To my parents, my wife, and my daughter
ACKNOWLEDGMENTS

From the bottom of my heart, I am grateful for the mentoring, guidance, and care from my advisor, Dr. Douglas Spearot. Including my master and Ph.D. times, I have worked under his supervision for 6 years. Needless to say, it has been a great journey for me to grow both professionally and personally. Throughout this journey, he has always been there for me, from my first conference presentation to my final Ph.D. defense or from my first manuscript to the final conclusion of this Ph.D. dissertation. During all of my personal struggles and difficulties, he has always been caring and supportive. I could not have asked for a greater mentor, who always puts his students, their success, and happiness above all. I owe him everything that I have achieved in my career.

I would also like to thank the other members of my doctoral committee: Dr. Arakere, Dr. Chen, and Dr. Phillip for the time and energy they have invested in this process. I would like to especially acknowledge Dr. Laurent Capolungo of Los Alamos National Laboratory for his guidance and support during my Ph.D. career. Working with an expert from a different simulation length scale has been an eye-opening experience for me. It helps me to understand the connection between different simulation techniques as well as the important connection between simulations and experiments.

This journey would not have been possible without the support of my family and friends. I am grateful for the unconditional support and love from my parents. They taught me to be happy, to be confident about myself, and to care for others. Following my parents’ footsteps as a Ph.D. in Mechanical Engineering, I have become familiar and recognize the challenges and difficulties in the work-life balance that they faced during their time. I am also thankful for my better half, Trang, for her constant love and
support for my goals and aspirations. Needless to say, my Ph.D. journey in the past several years has not been a smooth ride, both academically and personally. I truly thank Trang for sticking by my side, even when I had doubt about myself. I am thankful to my daughter Hannah for giving me strength and happiness to overcome all the challenges during the last year and a half.

I am also thankful for the members of Dr. Spearot’s research group: Brandon Witbeck, Darshan Barney, Doruk Aksoy, Luo Ke, and Robert Slapikas. Transferring to the University of Florida for my Ph.D. degree, this group of friends has become my second family. The debate, lunch, and group hangout as well as editing advice, ride to the airport, moving help, and friendship from you guys are deeply appreciated.
# TABLE OF CONTENTS

ACKNOWLEDGMENTS........................................................................................................... 4

LIST OF TABLES.................................................................................................................. 8

LIST OF FIGURES.................................................................................................................. 9

LIST OF ABBREVIATIONS.................................................................................................... 14

ABSTRACT............................................................................................................................ 16

CHAPTER............................................................................................................................... 18

1 INTRODUCTION .................................................................................................................. 18

1.1 What is a Dislocation? ........................................................................................................ 18
1.2 Role of Dislocations and Their Interaction with Other Defects in Metals ............ 19
1.3 Previous Dislocation Property Studies in FCC Metals ................................................. 22
   1.3.1 The Core Structure and the Peierls Stress of Dislocation in FCC Metals .......... 23
   1.3.2 The Mobility of Dislocations ................................................................................. 28
   1.3.3 Curved Dislocations and Dislocation Loops ......................................................... 32
   1.3.4 Summary of Prior Dislocation Studies ................................................................. 34
1.4 Goals and Objectives ........................................................................................................ 35

2 THEORY OF ATOMIC SIMULATION ............................................................................... 45

2.1 Atomistic Simulations ...................................................................................................... 45
2.2 Molecular Statics ............................................................................................................... 48
2.3 Molecular Dynamics Simulation ..................................................................................... 52
   2.3.1 The Microcanonical (NVE) Ensemble .................................................................... 52
   2.3.2 The Canonical (NVT) and the Isothermal-Isobaric (NPT) Ensembles ............... 53
   2.3.3 Molecular Dynamics Integration Algorithm and Initial Conditions ................. 55
   2.3.4 Virial Stress ............................................................................................................ 56
2.4 Interatomic Potential ......................................................................................................... 58
   2.4.1 Overview ................................................................................................................. 58
   2.4.2 The Embedded-Atom Method ................................................................................. 60

3 THEORY OF DISLOCATIONS ............................................................................................ 66

3.1 The Volterra Displacement Field of Infinitely Straight Dislocations .................... 66
3.2 The Displacement Field of a Triangular Dislocation Loop ....................................... 68
3.3 Dislocation Core Structure of FCC Metals ................................................................. 70

