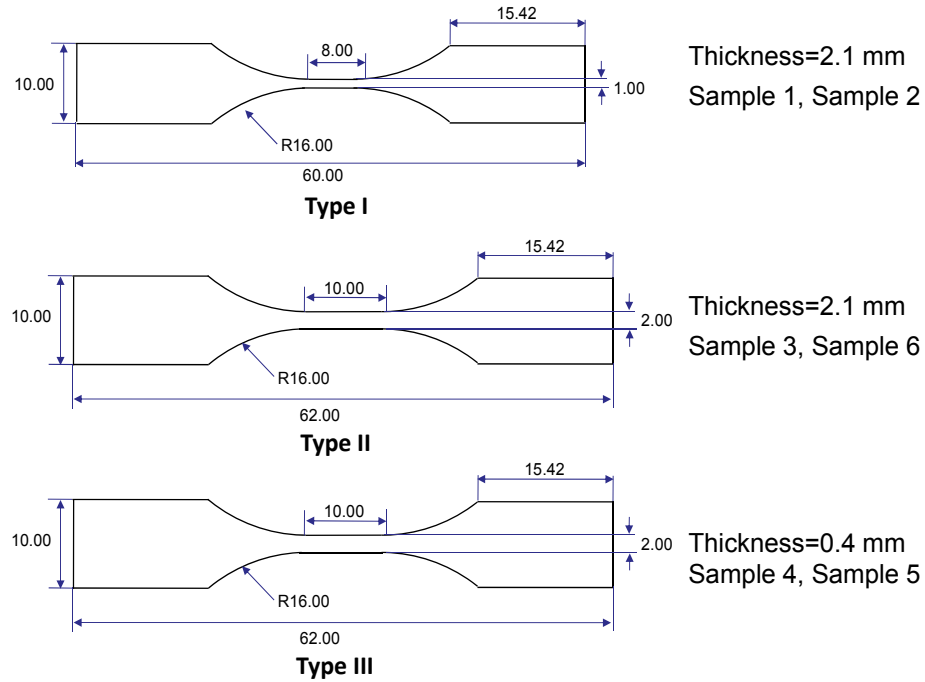


Figure 4.7: Dimensions of three different tensile sample types for multi-crystal minimum alloy steel (Unit: mm).

Grain orientations for each sample were then measured using OIM and a FEI-Philips XL-30 SFEG equipped with a DigiCam system. Figure 4.8 shows grain shapes within the entire reduced sections of six tensile specimens. Grain orientations corresponding to the grain numbers indicated in Figure 4.8 are listed in Appendix D.

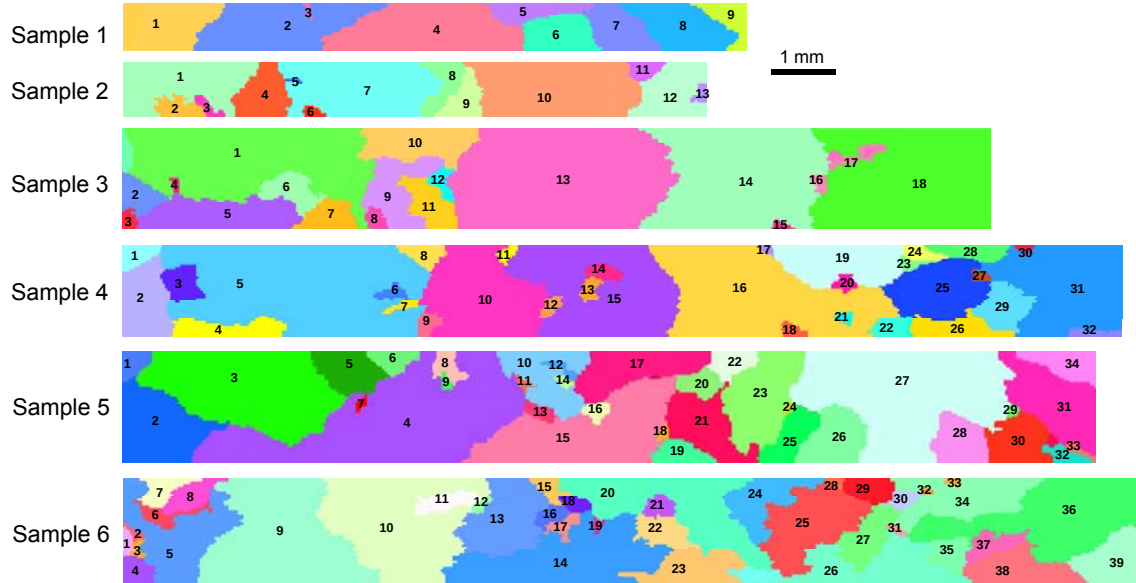


Figure 4.8: OIM grain map for reduced sections of six tensile specimens.

Uniaxial tensile tests were performed at a constant crosshead speed to obtain a nominal strain rate of $\sim 5 \times 10^{-4} \text{ s}^{-1}$ at room temperature using an MTS-810 tensing machine with 100 kN hydraulic grips. The extension of the reduced section was measured with a laser extensometer, Epsilon Tech Corp. LE-05. Figure 4.9 shows the stress-strain response of six tensile specimens.

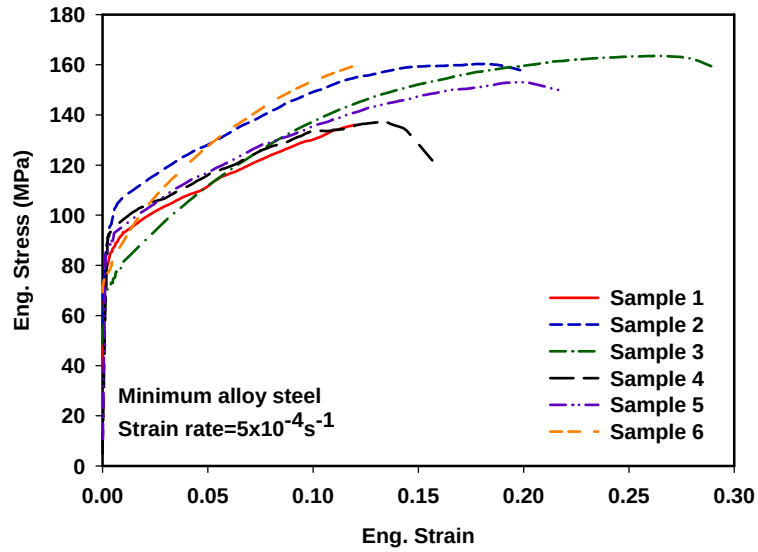


Figure 4.9: Measured engineering stress-strain response for 6 tensile samples.

4.4.2 Fe-3% Si tensile specimen

AK Steel has processed and provided the columnar Fe-3% Si in sheet form. The material is generally hot rolled, cold worked, annealed, decarburized, coated then box annealed. The thickness of sample is approximately 0.3mm and it is columnar-grained which has one grain through the thickness. Tensile specimens are water-jet fabricated to minimize local deformation near the cut surfaces, and at the same time minimizing temperature rise. Uniaxial tensile tests were performed at the strain rate of $1.25 \times 10^{-4} \text{ s}^{-1}$ using the Instron test frame up to 8% tensile strain with ASTM E8 standard specimens.

Crystallographic orientations and lattice curvature of grains in the gage region of Fe-3% Si tensile sample were measured using OIM before and after the deformation.

The primary objective of OIM analysis is to estimate the small changes in the orientation of the crystal lattice within the grain of same nominal orientation. This change has been reported to be associated with the pile-up of dislocation densities near the grain boundaries. The change in orientation with respect to the change in point of measurement is described by the lattice curvature tensor, κ_{ij} (Nye, 1953; Sun et al., 2000).

$$\kappa_{ij} = \frac{d\phi_i}{dx_j} \quad (4.21)$$

where, $d\phi_i$ is the change in orientation and dx_j is the change in position of the test point.

The diagonal components of κ_{ij} represent twisting of the lattice about the x_i axes, and the off-diagonal terms represent bending of the x_i plane, about the x_j direction. Under the assumption that the mean curvature $\bar{\kappa}$ associated with a specified grain boundary can be expressed as averaged value of six in-plane components (Adams and Field, 1992; Sun et al., 2000; El-Dasher et al., 2003).

$$\bar{\kappa} \cong \frac{1}{6} \sum_{i=1}^3 \sum_{j=1}^2 |\kappa_{ij}| = \frac{1}{6} \sum_{i=1}^3 \sum_{j=1}^2 \left| \frac{d\phi_i}{dx_j} \right| \quad (4.22)$$

4.5 Results

The two-scale simulation procedure was implemented into ABAQUS/ Standard (Hibbit, 2005) via user material subroutine UMAT. To assess the accuracy of the formulation, tensile tests of multicrystal specimens of minimum alloy steel and lattice curvature of Fe-3% Si alloy with simple two-dimensional columnar structure were

simulated and compared with that for the measured. Hardening behavior of multicrystal minimum alloy steel sample is also predicted using Taylor's iso-strain model (Taylor, 1938) and conventional PAN constitutive model (Peirce et al., 1982) to be compared with the two-scale model.

4.5.1 Prediction of Multi-Crystal Stress-Strain Response

The material constitutive response for the two-scale model, PAN model (Peirce et al., 1982), and Taylor's iso-strain model adopting SCCE-T and SCCE-D were fit to reproduce the measured stress-strain response of tensile sample 6, having the most number of grains (39). Bitmap data for each specimen's grain map from the OIM measurements was utilized to distinguish grains and a regular mesh with linear brick elements (C3D8) was superposed on the image using a total of 8671 elements. The size of the element was chosen to be smaller than the OIM measurement step size. Detailed procedures used to obtain the best-fit parameters and the effect of each variable were described previously (Lee et al., 2009). Anisotropic elasticity constants and shear modulus for minimum alloy steel used for the simulation are shown in Table 4.3.

μ	C_{11}	C_{12}	C_{44}
80	242	150	112

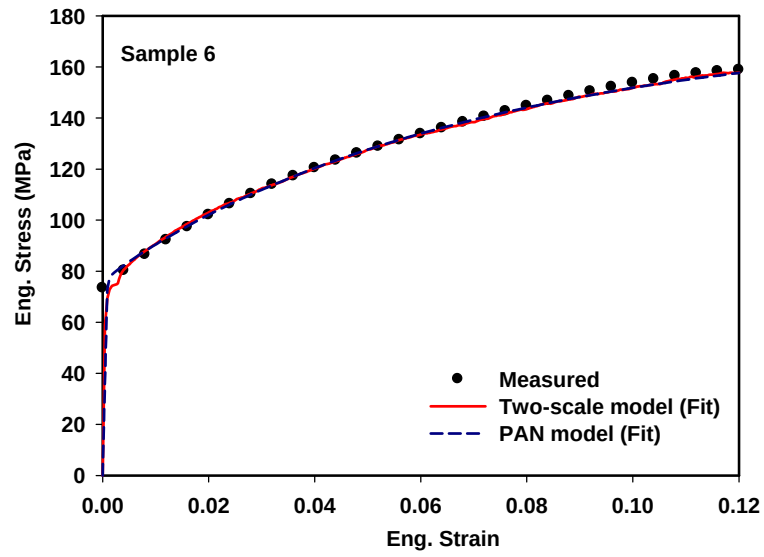
Table 4.3: Shear modulus and anisotropic elasticity constants (Hirth and Lothe, 1969)

(Unit: GPa)

SCCE-T			SCCE-D		
	PAN Model	Taylor Model		Two-Scale Model	Taylor Model
h_0 (MPa)	423	402	$\rho_0(m^{-2})$	9.4×10^{11}	1.2×10^{12}
g_s (MPa)	162	240	k_a	63	16
g_0 (MPa)	38	40	k_b	7b	25b
a	2	2			
Std. error of fit (MPa, %)	1.1 (0.8)	2.3 (1.7)	Std. error of fit (MPa)	1.1(0.8)	0.9 (0.7)

Table 4.4: Best fit parameters and standard error of fit for PAN model, two-scale model and Taylor's iso-strain model adopting SCCE-T and SCCE-D.

All models reproduced the measured stress-strain curve accurately, having standard errors of fit as shown in Figure 4.10 (a) and Table 4.4. The two-scale model employs SCCE-D while PAN utilizes SCCE-T, with three and four fitting parameters, respectively. Best-fit parameters for each model were then used to predict the mechanical response of the remaining five specimens having 9 to 34 grains. Predicted hardening curves using the best fit parameters are shown in Figure 4.10 (b)-(f). Hardening curves were obtained by subtracting the yield stress (0.2% offset) from the total flow stress for each model.