4 PRESSURE DEPENDENCE OF THE PEIERLS STRESS IN ALUMINUM* ............. 76
4.1 Background ........................................................................................................... 76
4.2 Simulation Methods .............................................................................................. 77
4.3 Results and Analysis ........................................................................................... 80
4.4 Summary ............................................................................................................... 83

5 STRESS STATE DEPENDENCE OF THE MOBILITY LAW IN ALUMINUM .......... 89
5.1 Background ......................................................................................................... 89
5.2 Simulation Methods ............................................................................................ 90
  5.2.1 Simulation Code and Interatomic Potential ...................................................... 90
  5.2.2 Mobility of Straight Dislocation and the Role of Stress State ......................... 90
5.3 Results and Analysis ............................................................................................ 93
  5.3.1 The Role of Interatomic Potential on the Mobility of Straight Dislocations ................................................................. 93
  5.3.2 Phonon Drag of Straight Dislocation and the Role of Stress State ............... 96
  5.3.3 Radiative Damping of Straight Dislocation and the Role of Stress State .... 101
5.4 Summary ............................................................................................................. 106

6 PROPERTIES OF NANOSCALE DISLOCATION SHEAR LOOP* ..................... 129
6.1 Background ......................................................................................................... 129
6.2 Simulation Methods ............................................................................................ 131
  6.2.1 Dislocation Shear Loop Algorithm ................................................................. 132
  6.2.2 Simulation Cell Geometries ............................................................................ 135
6.3 Results and Analysis ............................................................................................ 138
  6.3.1 Static Equilibrium Size and Shape of Dislocation Loops .............................. 138
  6.3.2 Temperature Dependence of the Effective Lattice Friction Stress ............... 141
  6.3.3 Expansion of the Dislocation Shear Loop under a Constant Schmid stress ........................................................................... 144
6.4 Summary ............................................................................................................. 147

7 CONCLUSIONS ...................................................................................................... 164
7.1 General Implications ........................................................................................... 164
7.2 Impact and Future Works .................................................................................... 165

LIST OF REFERENCES ................................................................................................. 169

BIOGRAPHICAL SKETCH ......................................................................................... 179
<table>
<thead>
<tr>
<th>Table</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-1</td>
<td>Dislocation character angle, lattice orientations and sizes for each simulation model.</td>
<td>84</td>
</tr>
<tr>
<td>4-2</td>
<td>Peierls Stress for each dislocation character angle.</td>
<td>84</td>
</tr>
<tr>
<td>5-1</td>
<td>Dislocation core width and stacking fault energies for different EAM potentials.</td>
<td>108</td>
</tr>
<tr>
<td>5-2</td>
<td>Damping parameters for different dislocation character angle under pure Schmid stress.</td>
<td>108</td>
</tr>
<tr>
<td>6-1</td>
<td>Stress tensor required to generate a state of pure Schmid stress in the dislocation loop slip plane.</td>
<td>149</td>
</tr>
<tr>
<td>Figure</td>
<td>Description</td>
<td>Page</td>
</tr>
<tr>
<td>--------</td>
<td>-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------</td>
<td>------</td>
</tr>
<tr>
<td>1-1</td>
<td>TEM micrograph showing the microstructure of Fe-20Mn-1.3C-3Cu steel at a true strain of 0.02</td>
<td>37</td>
</tr>
<tr>
<td>1-2</td>
<td>The stacking sequence of crystalline planes demonstrating prismatic dislocation loops formed from the clustering of the disc-shaped platelets</td>
<td>38</td>
</tr>
<tr>
<td>1-3</td>
<td>Schematic of a dislocation shear loop</td>
<td>38</td>
</tr>
<tr>
<td>1-4</td>
<td>Bright field TEM images of a UO$_2$ polycrystalline thin foil with marked prismatic dislocation loops</td>
<td>39</td>
</tr>
<tr>
<td>1-5</td>
<td>Deformation mechanism map of Al with a wide grain size range</td>
<td>39</td>
</tr>
<tr>
<td>1-6</td>
<td>View along the dislocation line of the core structure of the 60° dislocation</td>
<td>40</td>
</tr>
<tr>
<td>1-7</td>
<td>GSF energy curves for Al using EAM potentials compared to DFT results</td>
<td>40</td>
</tr>
<tr>
<td>1-8</td>
<td>Variation of the relative dislocation core energies for dissociated and undissociated screw dislocations as a function of normalized displacement traveled by the dislocation core</td>
<td>41</td>
</tr>
<tr>
<td>1-9</td>
<td>Variation of the Peierls stress with increasing Escaig stress for a screw dislocation in Cu</td>
<td>42</td>
</tr>
<tr>
<td>1-10</td>
<td>Al screw dislocation velocity as a function of the applied shear stress</td>
<td>42</td>
</tr>
<tr>
<td>1-11</td>
<td>Schematic of the three dynamic regimes observed in simulations of dislocation mobility</td>
<td>43</td>
</tr>
<tr>
<td>1-12</td>
<td>Snapshots of dislocation loop dynamics at 0, 2.5, 5 and 10ps with three different dislocation mobility laws</td>
<td>43</td>
</tr>
<tr>
<td>1-13</td>
<td>Influence of Escaig stress effect on the velocity versus the Schmid stress for screw dislocations in Cu</td>
<td>44</td>
</tr>
<tr>
<td>1-14</td>
<td>FR source operation using the Ercolessi-Adams Al EAM potential. Only atoms in the dislocation cores and ISF areas are shown. The orientation of applied stress and dislocation line senses (curved arrows) are also indicated...</td>
<td>44</td>
</tr>
<tr>
<td>2-1</td>
<td>Schematic of 2-D periodic boundary conditions in atomistic simulations</td>
<td>63</td>
</tr>
<tr>
<td>2-2</td>
<td>Graphical illustration of methods for energy minimization calculations</td>
<td>64</td>
</tr>
<tr>
<td>2-3</td>
<td>Diagram of types of interatomic potentials. Arrows point in the direction of increasing complexity.</td>
<td>65</td>
</tr>
</tbody>
</table>
3-1 Volterra displacement field of a right-handed screw dislocation .................... 73
3-2 Volterra displacement field of an edge dislocation ....................................... 73
3-3 Geometry associated with a triangular dislocation loop ................................ 74
3-4 The plane triangle ABC and its projection, the spherical triangle A'B'C', on the unit sphere .................................................................................................................. 74
3-5 Construction of a dislocation loop with complex geometry via addition and subtraction of triangular displacement fields .................................................. 75
3-6 Stacking faults in FCC metals ........................................................................... 75
4-1 Simulation cell after imposing the modified Volterra fields ............................... 85
4-2 Energy variation versus top layer displacement in the Burgers vector direction. Energy variation is computed relative to the original energy of the dislocation model .............................................................. 86
4-3 Peierls stress for screw, 30°, 60°, and edge dislocations using different EAM potentials ......................................................................................................................... 87
4-4 Deviation of the SFWs from integral multiples of the Peierls period for different EAM potentials ................................................................. 88
5-1 Simulation cell with a straight dislocation has 3 different regions. Blue: boundary region, yellow: thermostat region, and green: mid region. The dislocation core structure is colored red. ........................................... 108
5-2 Dislocation velocity versus Schmid stress for different EAM potentials ........... 109
5-3 Example dislocation velocity versus time for an edge dislocation under a Schmid stress of 100 MPa ................................................................. 110
5-4 Phonon drag coefficients for edge, screw, 30°, and 60° dislocations at 100K compared to Cho et al. and interpolation functions in DDD simulations ........... 111
5-5 Phonon drag coefficients for the edge, screw, 30°, and 60° dislocations at 100K .......................................................................................... 112
5-6 Dislocation core structure of the 60° dislocation .............................................. 113
5-7 Phonon drag coefficients for edge (black), screw (blue), 30° (red), and 60° (green) dislocations at 100K .............................................................. 113
5-8 Phonon drag coefficients and average SFW for different state of stress. Blue: positive, green: zero, and red: negative values. Circle: screw, triangle: 30°, square: 60°, and diamond: edge dislocations ........................................... 114
5-9 Mobility data and curves for different dislocation character angles under pure Schmid stress. 

5-10 Comparison between critical velocities and the minimum phase velocities for different dislocation character angles under pure Schmid stress.

5-11 Mobility data and curves for screw dislocations under different pressures normal to the (111) slip plane and Schmid stresses.

5-12 Mobility data and curves for 30° dislocations under different pressures normal to the (111) slip plane and Schmid stresses.

5-13 Mobility data and curves for 60° dislocations under different pressures normal to the (111) slip plane and Schmid stresses.

5-14 Mobility data and curves for edge dislocations under different pressures normal to the (111) slip plane and Schmid stresses.

5-15 Power law exponent for screw and 60° dislocations under different pressures normal to the (111) slip plane and Schmid stresses.