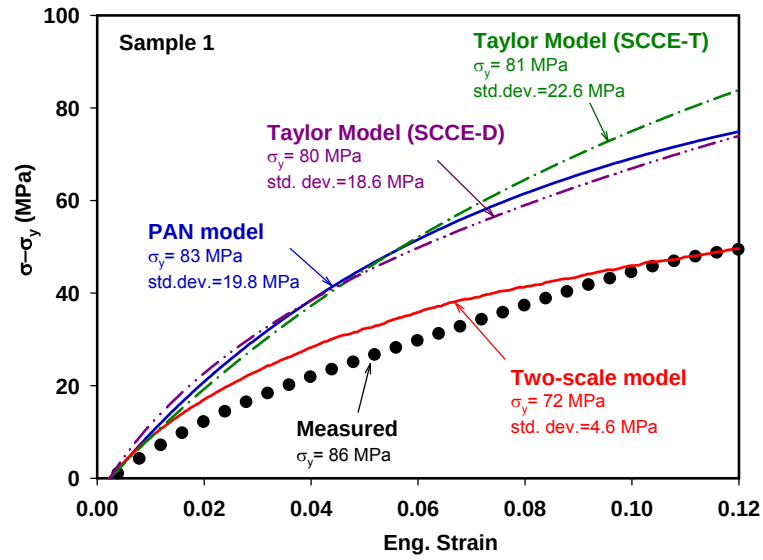


(a)

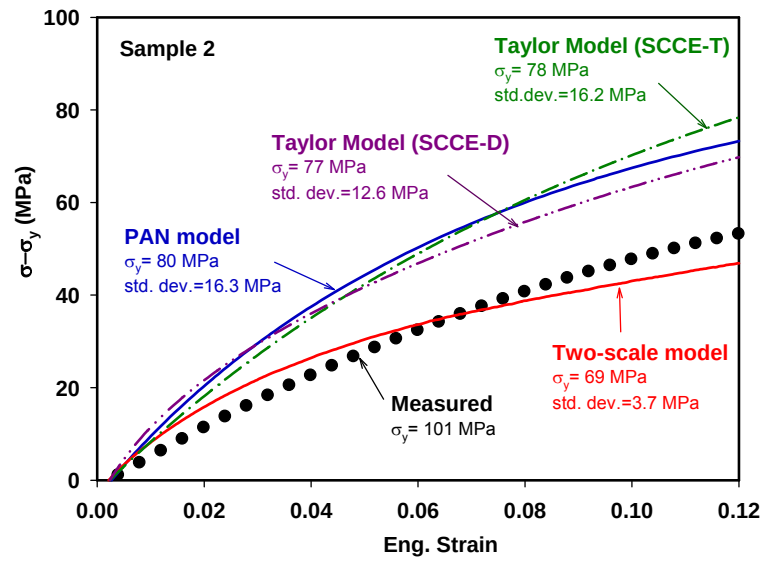
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Figure 4.10: Comparison of predicted stress-strain curves with the measurement for 6 samples for two-scale model, PAN model and Taylor model adopting SCCE-T and SCCE-D. The parameters for the constitutive models were fit to the sample 6.

Figure 4.10 continued



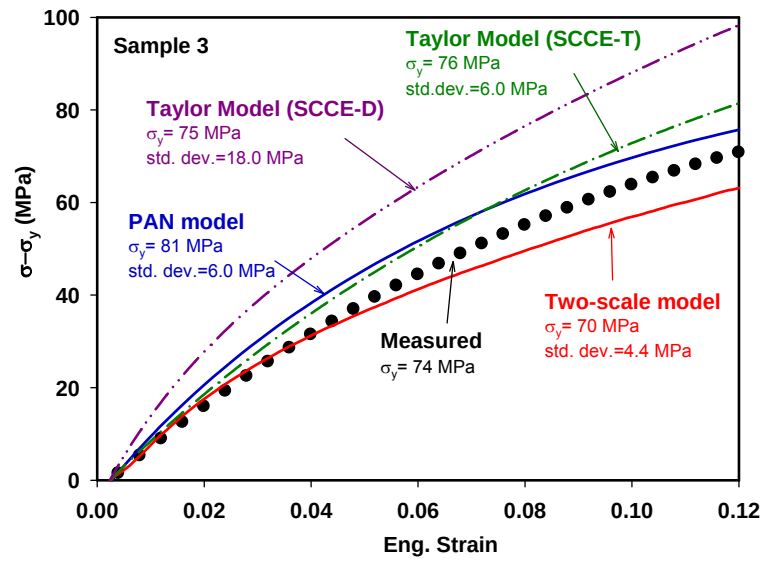
(b)



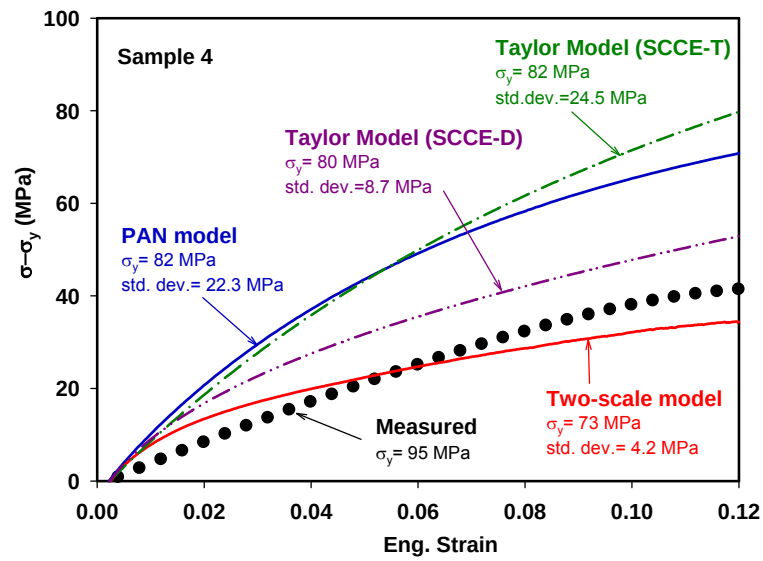
(c)

Continued

Figure 4.10 continued



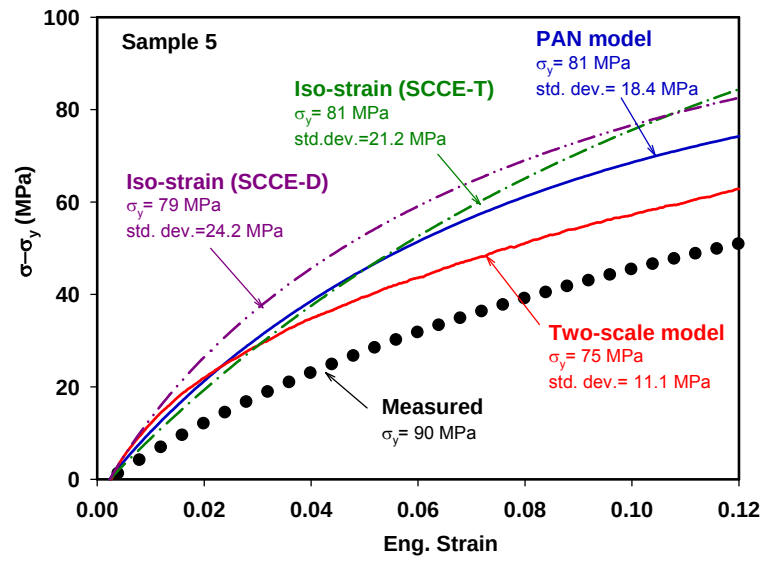
(d)



(e)

Continued

Figure 4.10 continued



(f)

Samples	# of grains	Standard deviations (MPa)				
		Two-scale	Two-scale (GSS only)	PAN Model	Iso-strain (SCCE-D)	Iso-strain (SCCE-T)
Sample 1	9	4.6	4.9	19.8	18.6	22.6
Sample 2	13	3.7	11.1	16.3	13.6	16.8
Sample 3	18	4.4	12.1	6.0	19.1	6.6
Sample 4	32	4.2	8.0	22.3	9.5	25.1
Sample 5	34	11.1	9.2	18.4	25.3	21.8
Average		5.6	9.1	16.6	17.2	18.6

Table 4.5: Standard deviations between predicted and measured stress-strain curves

(Unit: MPa).

Table 4.5 compares average standard deviations between predicted and measured stress-strain curves for each model. The averaged standard deviation between measurement and prediction is approximately three times larger for PAN model than for

the two-scale model (16.6 MPa vs. 5.6 MPa, respectively). In accordance with similar tests for single crystals (Lee et al., 2009), the two-scale model adopting SCCE-D agrees better with measurements compared to the PAN model in spite of having fewer arbitrary parameters. Taylor models, whether adopting SCCE-T or SCCE-D showed larger standard deviation compared to two-scale model and PAN model.

The likely source of error for the PAN model and Taylor models lies in ignoring the role of grain boundaries except as an integral part of the single-crystal constitutive equation. Figure 4.10 (b)-(f) illustrate that the PAN model tends to over-predict hardening of the multi-crystals. Recall that all models were fit to multi-crystals with the most number of grains and the stress-strain response was then predicted for samples with fewer grains. This over-prediction implies that the best-fit parameters obtained from Sample 6, which is the most polycrystal-like, do not represent well the hardening behavior for samples with fewer grains. The averaged standard deviation for prediction using GSS alone is 9.1 MPa, Table 4.5, larger than the full two-scale model. This indicates that the back stress and redistribution of mobile dislocations within the MSS increases accuracy of the prediction over a range of grain configurations.

Despite the two-scale model showing good agreement for hardening of multi-crystals, both models failed to predict the measured yield stresses accurately using the current prediction scheme. Values of ρ_0 and g_0 for SCCE-D and SCCE-T were determined from the initial yield stress of Sample 6 and the same values. The predicted yield stresses for the other specimens were 70 to 76 MPa and 81 to 84 MPa for the two-scale model and PAN model, respectively, while the measured yield stress ranged from

63 to 96 MPa. This deviation may be related to altered initial dislocation densities or defects created during specimen preparation and polishing.

4.5.2 Prediction of Hall-Petch Slopes

Hall-Petch Law (Hall, 1951; Petch, 1953) suggests that there exists a relation between the yield stress and the grain size of the material. This relationship has been confirmed by many experimental results, and it is agreed that this grain size hardening effect originates from mechanisms near the grain boundaries.

In order to assess the accuracy of the two-scale model for predicting the Hall-Petch effect, simulations and experiments of tensile tests with various grain sizes were conducted using the minimum alloy steel. Uniaxial tensile tests for minimum alloy steel were performed using ASTM E8 subsize specimens. Measured Hall-Petch slopes at the yield stress and the stress at 10% strain were 0.88 and 0.98 MN/m^{3/2}, respectively as shown in Figure 4.12.

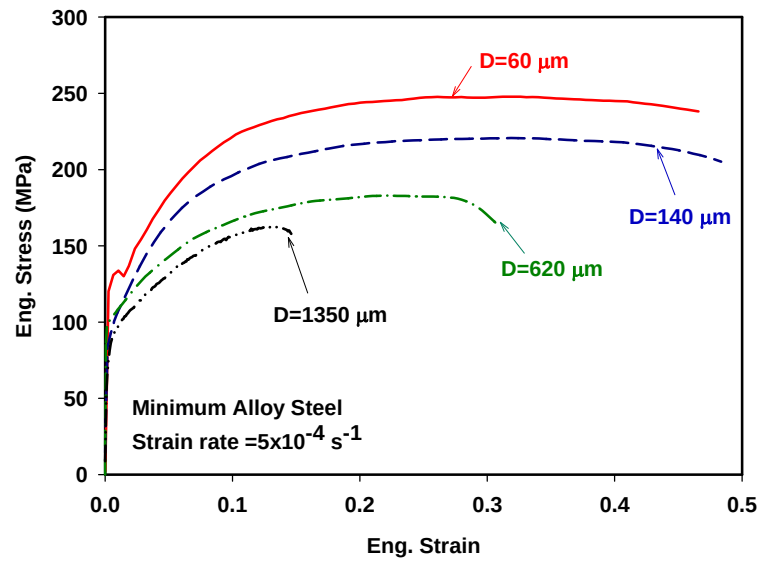


Figure 4.11: Stress-strain responses for minimum alloy steels with four different grain sizes.

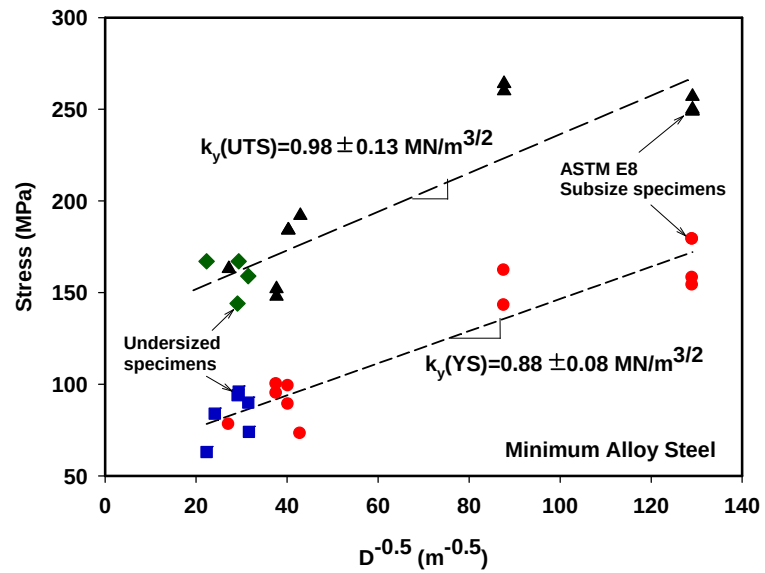


Figure 4.12: Measured Hall-Petch slope for minimum alloy steel at YS and UTS.

As shown in Figure 4.13, the uniaxial tension of 2D and 3D array of grain assemblies having 4 to 64 and 8 to 125 grains with four random crystal orientations were simulated using the two-scale model. Total of 8000 solid elements (C3D8) were used ($40 \times 40 \times 5$ for 2D and $20 \times 20 \times 20$ for 3D) with the dimensions of $1\text{mm} \times 1\text{mm} \times 0.1\text{mm}$ and $1\text{mm} \times 1\text{mm} \times 1\text{mm}$ for 2D and 3D case, respectively. Material parameters for minimum alloy steel (Table 4.4) and τ^* of 375 MPa (~ 5 times the yield stress) are adopted

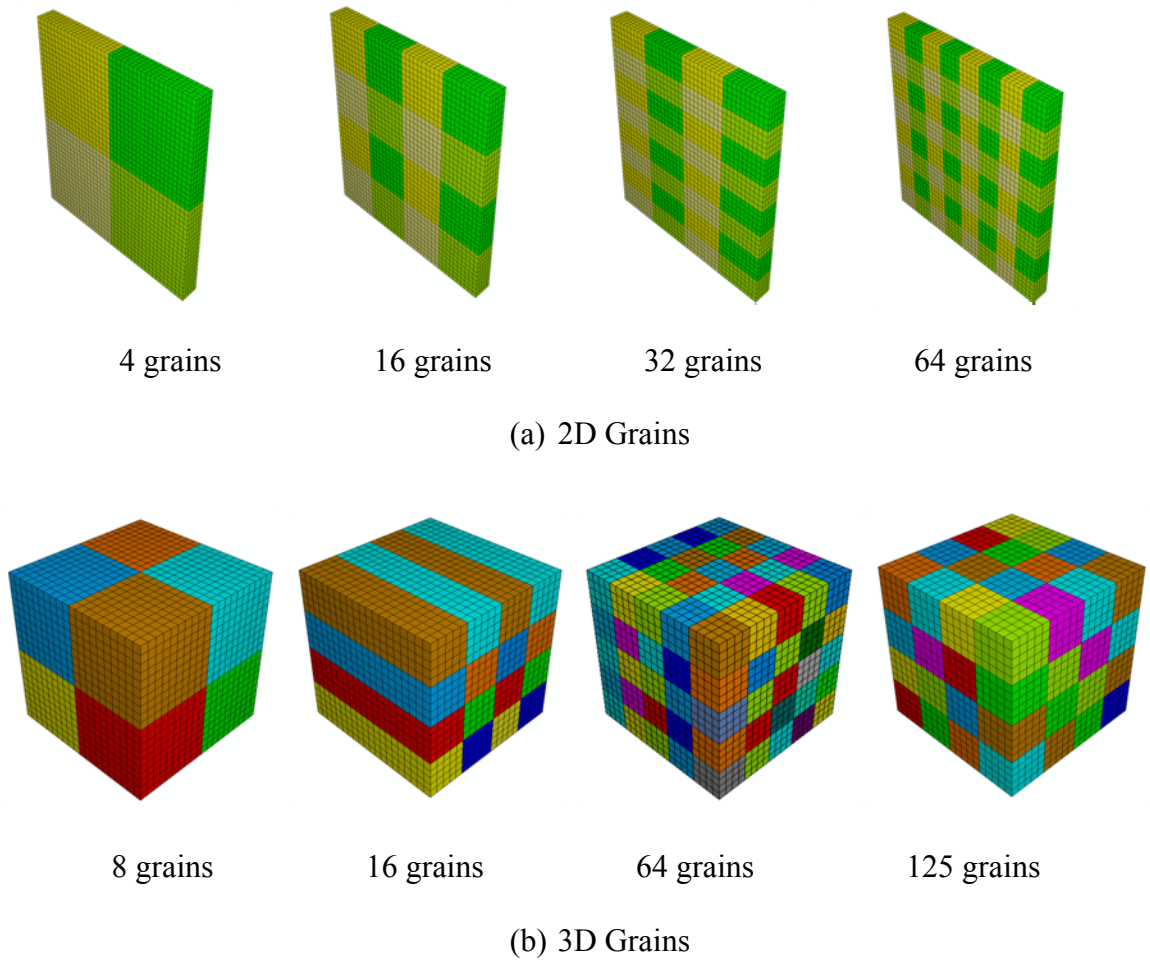


Figure 4.13: Schematics of imaginary samples with different numbers and sizes of the grain, (a) 2D array of 4 to 64 grains and (b) 3D array of 8 to 125 grains.

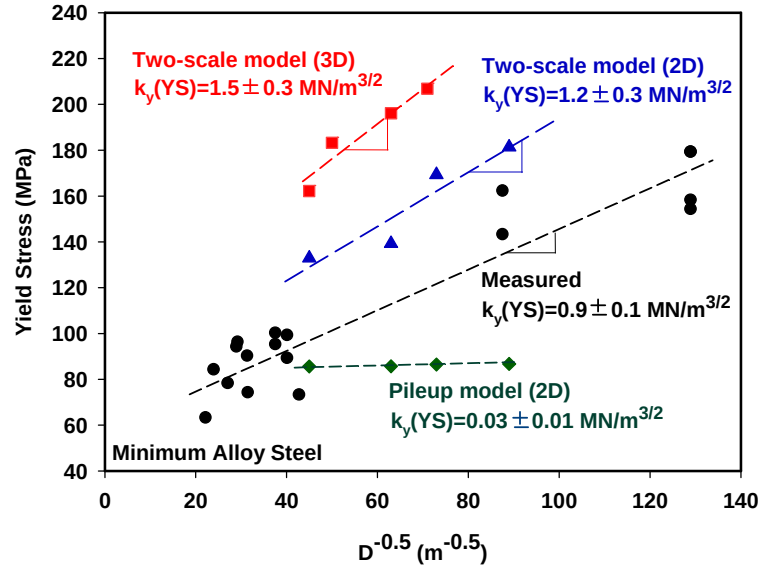


Figure 4.14: Measured and simulated Hall-Petch slope for 2D and 3D grain assemblies.

Figure 4.14 compares measured and simulated Hall-Petch slopes at the yield stress using the two-scale model (2D and 3D) and the pileup model (2D). For the 2D grain assemblies, the pileup model showed a negligible size dependence ($k_y = 0.03 \pm 0.01 \text{ MN/m}^{3/2}$), whereas the two-scale model predicted the magnitude of the Hall-Petch slope ($k_y = 1.2 \pm 0.3 \text{ MN/m}^{3/2}$), within the scatter of the measurements and simulations. For the 3D case, two-scale model over-predicted the Hall-Petch slope by a factor of 1.5 when τ^* of 375 MPa was used.

In accordance with the experimental data, the two-scale model predicted higher Hall-Petch slope at larger strains due to the increased strain hardening for smaller grain sizes. However, predicted Hall-Petch slope at 10% strain was larger than that for the

measured by a factor of 2-3 as shown in Table 4.6. This deviation was more significant for the 2D case, possibly due to an unrealistic surface to volume ratio compared to real polycrystal samples. This over-prediction may be attributed to neglecting the effect of the cross-slip near the grain boundary which may lower the effective grain boundary obstacle strength at larger strains.

	Measured k_y (MN/m ^{3/2})	Simulated k_y (MN/m ^{3/2})	
		2D	3D
YS	0.9 ± 0.1	1.2 ± 0.3	1.5 ± 0.3
e=0.05	0.9 ± 0.1	2.4 ± 0.4	1.9 ± 0.3
e=0.10	1.0 ± 0.1	2.9 ± 0.4	2.0 ± 0.3
UTS	1.0 ± 0.1	-	-

Table 4.6: Measured and simulated Hall-Petch slope (k_y) obtained at the YS, 5 % and 10% strains, and the UTS.

Figure 4.15 shows the effect of τ^* on the Hall-Petch slope for 3D grain assemblies. In order to obtain the measured Hall-Petch slope of $0.9 \text{ MN/m}^{3/2}$, τ^* of 150-200 MPa or 2-3 times the yield stress can be estimated for minimum alloy steel.

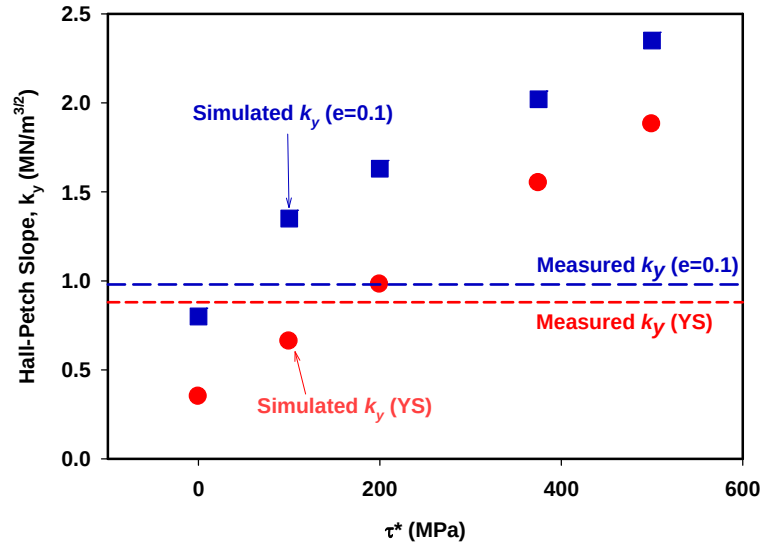


Figure 4.15: Effect of τ^* on Hall-Petch slope for 3D grain arrays.

4.5.3 Prediction of Lattice Curvature

The initial grain orientations in the gage region of Fe-3% Si tensile specimen are scanned using the OIM with the step size of 10 μm as shown in Figure 4.16. In order to measure the lattice curvature with finer OIM step sizes, smaller region of interest with four grains and two triple junctions is selected (Figure 4.16). The initial Bunge's Euler angles for the four grains are listed in Table 4.7. After 8% tensile strain was applied to the sample, the average lattice curvature is remeasured with 1 μm scanning step size. From the initial grain map, the region of interest is meshed with 9600 elements (C3D8) and measured stress-strain curve is fitted using the two-scale model, similar to procedure for minimum alloy steel samples. Best-fit parameters for Fe-3% Si sample are as follows: $\rho_0 = 7 \times 10^{12} \text{ m}^{-2}$, $k_a = 98$ and $k_b = 8b$.

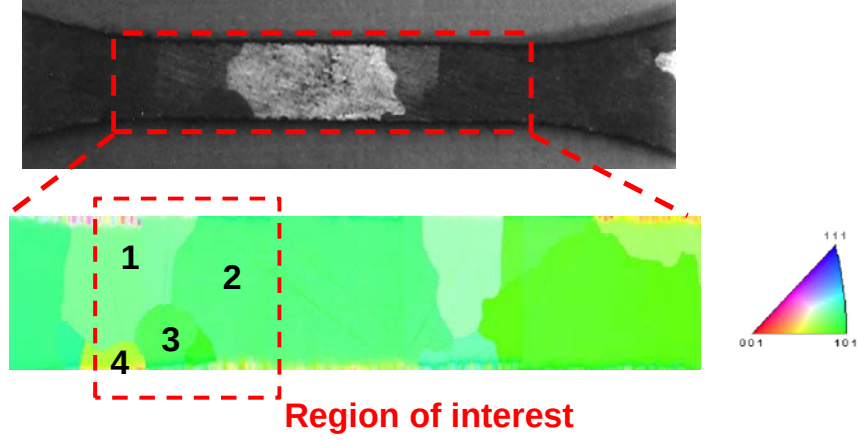


Figure 4.16: Surface image (optical microscope) and inverse pole figure (OIM) for Fe-3% Si tensile samples.

Grain	φ	Φ	φ_2
1	61	38	282
2	266	41	81
3	74	41	265
4	248	30	88

Table 4.7: Initial grain orientations for four grains in the region of interest in the form of Bunge's Euler angles (degrees).

In order to verify the prediction capability of the present two-scale simulation procedure, measured distribution of lattice curvature for the tensile sample is compared with that of simulations. The lattice curvature is related to the dislocation tensor through the expression (Nye, 1953; Sun et al., 2000; Hartley, 2003),

$$\kappa_{ij} = -\alpha_{ij} + \frac{1}{2} \delta_{ij} \alpha_{kk} - e_{ijk} \varepsilon_{jk,l}^e \quad (4.23)$$

where α_{ij} is dislocation tensor, e_{ijk} denotes components of the permutation tensor. As shown by Nye (Nye, 1953), there exists a relation between the dislocation tensor and the network of dislocations as:

$$\boldsymbol{\alpha} = \sum_{s=1}^{NS} \rho^{(s)} \mathbf{b}^{(s)} \otimes \mathbf{z}^{(s)} \quad \text{or} \quad \alpha_{ij} = \sum_{s=1}^{NS} \rho^{(s)} b_i^{(s)} z_j^{(s)} \quad (4.24)$$

where $\rho^{(s)}$ denotes the density of dislocation type s , $\mathbf{b}^{(s)}$ is the Burgers vector of that type, and $\mathbf{z}^{(s)}$ is the line direction of the dislocation type. Since only edge dislocation is considered in the present two-scale model, the dyadic in equation (4.24) is uniquely determined with a geometric definition of dislocation on each slip system.

Using equations (4.22), (4.23) and (4.24), the average lattice curvatures are calculated from the lattice misorientation and dislocation distribution inside the grains. Figure 4.17 (c)-(e) show the first example of simulated lattice curvature for a Fe-3% Si specimen after 8% strain. As shown in this figure, high curvatures are developed near the grain boundaries and near the two triple junctions with predicted curvature distribution confirmed by the measurements.

Note that high lattice curvatures were measured near the specimen edges due to surface irregularities. Excluding high lattice curvatures measured near the specimen edges (dotted line in Figure 4.17 (c)), the difference in maximum magnitude of curvatures is within 4%: 9.2×10^{-3} rad/ μm for the prediction using the two-scale model and 9.5×10^{-3} rad/ μm for the measurement. Two-scale model accurately predicted maximum lattice curvature and notably low lattice curvature at some grain boundaries, i.e. the vertical boundary in Figure 4.17 (c). On the other hand, measured averaged lattice

curvature was 5.8×10^{-4} rad/ μm for the measured while the simulated value using the two-scale model smaller by a factor of 8, 7.3×10^{-5} rad/ μm . This discrepancy may be due to the initial lattice curvature before the deformation and trapping of dislocations within the sample as deformation proceeds. The two-scale model utilizes average grain orientations for each grain so that the small differences in the orientation of the crystal lattice within the grain are neglected.