5-16 Mobility data and curves for screw dislocations under different Escaig and Schmid stresses.

5-17 Mobility data and curves for 30° dislocations under different Escaig and Schmid stresses.

5-18 Mobility data and curves for 60° dislocations under different Escaig and Schmid stresses.

5-19 Mobility data and curves for edge dislocations under different Escaig and Schmid stresses.

5-20 Power law exponent for screw and 60° dislocations under different Escaig and Schmid stresses.

5-21 Dislocation core widths of edge and 30° dislocations under different combinations of Schmid stress, Escaig stress, and pressure normal to the (111) slip plane.

5-22 Dislocation core widths of screw and 60° dislocations under different combinations of Schmid stress, Escaig stress, and pressure normal to the (111) slip plane.

6-1 Bisection algorithm to determine the resolved Schmid stress necessary for dislocation loop equilibrium at 0 K.
Bisection algorithm to determine the minimum resolved Schmid stress necessary to expand each dislocation loop at finite temperature .................. 150

Schematic of the “plate” simulation cell with a dislocation loop. ...................... 150

Equilibrium resolved Schmid stress for different loop radii and different Al EAM potentials ............................................................................................................. 151

Temperature dependence of elastic properties in Al predicted by different EAM potentials ............................................................................................................. 152

Statics properties of dislocation loops in Al ......................................................... 153

Temperature effects on different stress for different starting dislocation loop radius in Al ............................................................................................................. 154

Normalized stress field with \( \tau_{ss} \) around edge and screw segments of dislocation loop with different dislocation loop radius ........................................... 155

Snapshots of dislocation shear loop under pure Schmid stress of 380 MPa at different time steps. The locations of dislocation segments are marked as red. ............................................................................................................. 156

Dislocation velocity versus Schmid stress for 60° types of dislocations using the Zope and Mishin potential ............................................................................................................. 157

Snapshots of dislocation shear loop under the Schmid stress of 380 MPa and compressive pressure normal to the (111) slip plane of 500 MPa at 100 K and different time steps. ............................................................................................................. 158

Snapshots of dislocation shear loop under the Schmid stress of 380 MPa and tensile pressure normal to the (111) slip plane of -500 MPa at 100 K and different time steps. ............................................................................................................. 159

Snapshots of dislocation shear loop under the Schmid stress of 380 MPa and the Escaig stress of -250 MPa at 100 K and different time steps. ...................... 160

Snapshots of dislocation shear loop under the Schmid stress of 380 MPa and the Escaig stress of 250 MPa at 100 K and different time steps ...................... 161

Dislocation core widths at different locations on the dislocation loops under different pressures normal to the (111) slip plane at different time. .............. 162

Dislocation core widths at different locations on the dislocation loops under different Escaig stress at different time .......................................................... 163
7-1 Comparison between MD and DDD data at 300 and 400 K. The core width parameter in DDD is tuned to match the MD data using the temperature dependence of the elastic moduli and friction stress extracted from MD........ 167

7-2 Simulation setting of a system with a dislocation loop and two \( \Sigma 3(112) \) grain boundaries. Only atoms with the centrosymmetry values greater than 2 Å² are shown................................................................. 168
<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Å</td>
<td>Ångström</td>
</tr>
<tr>
<td>BCC</td>
<td>Body centered cubic</td>
</tr>
<tr>
<td>CAC</td>
<td>Concurrent atomistic-continuum</td>
</tr>
<tr>
<td>CG</td>
<td>Conjugate gradient</td>
</tr>
<tr>
<td>DDD</td>
<td>Discrete dislocation dynamics</td>
</tr>
<tr>
<td>DFT</td>
<td>Density functional theory</td>
</tr>
<tr>
<td>DXA</td>
<td>Dislocation Extraction Algorithm</td>
</tr>
<tr>
<td>EAM</td>
<td>Embedded atom method</td>
</tr>
<tr>
<td>FCC</td>
<td>Face centered cubic</td>
</tr>
<tr>
<td>FIRE</td>
<td>Fast Inertial Relaxation Engine</td>
</tr>
<tr>
<td>FR</td>
<td>Frank-Read</td>
</tr>
<tr>
<td>GSFE</td>
<td>Generalized stacking fault energy</td>
</tr>
<tr>
<td>HCP</td>
<td>Hexagonal close packed</td>
</tr>
<tr>
<td>LAMMPS</td>
<td>Large-scale Atomic/Molecular Massively Parallel Simulator</td>
</tr>
<tr>
<td>MD</td>
<td>Molecular dynamics</td>
</tr>
<tr>
<td>MEAM</td>
<td>Modified embedded atom method</td>
</tr>
<tr>
<td>NEB</td>
<td>Nudged elastic band</td>
</tr>
<tr>
<td>NPT</td>
<td>Isothermal-isobaric ensemble</td>
</tr>
<tr>
<td>NVE</td>
<td>Microcanonical ensemble</td>
</tr>
<tr>
<td>NVT</td>
<td>Canonical ensemble</td>
</tr>
<tr>
<td>OFDFT</td>
<td>Orbital-free density functional theory</td>
</tr>
<tr>
<td>OVITO</td>
<td>Open Visualization Tool</td>
</tr>
<tr>
<td>PBC</td>
<td>Periodic boundary condition</td>
</tr>
<tr>
<td>PN</td>
<td>Peierls-Nabarro</td>
</tr>
<tr>
<td>Abbreviation</td>
<td>Full Form</td>
</tr>
<tr>
<td>--------------</td>
<td>-----------</td>
</tr>
<tr>
<td>SF</td>
<td>Stacking fault</td>
</tr>
<tr>
<td>SFW</td>
<td>Stacking fault width</td>
</tr>
<tr>
<td>SIA</td>
<td>Self interstitial atom</td>
</tr>
<tr>
<td>SVPN</td>
<td>Semi-discrete variational Peierls – Nabarro</td>
</tr>
<tr>
<td>TEM</td>
<td>Transmission electron microscopy</td>
</tr>
</tbody>
</table>
Plastic deformation is governed by the motion of dislocations. The objective of this dissertation is to investigate dislocation properties in Al such as core structures, the Peierls stress, the mobility of dislocations, and the role of stress state on these properties. First, the effects of local stress state on the movement of edge, screw, 30°, and 60° straight dislocations are studied via atomistic simulations. In general, a negative Escaig stress or compressive pressure decreases the mobility, while a positive Escaig stress or tensile pressure increases the mobility of a dislocation. Moreover, the role of local stress state on the mobility of dislocations varies for different dislocation character angles and applied Schmid stresses. The combined effects of the Escaig stress and pressure applied normal to the (111) slip plane on the Peierls stress and the mobility of each dislocation is correlated to the role of stress state on the dislocation core structure and the direction of dislocation motion. Second, static and finite temperature properties of nanoscale dislocation shear loops are investigated. Dislocation loops with different sizes and shapes are created via superposition of elemental triangular dislocation displacement fields in the presence of an externally imposed shear stress. It is found that the equilibrium shape of a dislocation loop becomes more circular with increasing
loop size. An approach is presented to compute the effective lattice friction stress, including temperature dependence, for dislocation loops in Al. The temperature dependence of the effective lattice friction stress can be reliably computed for dislocation loops larger than 16.2 nm. When subjected to a pure Schmid stress, the ellipsoidal dislocation loop becomes faceted in the screw and 60° segments during motion due to the much lower mobility of these two dislocation character angles. As the dislocation loop moves at velocities associated with the radiative damping regime, it becomes asymmetric due to the difference in mobility between the 60° and 120° dislocations. The role of both Escaig stress and pressure normal to the (111) slip plane on the core structure and the mobility of dislocation loops is consistent with results for straight dislocations.
CHAPTER 1
INTRODUCTION

1.1 What is a Dislocation?

Dislocations are line defects associated with plastic deformation in crystalline materials and are characterized by a Burgers vector magnitude and direction \([1,2]\). The core of a dislocation exists along a line within the crystal lattice; thus, dislocations are known as linear defects, distinguishing them from point defects, such as vacancies or interstitials, and planar defects, such as grain boundaries. Dislocations usually appear in curves or loops, as shown in Figure 1-1. Dislocation loops can be categorized into prismatic, glide/shear, or mixed types based on the relative alignment between the Burgers vector and the slip plane \([1,2]\). As shown in Figure 1-2, the Burgers vector of a prismatic dislocation loop is perpendicular to the slip plane. Prismatic dislocation loops are further categorized into interstitial and vacancy prismatic dislocation loops, depending on the clustering of either missing or extra layers of atoms in the slip plane.