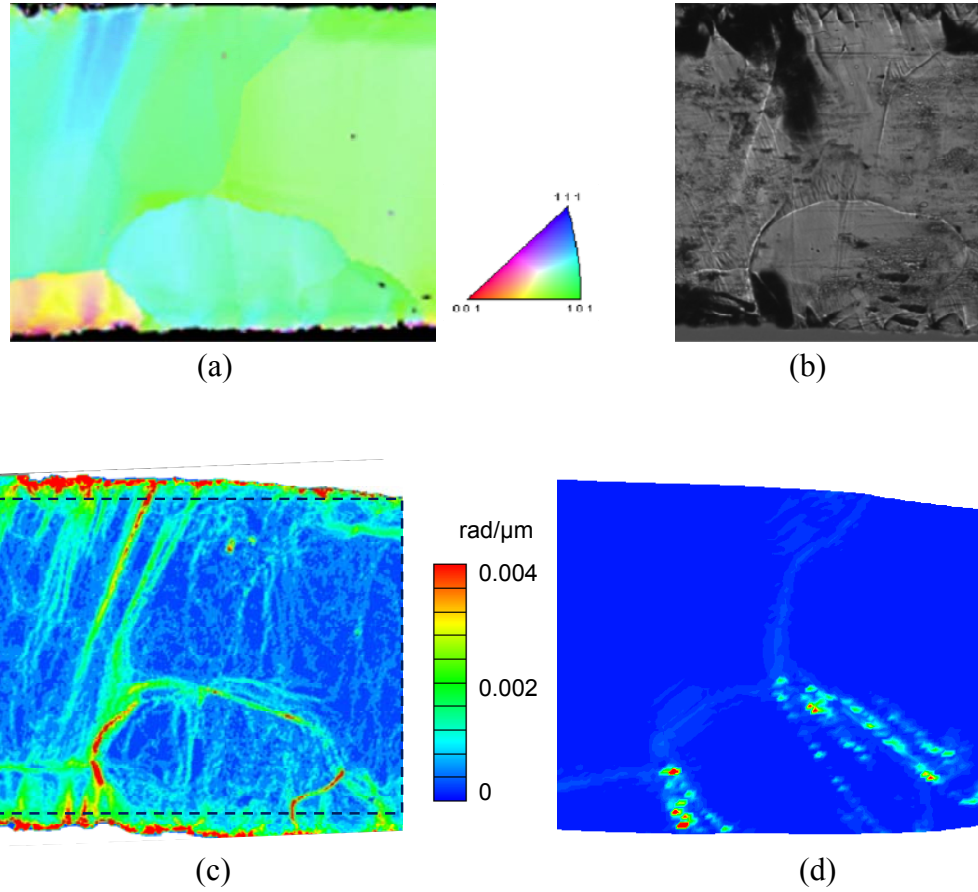


Figure 4.17: Deformed Fe-3% Si specimen images after 8% strain (a) Inverse pole figure, (b) surface image using optical microscope, (c) measured lattice curvature (d) predicted lattice curvature using the two-scale model

4.6 Discussions

Parametric tests are conducted using the two-scale model with material properties obtained for minimum alloy steel. Uniaxial tension of rectangular bicrystal is simulated to see how the dislocation densities evolve at different strains and slip systems. Reversal loading at different strains was simulated to observe Bauschinger effect using 16 grain samples.

4.6.1 Evolution of Dislocation Densities

Simple parametric test is performed to predict spatial distributions of dislocations for different strains and slip systems. A rectangular sample with embedded cylindrical grain is constructed. The crystal orientation of the cylindrical grain is misoriented by 45° relative to the rectangular grain (Figure 4.18 (a)) and uniaxial tension is applied up to 10%. The two-scale model predicted the overall stress levels (Figure 4.18 (a)) and simulated development of dislocation density as a function of strain (1%, 5% and 10%), Figure 4.18 (b). Upon straining, dislocation density built up more rapidly near the grain boundary. Upon 10% strain, initial dislocation density of $9.4 \times 10^{11} \text{ m}^{-2}$ is increased up to an average and a maximum dislocation density of $6.9 \times 10^{12} \text{ m}^{-2}$ and $3.4 \times 10^{13} \text{ m}^{-2}$, respectively. Figure 4.18 (c) shows the partitioning of dislocation density on slip systems at 10% strain. Two different slip systems, $(-21-1)[-1-11]$ and $(1-12)[-111]$ represent most active slips for each grain or the slip systems of the highest density at a strain of 10%.

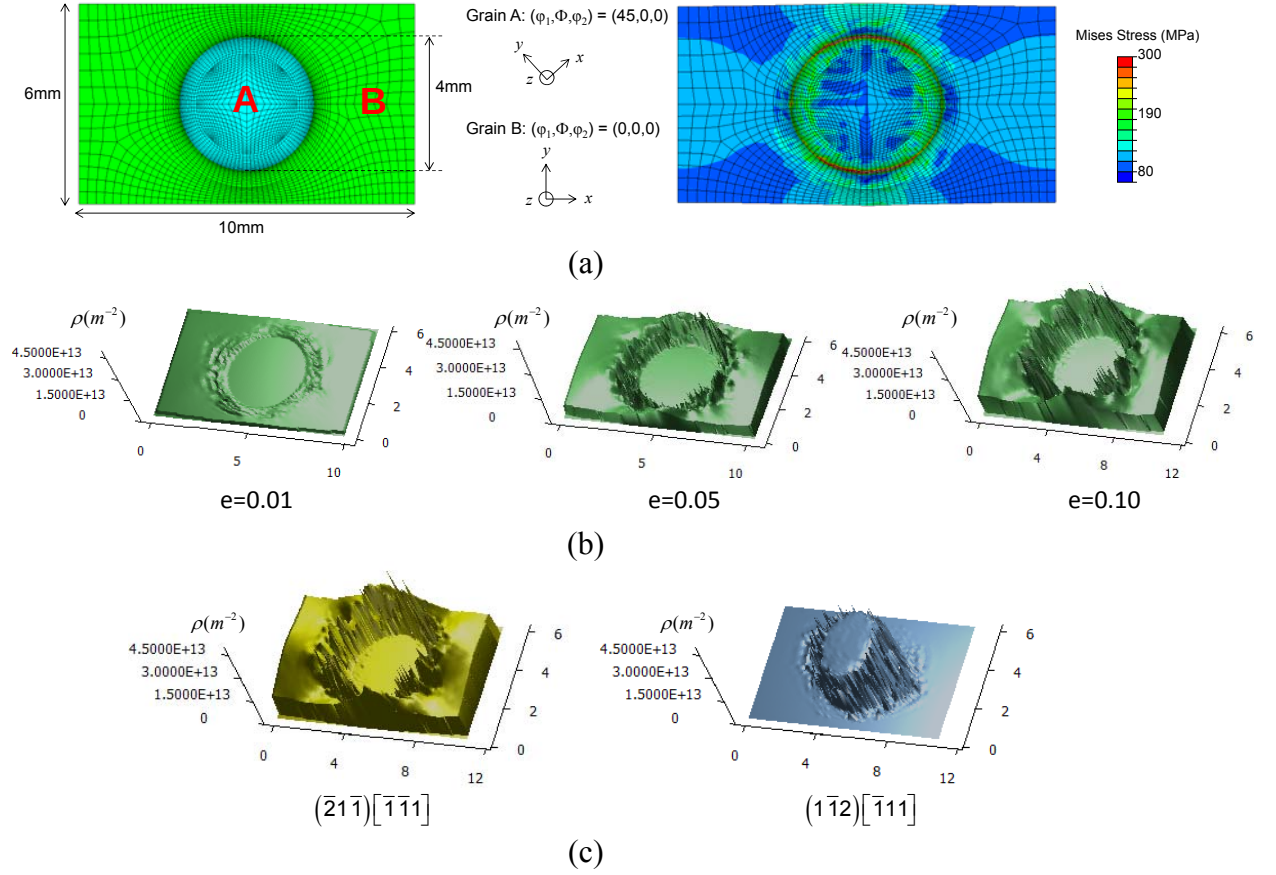


Figure 4.18: Two-scale simulation of a cylindrical grain within a rectangular grain, lattices misoriented by 45° . (a) Schematics of test geometry and Mises stress at 10% strain, (b) evolution of dislocation densities at various strains (1%, 5% and 10%), and (c) dislocation densities for different slip systems.

In order to assess the effect of grain orientations on the evolution of dislocation densities, identical tests with the different crystal orientations for inner cylindrical grains were performed. Figure 4.19 compares total dislocation densities at 10% strain for three cases; inner grain is misoriented by 15, 30 and 45 degrees relative to outer grain. As the misorientation between two grains increased, differences in total dislocation densities

between two grains increased. Differences in dislocation densities between the inner and outer grains were 12, 23 and 27% for 15, 30 and 45°, respectively.

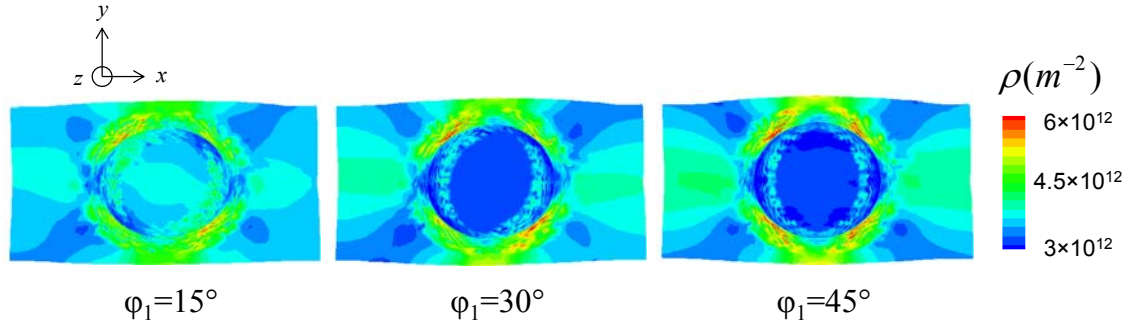


Figure 4.19: Dislocation densities at 10% strain for inner grain misoriented by 15, 30 and 45 degrees.

4.6.2 Bauschinger Effect

In order to investigate the effect of the back stress on the reversal loading, simulations of tension-compression and compression-tension tests are conducted using the two-scale model. Parametric tests are performed using an imaginary square polycrystal with 16 grains having four random crystal orientations (A, B, C and D) as shown in Figure 4.20. Material constants for minimum alloy steel are used as listed in Table 4.4.

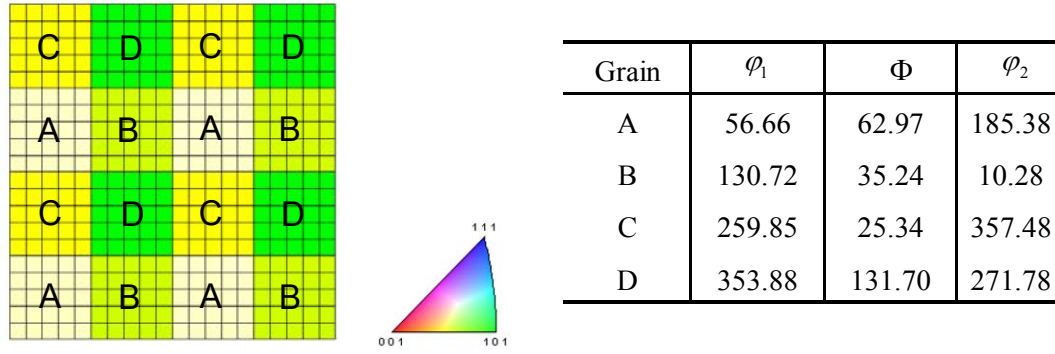
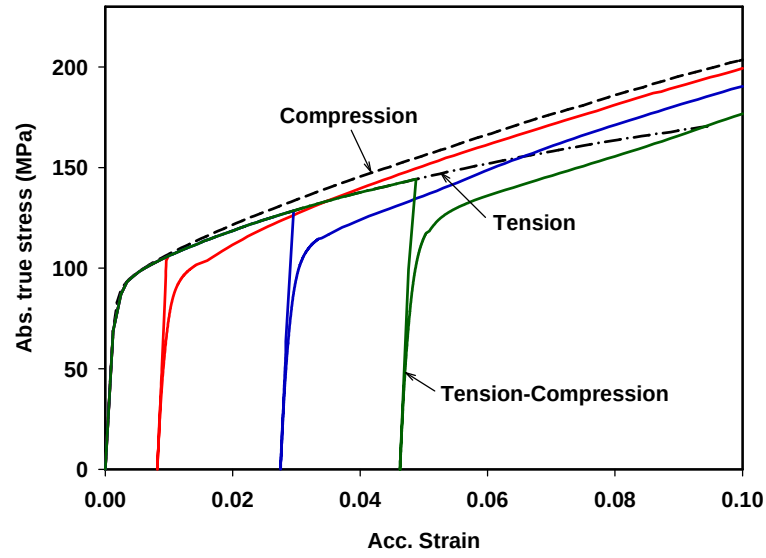
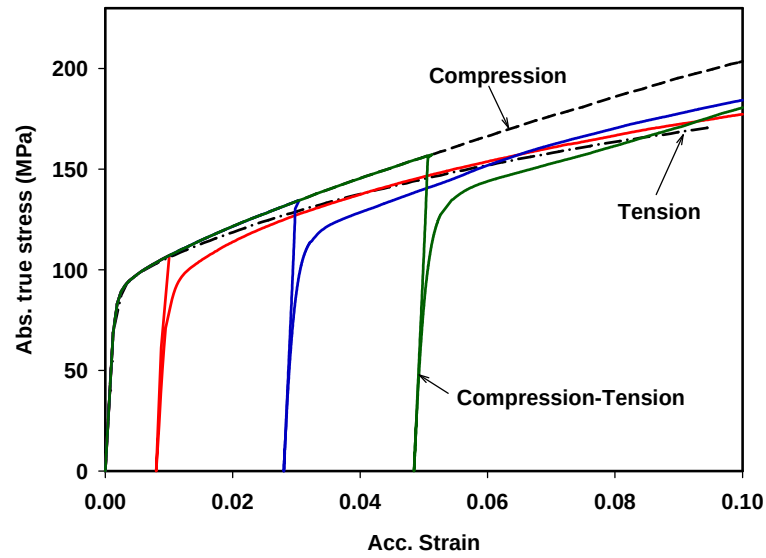


Figure 4.20: Square polycrystal sample with 16 grains and crystal orientations for each grain in terms of Bunge's Euler angles (degrees).

Figure 4.21 (a) and (b) show simulated tension-compression and compression-tension tests with reversal loadings at 1, 3, and 5% strains. Contrary to most conventional continuum models, e.g. PAN model, the two-scale model predicted lower yield stress at the reversal loading due to the back stress. The two-scale model does not require any fitting parameters to obtain back stress since it is explicitly obtained using interaction forces among dislocations, equation (4.15) .



(a)



(b)

Figure 4.21: Simulated (a) tension-compression and (b) compression- tension of 16 grain square sample with 1%, 3% and 5% pre-strains using the two-scale model.

4.6.3 Efficiency of the Model

The two-scale model was computationally efficient, CPU times required to simulate 64 grains with 8000 elements was 6.5 hours while that for the pileup model was 13.5 hours. Computational time for the GSS alone was around 6.2 hours so that MSS contributed only 5% of the total CPU time. Therefore, two-scale model is an efficient and promising method for treating 100 or more grains.

4.7 Conclusions

A computationally efficient two-scale model was developed capable of predicting the Hall-Petch effect quantitatively with no arbitrary length scales and only three arbitrary parameters corresponding to measured strain hardening rates for a single specimen and grain size. Here are the main conclusions of the work.

1. A two-scale model was developed that is capable of effective and practical simulation of dislocation densities in polycrystals and their interactions with grain boundaries based on local boundary/grain properties while reproducing simple dislocation pile-up solutions. The CPU time to simulate 64 grains with 8000 finite elements deformed to a strain of 10% was 6.5 hours, 95% of which was used in the standard finite element routine at the larger length scale.
2. The two-scale model accurately predicted the strain hardening of 5 multi-crystal tensile samples having 9 to 39 grains. Standard texture-type simulations exhibited standard deviations 3 times greater than those of the two-scale model in spite of

having additional undetermined parameters. The average standard deviation predicted by the two-scale model is 6 MPa as compared with those for the PAN (Peirce, Asaro, Needleman) / Taylor models with SCCE-D or SCCE-T of 17-19 MPa.

3. PAN and Taylor iso-strain models failed to predict the hardening of multi-crystal tensile samples accurately. The PAN model was back-fitted from the polycrystal flow curve (as is usual) and did not adequately represent the behavior of multi-crystals with fewer numbers of grains. The discrepancy presumably arises from neglecting the effect of grain boundaries and interaction with dislocations.
4. The two-scale model accurately predicted maximum lattice curvature for a Fe-3% Si specimen after 8% strain. The maximum lattice curvature predicted by the two-scale model is 9.5×10^{-3} rad/ μm while that for the measured is 9.2×10^{-3} rad/ μm , within 5% deviation.
5. The two-scale model predicted the Hall-Petch effect and its magnitude without involving related arbitrary parameters. (Only three arbitrary parameters related to strain hardening were fit, none related to grain size or other lengths scales.) The simulated Hall-Petch slopes for minimum alloy steel were 1.2 ± 0.3 and 1.5 ± 0.3 MN/m^{3/2} for 2D and 3D grain assemblies respectively while the corresponding measured slope was 0.9 ± 0.1 MN/m^{3/2}, approximately within the scatter of the experiment and simulation.

6. Parametric tests showed that if grain boundary strength were treated as an undetermined parameter, a value 2-3 times the yield stress would match measured Hall-Petch slopes for minimum alloy steel.
7. Quantitative prediction of spatial distribution of dislocation density has been carried out and presented. Accumulation of dislocations near grain boundaries occurs.

5. CONCLUSIONS

A computationally efficient two-scale model based on inhomogeneous dislocation generation, annihilation and accumulation was formulated, implemented and tested (Chapter 4). In order to implement the two-scale model, a new, more accurate constitutive model for single crystals was developed (Chapter 3).

1. SCCE-D (the proposed single-crystal constitutive model) reproduces flow curves for single slip and multi slip in FCC and BCC single crystals. SCCE-D have better accuracy than SCCE-T (the dominant constitutive model appearing in the literature) while using a smaller number of adjustable parameters. The average standard deviation predicted by SCCE-D is 14 MPa while that for the SCCE-T is 31 MPa.
2. SCCE-T, which are usually back-fitted from polycrystal flow curves, do not adequately represent orientation - dependent single crystal behavior. The discrepancy may arise from neglecting the effect of grain boundaries, grain size and relative misorientation between pairs of grains.
3. Polycrystal simulations using SCCE-T fit to multiple-slip single-crystal data predict higher flow stresses than SCCE-D, correlated with the high flow stresses predicted by the former for single crystals oriented for limited slip system

activation. This correlation implies that there may exist significant regions of limited slip activation in polycrystals, contrary to the usual assumption.

4. Texture evolution has little sensitivity to the type of constitutive equation. Simulated textures for SCCE-T and SCCE-D for FCC and BCC polycrystals are similar, while the simulated macroscopic stress-strain responses differ.

The following conclusions were drawn from the work presented in Chapter 4:

1. A two-scale model was developed that is capable of effective and practical simulation of dislocation densities in polycrystals and their interactions with grain boundaries based on local boundary/grain properties while reproducing simple dislocation pile-up solutions. The CPU time to simulate 64 grains with 8000 finite elements deformed to a strain of 10% was 6.5 hours, 95% of which was used in the standard finite element routine at the larger length scale.
2. The two-scale model accurately predicted the strain hardening of 5 multi-crystal tensile samples having 9 to 39 grains. Standard texture-type simulations exhibited standard deviations 3 times greater than those of the two-scale model in spite of having additional undetermined parameters. The average standard deviation predicted by the two-scale model is 6 MPa as compared with those for the PAN (Peirce, Asaro, Needleman) / Taylor models with SCCE-D or SCCE-T of 17-19 MPa.
3. PAN and Taylor iso-strain models failed to predict the hardening of multi-crystal tensile samples accurately. The PAN model was back-fitted from the polycrystal

flow curve (as is usual) and did not adequately represent the behavior of multi-crystals with fewer numbers of grains. The discrepancy presumably arises from neglecting the effect of grain boundaries and interaction with dislocations.

4. The two-scale model accurately predicted maximum lattice curvature for a Fe-3% Si specimen after 8% strain. The maximum lattice curvature predicted by the two-scale model is 9.5×10^{-3} rad/ μm while that for the measured is 9.2×10^{-3} rad/ μm , within 5% deviation.
5. The two-scale model predicted the Hall-Petch effect and its magnitude without involving related arbitrary parameters. (Only three arbitrary parameters related to strain hardening were fit, none related to grain size or other lengths scales.) The simulated Hall-Petch slopes for minimum alloy steel were 1.2 ± 0.3 and 1.5 ± 0.3 MN/m^{3/2} for 2D and 3D grain assemblies respectively while the corresponding measured slope was 0.9 ± 0.1 MN/m^{3/2}, approximately within the scatter of the experiment and simulation.
6. Parametric tests showed that if grain boundary strength were treated as an undetermined parameter, a value 2-3 times the yield stress would match measured Hall-Petch slopes for minimum alloy steel.
7. Quantitative prediction of spatial distribution of dislocation density has been carried out and presented. Accumulation of dislocations near grain boundaries occurs.

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APPENDIX A: Pileup and Drainage Formulation

Alternative MSS scheme is the pileup and drainage formulation that is based on a 3D generalization of a dislocation pileup model where an assumed mobile fraction (here $\frac{1}{2}$) of the dislocation density is redistributed to satisfy inter-dislocation force equilibrium. The ratio of mobile to immobile incremental dislocation density would likely vary with immobilizing and mobilizing rates of dislocation density by the formation of sessile Lomer-Cottrell locks, dislocation dipoles and other factors, but there is little guidance in the literature on such variation, so an arbitrary constant value of $\frac{1}{2}$ was selected.

Each dislocation experiences a net force from other dislocations and from the applied stress field. Equilibrium requires that the sum of forces on any dislocation is zero. Hence, using the superdislocation concept, and ignoring lattice friction stresses or other local constraints to dislocation motion, the defect equilibrium equation condition may be expressed as equation (4.20). The stress tensor in equation (4.20) is obtained from the GSS, and thus reflects elastic incompatibilities among grains, but not internal contributions of the dislocation or superdislocation stress fields.

Constraints are required in order to obtain a nontrivial solution of equation (4.20) because like dislocations repel each other and mobile dislocations will move infinitely apart in the unconstrained case. Equation (4.20) may be solved in two ways. First approach, method used for discrete dislocation equilibration (Wagoner et al., 1981),

calculates the positions of each dislocation or superdislocation where the force acting on them is within some specified tolerance. Alternatively, equation (4.20) can be solved by finding the superdislocation content at fixed spatial locations, i.e. at the centers of the elements, while maintaining the overall dislocation content on each slip system ($\mathbf{B}^{(\alpha)}$) constant. The constraint can be enforced by ignoring equilibrium requirements for superdislocations adjacent to grain boundaries, prohibiting a transfer of dislocation content out of the grain.

Dislocations are transmitted across the grain boundary or nucleate new dislocations in the adjacent grain if the stress at the head of the accumulated dislocation is sufficient (Shen et al., 1986, 1988). Therefore, a more realistic constraint will involve slip transmission or absorption whenever the tip stress exceeds critical obstacle force at the grain boundary. If $\sigma_{obs} = 0$, dislocations are free to pass through the grain boundary.

In order to test the concept of pileup model, a 1D implementation for a single slip system was derived. The procedure is equivalent to solving for the generalized dislocation pileup mechanism using the superdislocation concept. Isotropic elasticity is used to calculate interaction between dislocations and a fixed number of dislocations are injected into finite elements while infinite obstacle strength is imposed at one end of the 1D mesh. For simplicity, dislocations with infinite line length and a constant applied stress field (σ) is assumed. Equation (4.20) can be represented as:

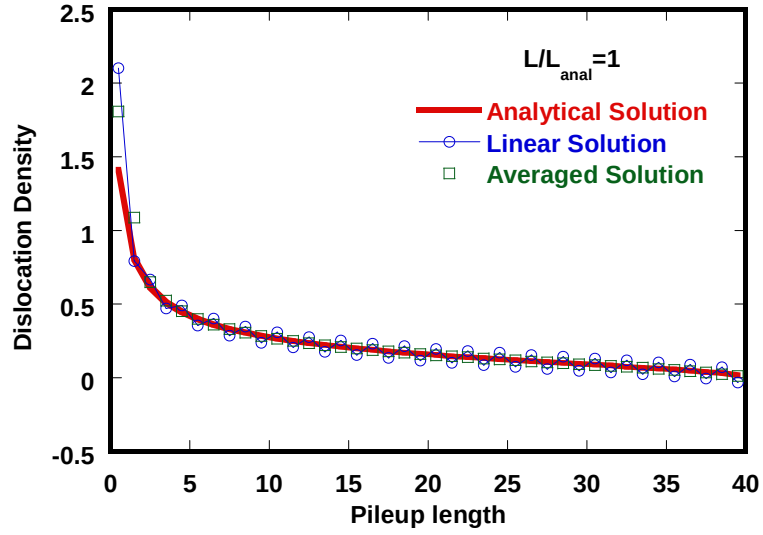
$$\mathbf{F}_i = \sum_{\substack{j=1 \\ j \neq i}}^{N_E} \frac{\mathbf{K}^j \mathbf{B}^i}{x_i - x_j} - \sigma \mathbf{B}^i = 0 \quad (i = 1, 2, \dots, N_E) \quad (\text{A.1})$$

where $\mathbf{K}^j$ is the material constant associated with the character of the j-th superdislocation where $\mathbf{K}^j = \frac{\mu \mathbf{B}^j}{2\pi(1-\nu)}$ for edge and $\mathbf{K}^j = \frac{\mu \mathbf{B}^j}{2\pi}$ for screw dislocations, respectively. $\mathbf{B}^j$ is the Burgers vector and N_E is number of superdislocations (or elements). Note that the unknowns are the $\mathbf{B}^j$, while the spatial positions are prescribed at the center of the elements. Therefore, the numerical procedure to solve the dislocation contents (or Burgers vector of superdislocation) in fixed positions becomes linear system on the dislocation contents, which makes the problem more numerically tractable. In the following section, solving a simple 1D stressed pileup using this method will be addressed.

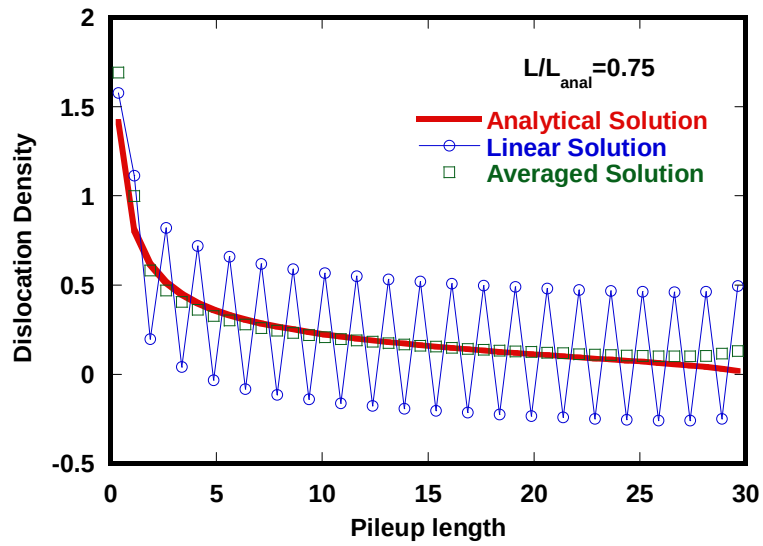
In the case of 1D pileup, by taking $\frac{\mathbf{K}}{2\sigma}$ as unity and assuming that the magnitude of dislocations is identical ($|\mathbf{b}_i| = |\mathbf{b}_j|$), equation (A.1) can be simplified as follows:

$$\frac{1}{x_i} N'_1 + \sum_{\substack{j=2 \\ i \neq j}}^{N_E} \frac{1}{x_i - x_j} N'_j = \frac{1}{2} \quad (i = 2, \dots, N_E) \quad (\text{A.2})$$

In equation (A.3), N'_i defines the Burgers vector of i-th superdislocation and N'_1 represents the dislocation content of the element adjacent to the obstacle. For a current numerical test, total of 10 dislocations are injected to the domain (or the slip plane on which the dislocations glide), discretized by 100 regular elements for three different domain lengths (L), 30, 40 and 50. It should be noted that an analytical solution for a pileup length, L^{an} , for a given condition is 40 (Hirth and Lothe, 1969).



(a)

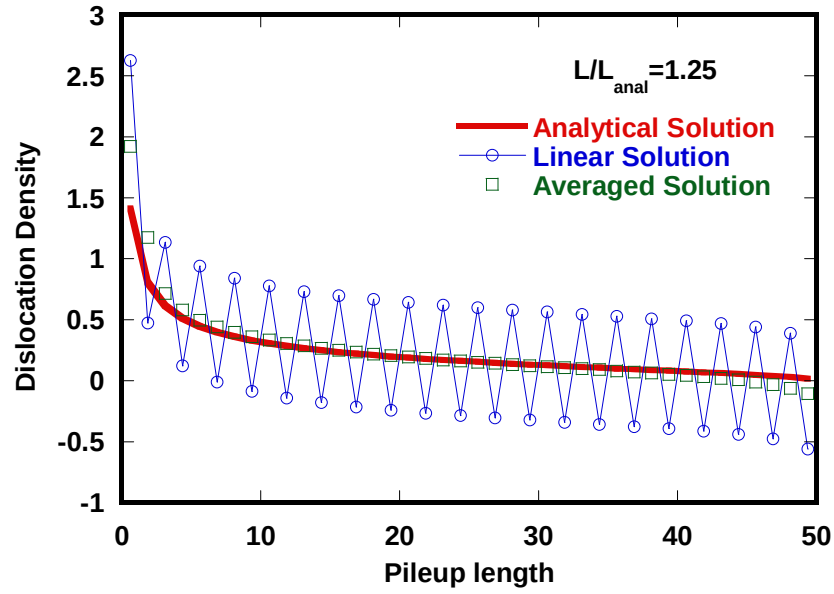


(b)

Continued

Figure A.1: Equilibrated dislocation densities with respect to the different pileup domain length: (a) $L/L^{an}=1$, (b) $L/L^{an}=0.75$, and (c) $L/L^{an}=1.25$

Figure A.1 continued



(c)

Figure A.1 (a)-(c) show the dislocation density with domain length of 40 ($L/L^{an}=1$), 30 ($L/L^{an}=0.75$) and 50 ($L/L^{an}=1.25$), respectively. For $L=40$ ($L/L^{an}=1$), calculated dislocation densities agree well with the analytical solution with small oscillation. Better agreement is achieved by averaging the dislocation densities among the neighboring elements. In the cases when domain length is different from the analytical pileup length ($L/L^{an} \neq 1$), the equilibrated configurations show significant oscillation (Figure A.1 (b) and (c)). However, averaged dislocation densities between two adjacent elements agree well with analytical solution except for small deviation at the end of the pileup.

Since constraint method does not impose any constraints for the polarity (sign) of dislocation contents, each element can have both positive and negative dislocation contents for a possible equilibrium solution. In the cases where the domain length is different from the analytical pileup length, it was shown that different signs of dislocations may be mixed to get equilibrated configurations. However, in real materials, dislocations with opposite polarities at the same slip plane would annihilate each other and the averaged dislocation density between two neighboring elements is equivalent to the net dislocation density as schematically shown in Figure A.2.

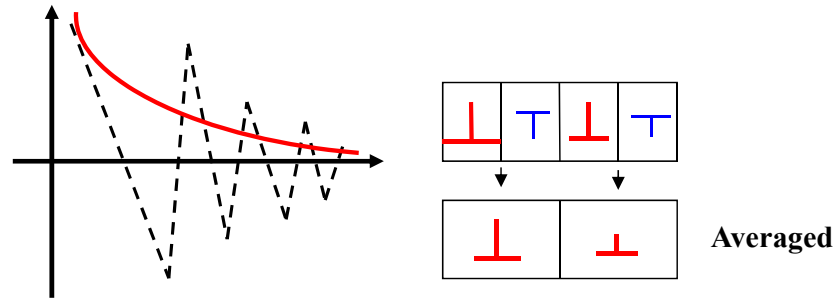


Figure A.2: Schematic view of dislocation density configuration that shows oscillatory behavior and its averaged sense.

In order to make the equilibration problem more systemically solvable, stable domain length ($L=L^{\text{an}}$) can be obtained as schematically shown in Figure A.3. The domain length is altered iteratively until the average force at the end of the pileup is within the specified tolerance. If the force is repulsive (or positive) the solution procedure is repeated with prolonged length ($L^{k+1}=\beta L^k$, $\beta>1$), while the length is shortened

($L^{k+1} = \beta L^k$, $\beta < 1$) if the force is attractive (or negative). Here, L^k represents the domain length during the k-th iteration.

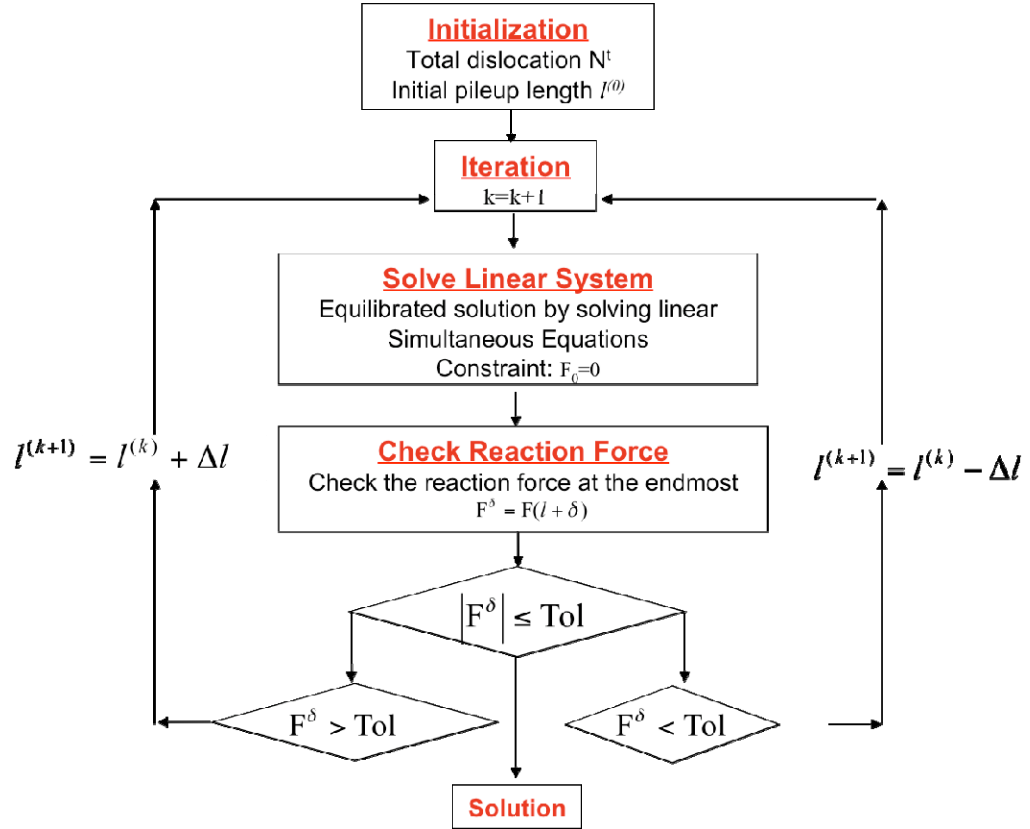


Figure A.3: Numerical algorithm to find the stabilized length of pileup.

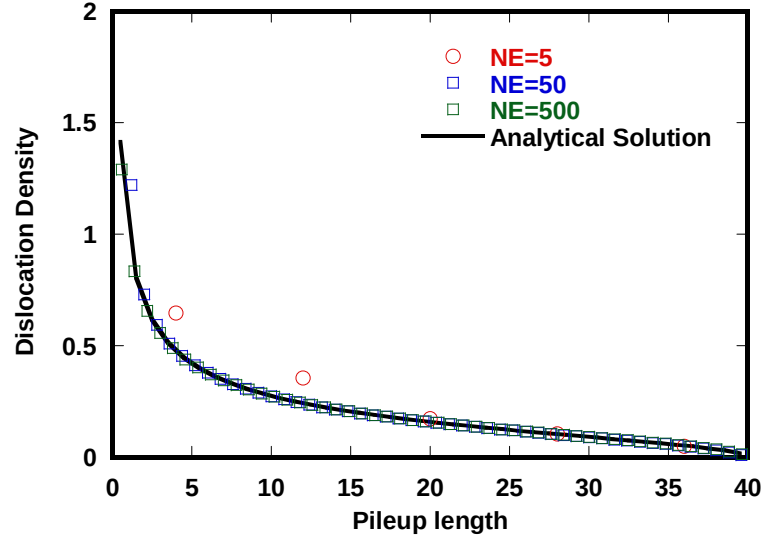


Figure A.4: 1D Pileups under constant stress field for different element sizes.

Figure A.4 shows the mesh independence of the proposed numerical algorithm for a 1D pileup. Equilibrated dislocation densities with four different mesh sizes agree well with analytical solution and show no significant mesh dependence. In addition, the robustness of the algorithm is checked by a convergence of force norm and pileup length during iterations for two unstable pileup cases ($L/L^{an}=0.75$ and 1.25). The force norms and updated pileup lengths show that the convergence is easily achieved within 5 iterations in these particular cases as shown in Figure A.5.

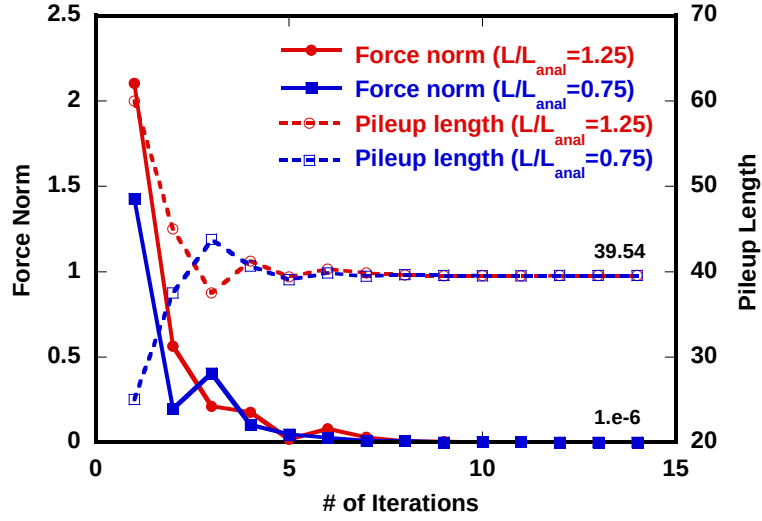
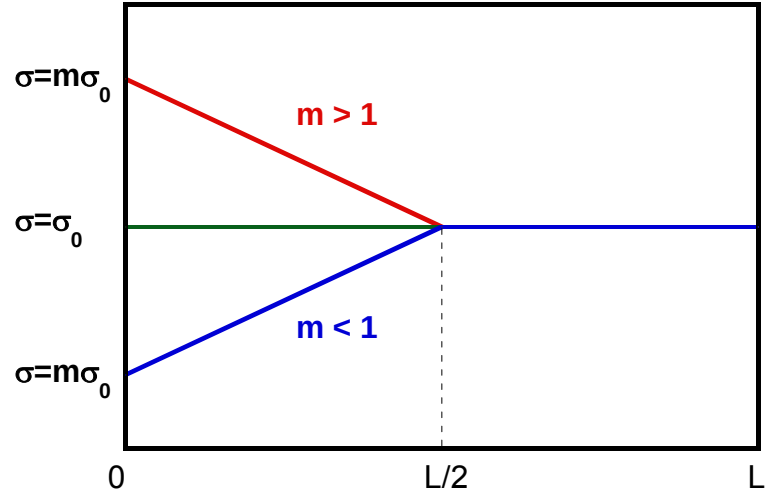
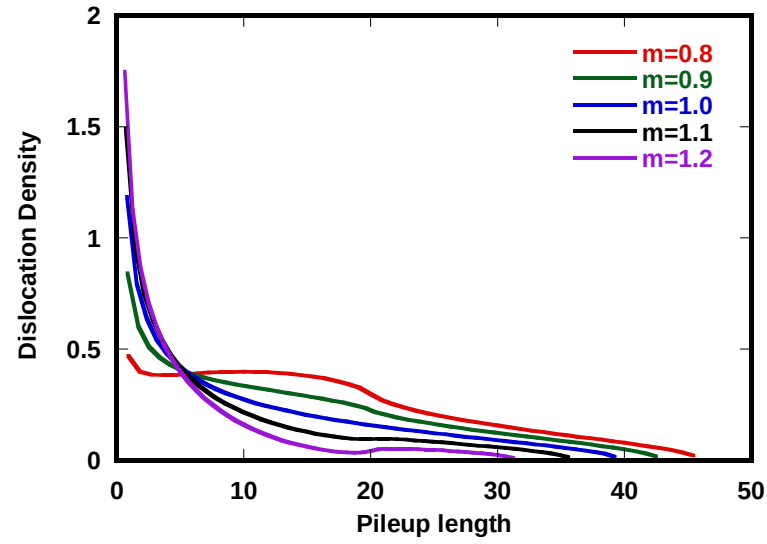


Figure A.5: Convergence of force norms and pileup lengths for $L/L^{an} = 0.75$ and 1.25 .

In real materials, the stress fields near the grain boundaries may be different from that of grain interior due to the incompatibility induced by the anisotropic nature of crystal and concentration of dislocation densities. In order to test the numerical algorithm for non-constant stress field, dislocation pileups with different stress fields are compared as shown in Figure A.6 (a). As shown in Figure A.6 (b), the higher dislocation density is accumulated near the boundary and shorter dislocation pileup length is obtained when the stress field is larger near the boundary.



(a)



(b)

Figure A.6: Dislocation pileup with varying stress field: (a) Stress profiles applied in the direction of pileup, and (b) Dislocation pileups with different external stress profiles.

Alternative method to solve the equilibrium equation, equation (A.1) with the superdislocation concept is to use energy minimization procedure as in Monte Carlo method. The general equilibrium equation, equation (B.3), can be rewritten as:

$$\left(\frac{1}{x_i} N_1 + \sum_{\substack{j=2 \\ i \neq j}}^{N_E} \frac{1}{x_i - x_j} N_j - \frac{1}{2} \right) \cdot N_i = 0 \quad (i = 2, \dots, N_E) \quad (\text{A.3})$$

In order to obtain static solution, small fraction of dislocation content is moved into neighboring element from the initial dislocation distribution and the norm of force imbalance is checked. If the force norm is decreased compared with that of previous time step, new distribution is accepted. This iterative procedure continues until the force norm is within the prescribed tolerance. The brief summary of this algorithm is illustrated in Figure A.7.

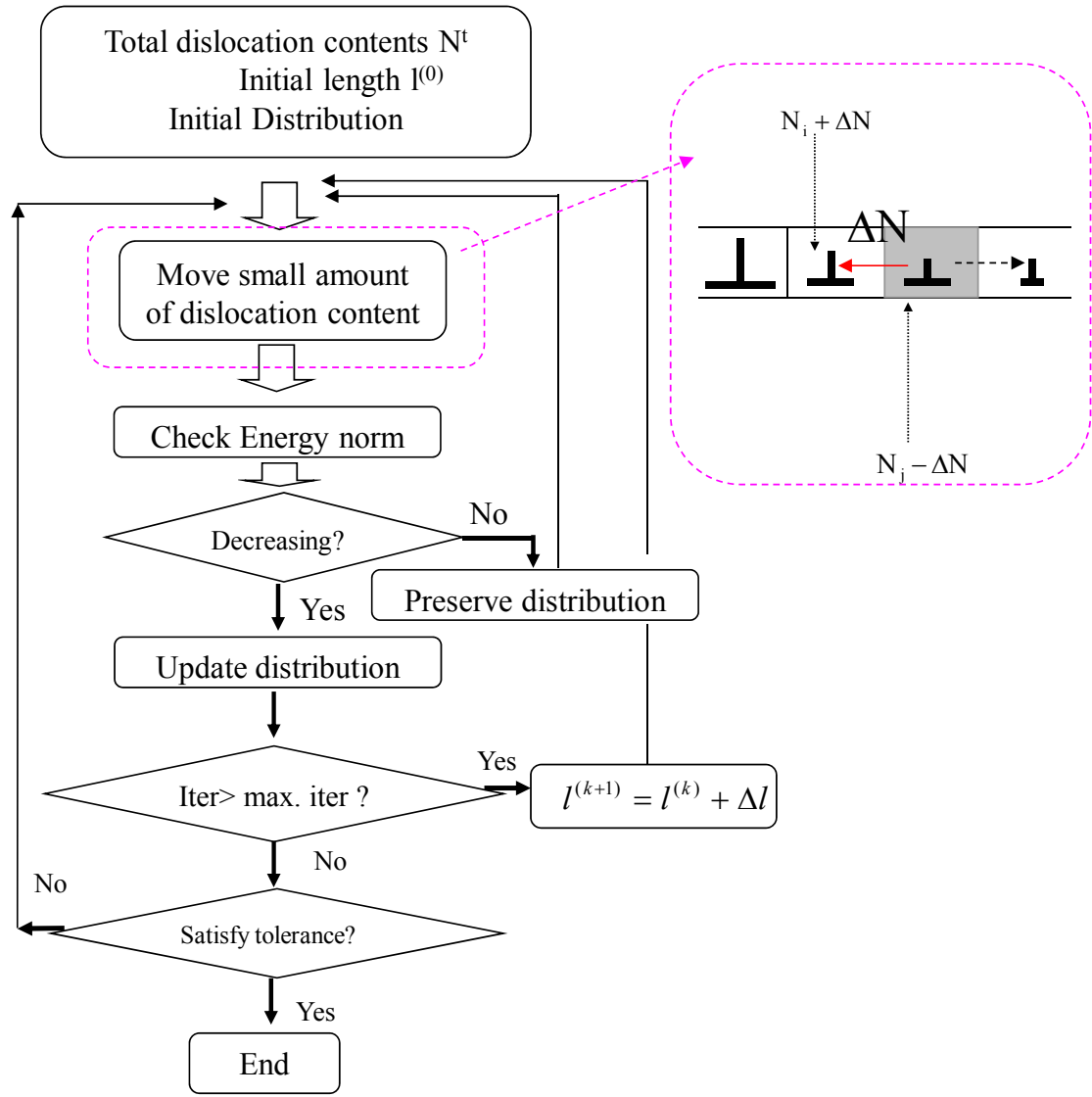


Figure A.7: Numerical algorithm for the energy minimization (non-constraint) method.

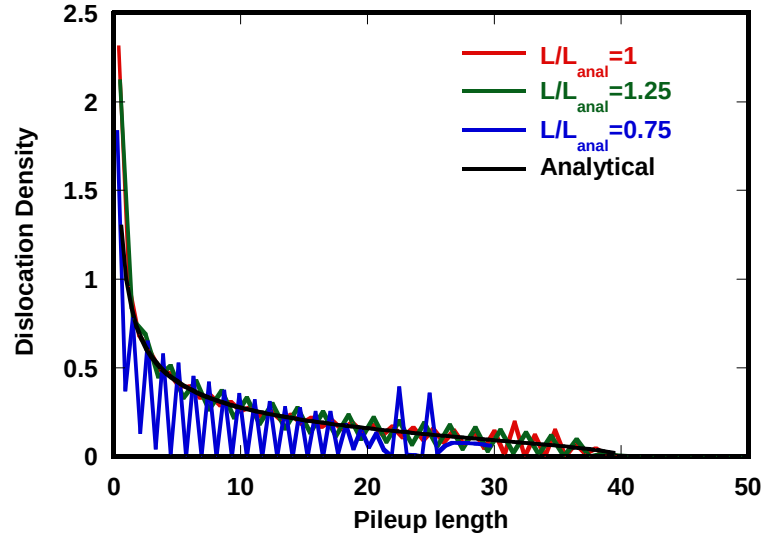


Figure A.8: Configurations of dislocation pileup using energy minimization (non-constraint) method.

Dislocation equilibration using non-constraint method with same material constants and applied stress as Figure A.1 is shown in Figure A.8. When the given domain length is larger than stable pileup length, the convergence is easily obtained and the pileup agrees well with analytic solution. However, when the domain length is shorter than stable pileup length, it is hard to get converged solution with reasonable tolerance and the equilibrated dislocation density is quite oscillatory. In these cases, the domain length needs to be adjusted until the stabilized solution is obtained as in non-constraint method.

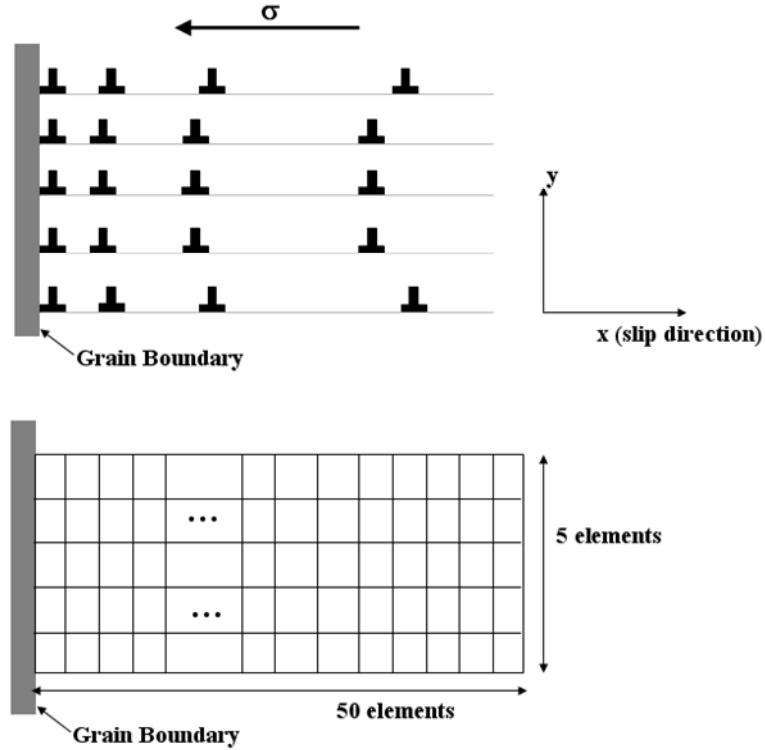
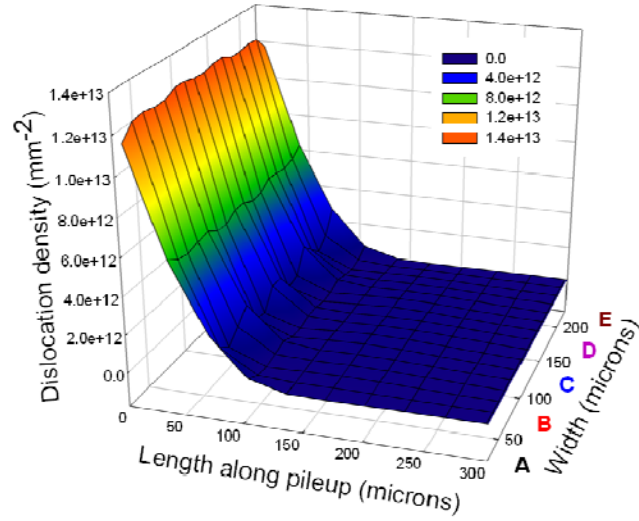


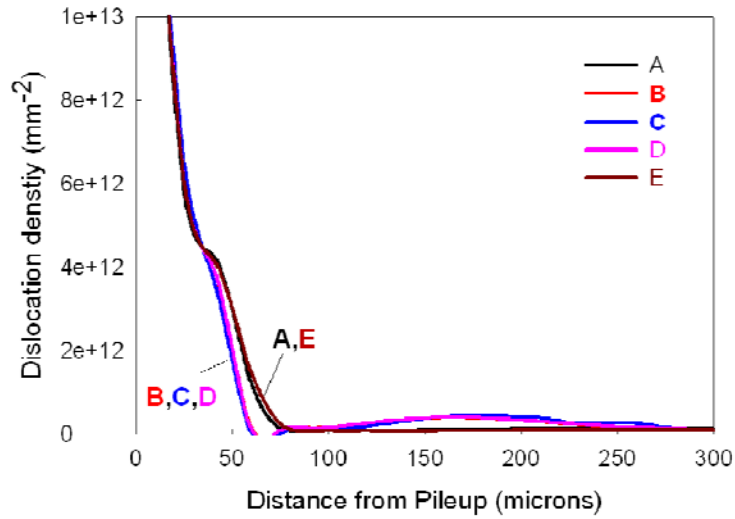
Figure A.9: 2D dislocation pileup: multi-layer pileup of discrete dislocations and corresponding mesh.

The equilibration of 2D pileup follows similar procedure as that of 1D problem. As shown in Figure A.9, the pileup of discrete edge dislocations with multi-layer pileups near the grain boundaries is considered. A mesh of 50×5 elements is used with dimensions of $300 \times 125 \mu\text{m}$. A constant stress of $10^{-5} \mu$, to the direction of slip is applied and a total of 2,500 dislocations with Burger's vector, $b=0.25\text{nm}$, is equilibrated using non-constraint method. The equilibrated dislocation density of 2D pileup is shown in Figure A.10 (a) and (b). The dislocations are accumulated near the boundary similar to

1D pileup and the distribution along the y-direction is almost uniform in this particular example as shown in Figure A.10 (b).



(a)



(b)

Figure A.10: 2D dislocation distribution in pileup under constant stress in the pileup direction: (a) surface plot, and (b) profiles along constant y-path.

APPENDIX B: Interaction Force Between Two Edge Dislocation Segments

In this section, the glide force on an edge dislocation segment (1) by a parallel edge dislocation segment (2) with parallel Burgers vectors is derived. The position vector from the centers of segment (1) to segment (2) is $\vec{r} = r_1 \hat{\mathbf{x}} + r_2 \hat{\mathbf{y}} + r_3 \hat{\mathbf{z}}$. dl_1 and dl_2 are segment lengths; and the Cartesian coordinate system is as shown in Figure 4.3 ($\hat{\mathbf{x}}$ = glide direction $\hat{\mathbf{z}}$ = line direction). Following the approach of Hirth and Lothe (Hirth and Lothe, 1969), the force on dl_1 by the segment $y_1 y_2$ is given as

$$\delta \mathbf{F} = \delta \mathbf{F}(y_2 - x_1) - \delta \mathbf{F}(y_1 - x_1) \quad (\text{B.1})$$

where $\delta \mathbf{F}$ is a total force acting on dl_1 . When $y_2 \rightarrow y_1$,

$$\frac{d\delta \mathbf{F}}{dl_2} = \lim_{y_2 \rightarrow y_1} \frac{\delta \mathbf{F}(y_2, x_1) - \delta \mathbf{F}(y_1, x_1)}{y_2 - y_1} = \frac{d\delta \mathbf{F}(y, x_1)}{dy} \quad (\text{B.2})$$

By assuming Burgers vector is in $\mathbf{e}_2$ direction and considering only the glide component,

$\delta \mathbf{F}(y, x)$ can be represented as:

$$\delta \mathbf{F}(y, x) = \frac{\mu b_1 b_2}{4\pi(1-\nu)} \frac{r_1}{R(R+r_3)} \left[1 - \frac{r_2^2}{R^2} - \frac{r_2^2}{R(R+r_3)} \right] dl_1 \quad (\text{B.3})$$

where $R = \sqrt{r_1^2 + r_2^2 + (y-x)^2}$. Equation (B.3) can be rewritten as:

$$\delta \mathbf{F} = \delta \mathbf{F}(y_2 - x_1) - \delta \mathbf{F}(y_1 - x_1) = \frac{\mu b_1 b_2}{4\pi(1-\nu)} \sum_{k=1}^N \Delta f_i^k \quad (\text{B.4})$$

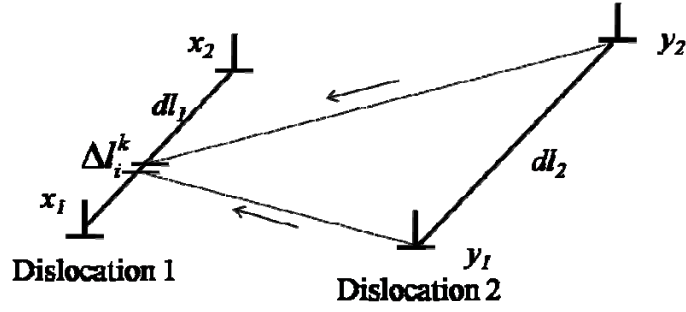


Figure B.1: Interaction between two segmented edge dislocations

$$\begin{aligned}
 \Delta f_i^k &= \left[\frac{r_1}{R(R+r_3)} \left(1 - \frac{r_2^2}{R^2} - \frac{r_2^2}{R(R+r_3)} \right) \Delta I_i^k \right]_{y_1}^{y_2} \\
 &= \left[\frac{r_1}{R_2(R_2+r_{32})} \left(1 - \frac{r_2^2}{R_2^2} - \frac{r_2^2}{R_2(R_2+r_{32})} \right) \Delta I_i^k \right] \\
 &\quad - \left[\frac{r_1}{R_1(R_1+r_{32})} \left(1 - \frac{r_2^2}{R_1^2} - \frac{r_2^2}{R_1(R_1+r_{31})} \right) \Delta I_i^k \right]
 \end{aligned} \tag{B.5}$$

where $R_1 = R(y_1, x)$, $R_2 = R(y_2, x)$

$$\begin{aligned}
 \delta F &= \frac{\mu b_1 b_2}{4\pi(1-\nu)} \int_{x_1}^{x_2} \left[\frac{r_1}{R_2(R_2+r_{32})} \left(1 - \frac{r_2^2}{R_2^2} - \frac{r_2^2}{R_2(R_2+r_{32})} \right) \right] dx \\
 &\quad - \frac{\mu b_1 b_2}{4\pi(1-\nu)} \int_{x_1}^{x_2} \left[\frac{r_1}{R_1(R_1+r_{31})} \left(1 - \frac{r_2^2}{R_1^2} - \frac{r_2^2}{R_1(R_1+r_{31})} \right) \right] dx
 \end{aligned} \tag{B.6}$$

Integrating the right term,

$$\mathbf{F} = \left[\frac{\mu b_1 b_2}{4\pi(1-\nu)} \left[\frac{r_1}{r_1^2 + r_2^2} \right] \left[\frac{r_2^2}{R} + (x+R) \left(\frac{r_1^2 - r_2^2}{r_1^2 + r_2^2} \right) \right] \right]_{x_1, y_2}^{x_2, y_2} - \left[\frac{\mu b_1 b_2}{4\pi(1-\nu)} \left[\frac{r_1}{r_1^2 + r_2^2} \right] \left[\frac{r_2^2}{R} + (x+R) \left(\frac{r_1^2 - r_2^2}{r_1^2 + r_2^2} \right) \right] \right]_{x_1, y_1}^{x_2, y_1} \quad (\text{B.7})$$

Then the force per unit length applied on the first edge dislocation can be represented as:

$$\frac{F_{\text{glide}}}{dl_1} = \frac{\mu b_1 b_2}{4\pi(1-\nu)} \frac{1}{(x_2 - x_1)} \left[\frac{r_1}{r_1^2 + r_2^2} \right] [g_{11} + g_{22} - g_{12} - g_{21}] \quad (\text{B.4})$$

Where $g_{ij} = \sqrt{\frac{r_2^2}{R_{ij}} + (x + R_{ij}) \left(\frac{r_1^2 - r_2^2}{r_1^2 + r_2^2} \right)}$. For 1D case ($r_1 = r$, $r_2 = r_3 = 0$), equation (B.4)

can be reduced to

$$\frac{F_{\text{glide}}}{dl_1} = \frac{\mu b_1 b_2}{4\pi(1-\nu)} \left[\frac{1}{r(x_2 - x_1)} \right] [g'_{11} + g'_{22} - g'_{12} - g'_{21}] \quad (\text{B.5})$$

Where $g'_{ij} = \sqrt{r^2 + (y_j - x_i)^2}$.

APPENDIX C: Slip systems for FCC and BCC

FCC					
Slip system	Slip normal	Slip direction	Slip system	Slip normal	Slip direction
1	(111)	$[1\bar{1}0]$	7	$(\bar{1}11)$	$[110]$
2	(111)	$[10\bar{1}]$	8	$(\bar{1}11)$	$[\bar{1}\bar{1}1]$
3	(111)	$[01\bar{1}]$	9	$(\bar{1}11)$	$[10\bar{1}]$
4	$(\bar{1}11)$	$[110]$	10	(111)	$[1\bar{1}0]$
5	$(\bar{1}11)$	$[101]$	11	(111)	$[101]$
6	$(\bar{1}11)$	$[01\bar{1}]$	12	(111)	$[011]$
BCC					
Slip system	Slip normal	Slip direction	Slip system	Slip normal	Slip direction
1	(011)	$[11\bar{1}]$	13	$(\bar{2}1\bar{1})$	$[\bar{1}\bar{1}1]$
2	(101)	$[11\bar{1}]$	14	$(1\bar{2}\bar{1})$	$[\bar{1}\bar{1}1]$
3	$(1\bar{1}0)$	$[11\bar{1}]$	15	(112)	$[\bar{1}\bar{1}1]$
4	$(01\bar{1})$	$[1\bar{1}\bar{1}]$	16	$(\bar{2}\bar{1}\bar{1})$	$[\bar{1}11]$
5	(101)	$[1\bar{1}\bar{1}]$	17	$(12\bar{1})$	$[\bar{1}11]$
6	(110)	$[1\bar{1}\bar{1}]$	18	$(1\bar{1}2)$	$[\bar{1}11]$
7	(011)	$[1\bar{1}1]$	19	$(21\bar{1})$	$[1\bar{1}1]$
8	$(10\bar{1})$	$[1\bar{1}1]$	20	$(\bar{1}2\bar{1})$	$[1\bar{1}1]$
9	(110)	$[1\bar{1}1]$	21	$(\bar{1}12)$	$[1\bar{1}1]$
10	$(01\bar{1})$	$[111]$	22	$(2\bar{1}\bar{1})$	$[111]$
11	$(10\bar{1})$	$[111]$	23	$(\bar{1}2\bar{1})$	$[111]$
12	$(1\bar{1}0)$	$[111]$	24	$(\bar{1}\bar{1}2)$	$[111]$

APPENDIX D: Grain Orientations for 6 Minimum Alloy Steel Samples

Sample 1											
Grain	φ_1	Φ	φ_2	Grain	φ_1	Φ	φ_2	Grain	φ_1	Φ	φ_2
1	62.6	20.0	276.3	4	354.6	17.9	332.9	7	305.0	42.6	55.7
2	161.2	44.3	236.0	5	90.1	35.1	233.9	8	160.4	48.5	209.7
3	34.0	20.9	302.5	6	112.3	45.1	253.5	9	286.2	27.7	91.8
Sample 2											
Grain	φ_1	Φ	φ_2	Grain	φ_1	Φ	φ_2	Grain	φ_1	Φ	φ_2
1	95.9	2.5	292.2	6	199.6	33	192	11	147	44.3	256.5
2	220.1	16.8	148.3	7	104.9	26.2	237.7	12	341.6	49.4	51.8
3	233.8	26.9	138.2	8	293.6	42.7	50.2	13	48.2	40.6	311.4
4	201.9	39.2	140.4	9	129.3	28.3	212.4				
5	74.3	25.4	273.2	10	152.7	28.3	201.6				
Sample 3											
Grain	φ_1	Φ	φ_2	Grain	φ_1	Φ	φ_2	Grain	φ_1	Φ	φ_2
1	189.7	50.5	180.7	7	241	15.8	87.8	13	197.5	23.5	151.1
2	103.8	43.9	211.6	8	23.6	19.7	306.3	14	191.6	575	192.2
3	24.3	4.2	327.2	9	172.8	33.6	214.1	15	207.8	13.5	131.4
4	283.0	13.7	43.1	10	15.9	18.7	2.6	16	220.0	22.1	121.8
5	253.5	40.3	140.7	11	273.9	20.6	84.5	17	266.3	20.3	124.1
6	246.1	36.7	104.9	12	43.5	30.5	357.2				
Sample 4											
Grain	φ_1	Φ	φ_2	Grain	φ_1	Φ	φ_2	Grain	φ_1	Φ	φ_2
1	108.6	46.7	244.4	12	180.0	44.6	225.1	23	285.9	43.0	33.0
2	1.2	22.3	28.2	13	178.2	44.5	138.7	24	163.4	50.6	226.9
3	324.5	19.7	352.1	14	194.0	45.9	130.5	25	94.4	37.0	267.1
4	284.6	43.8	103.8	15	2.7	32.9	36.9	26	155.0	37.8	195.7
5	121.5	49.6	256.9	16	168.2	47.0	144.3	27	89.3	36.6	263.6
6	116.0	44.8	261.1	17	306.0	42.3	12.6	28	284.7	39.6	39.7
7	234.4	37.0	151.4	18	181.3	37.3	223.0	29	22.3	42.0	309.9
8	155.0	20.7	251.2	19	295.4	44.1	26.2	30	196.0	36.9	134.0
9	164.7	28.9	152.4	20	57.0	52.1	326.1	31	17.1	36.0	313.5
10	157.5	32.7	157.9	21	23.0	18.5	9.3	32	310.2	49.1	66.9
11	170.0	36.6	146.4	22	358.4	14.5	32.1				
Sample 5											
Grain	φ_1	Φ	φ_2	Grain	φ_1	Φ	φ_2	Grain	φ_1	Φ	φ_2
1	55.8	52.5	331.0	13	40.2	11.9	322.0	25	86.8	38.6	271.9

2	59.8	57.0	321.0	14	169.6	30.6	170.3	26	259.1	37.4	102.3
3	218.2	42.2	181.3	15	71.0	18.3	296.4	27	283.1	34.6	72.3
4	58.8	60.9	298.1	16	81.5	28.7	285.3	28	128.7	23.2	227.9
5	38.0	41.9	357.5	17	138.7	16.5	215.0	29	350.1	40.3	6.6
6	226.1	33.8	175.4	18	93.8	14.6	271.8	30	198.7	2.9	194.4
7	167.3	21.5	202.4	19	74.9	46.1	281.0	31	355.7	21.1	44.2
8	200.4	24.5	161.5	20	254.8	36.4	102.5	32	330.7	49.6	28.9
9	180.6	33.2	184.9	21	84.3	7.1	318.3	33	329.9	12.8	66.2
10	71.5	37.9	293.1	22	248.3	32.2	110.5	34	202.8	27.1	140.7
11	239.5	11.2	160.6	23	258.2	36.1	96.8				
12	77.6	43.2	297.2	24	272.1	26.8	80.7				
Sample 6											
Grain	φ_1	Φ	φ_2	Grain	φ_1	Φ	φ_2	Grain	φ_1	Φ	φ_2
1	59.7	30.7	301.0	14	306.5	51.1	30.9	27	162.6	38.8	189.0
2	353.0	13.3	26.9	15	294.0	19.6	97.7	28	358.6	10.2	14.9
3	24.2	15.0	357.3	16	54.4	54.1	326.9	29	163.1	1.6	212.4
4	326.9	37.9	40.8	17	261.7	18.0	111.7	30	215.7	36.1	152.9
5	44.9	52.9	299.0	18	43.5	45.7	315.8	31	297.3	20.2	21.6
6	318.7	9.0	61.2	19	237.4	14.5	137.5	32	226.5	13.8	173.1
7	293.8	29.0	106.5	20	4.6	43.0	343.4	33	225.3	16.2	172.9
8	218.1	23.4	129.7	21	87.7	34.5	310.3	34	74.0	38.5	285.0
9	189.1	37.8	161.9	22	207.9	22.8	167.8	35	239.5	39.3	75.9
10	281.5	31.0	73.6	23	48.1	20.4	349.2	36	336.3	43.1	6.6
11	21.1	31.1	22.6	24	225.1	46.9	119.3	37	260.7	20.9	124.6
12	24.1	36.5	346.6	25	133.2	8.0	246.6	38	134.6	15.0	204.7
13	109.8	44.7	237.2	26	291.9	41.3	71.7	39	102.4	36.8	287.9