On the other hand, Figure 1-3 shows a dislocation shear loop where the Burgers vector is parallel to the slip plane. The core structure of segments on a dislocation loop with the same Burgers vector varies, depending on the character angle between the dislocation axis and the Burgers vector. Two special cases are where the dislocation axis is perpendicular and parallel to the Burgers vector, which results in edge and screw dislocation segments, respectively. For FCC metals, a dislocation typically dissociates into two Shockley partial dislocations connected by a stacking fault, which is more energetically favorable. For edge and screw dislocations, these partial dislocations are the same type, resulting in symmetric dislocation core structures. On the other hand, mixed dislocations with arbitrary dislocation character angles have partial dislocations of
1.2 Role of Dislocations and Their Interaction with Other Defects in Metals

The nucleation, motion, and interaction of dislocations influence the strength of metals. As shown in [1], the theoretical shear strength of a metal at room temperature is approximately $\mu/15$, where $\mu$ is the shear modulus, while experimental results indicate plastic deformation at stresses on the order of $10^{-9}\mu$. This much lower mechanical strength, compared to the theoretical strength of perfect crystals, can be explained by the presence of dislocations since the stress required to move dislocations is much lower than to break every bond between two planes of atoms.

Dislocations also influence mechanical properties and failure mechanisms such as creep, fracture, void growth, and radiation damage. For instance, the creep strain-rate, which is a constant rate in the secondary stage of creep, is a function of the mobile dislocation density, the Burgers vector, and the dislocation velocity [4]. For steel, the glide of existing dislocations under a creep stress resulted in room temperature creep deformation [4,5]. At room temperature, this mechanism dominates over the common dislocation climb mechanism in creep. Dislocation emission near a crack tip is also essential in the study of crack propagation in ductile materials. The comparison between the critical stress intensity factor for dislocation nucleation versus brittle fracture is considered as a criterion for determining the ductile versus brittle behavior of a metal [6].

Moreover, dislocation plasticity has been shown as the main mechanism for void nucleation, growth, and coalescence at room temperature in the absence of diffusive
effects [7–10]. In particular, the emission of nanoscale dislocation loops (both prismatic and shear) accounted for the growth of voids, which was proved by Lubarda et al. using laser shock experiments on monocrystalline Cu [9]. It was shown that the critical stress required for dislocation nucleation decreased with an increasing void size. This indicated a streamline emission of prismatic and shear dislocation loops, assisting and accelerating the growth of the void. It was also found that the emission rate depended on the dislocation structure. In particular, dislocations with a narrower dislocation core width are more difficult to nucleate than the ones with a wider dislocation core. These nanoscale dislocation loops, with diameters less than 100 nm, were also observed in materials under radiation [11–13] or deformation [14,15]. As shown in Figure 1-4, prismatic dislocation loops formed via the clustering of vacancies have been shown as the primary factor for radiation embrittlement in metals, which is critical for nuclear reactor pressure vessels [16,17].

Since plastic deformation is governed by the motion of dislocations, interactions between dislocations and other defects, which potentially serve as barriers for motion, have a great influence on mechanical hardening and failure mechanisms. Dislocations and their interaction with solute atoms, grain boundaries, and other dislocations also affect the strain hardening of a metal. For example, Al-Mg alloys under severe plastic deformations have higher hardness for higher Mg content due to the increase in dislocation density coupled with the decrease in grain size [18]. Moreover, Tsuru and Chrzan studied the effect of dislocation - solute interaction on dislocation behavior in Mg [19]. The interaction of Y solute atoms with dislocations within Mg shrank the dissociated dislocation in the basal plane. This reduced the energy barrier for
dislocation cross-slip into the prismatic plane significantly since the constriction of partial dislocations on the basal plane accounts for most of the Peierls barrier. As a result, 1 at% of Y increased the yield stress of the basal glide plane by approximately 90 MPa [19]. Void strengthening [20] and irradiation hardening [21] due to the interaction between dislocations and voids have also been observed experimentally in FCC materials. The yield strength of void strengthened Al increased and was sensitive to both the temperature and the strain rate [20]. Computational simulations via molecular dynamics (MD) simulations were performed to study the interaction between edge dislocations and voids in Ni. The void strength increased with increasing void size. The mobility of the dislocation also had a noticeable influence on the behavior of the dislocation – void interaction. The shear stress at which the dislocation bypassed a void was consistently larger by a factor of 1.5 if the shear stress was gradually increased instead of a constant applied stress.

For polycrystals, the interaction between dislocations and grain boundaries is essential. There are four possible scenarios that can happen when the incoming dislocations interact with the grain boundaries [22]: (a) direct slip transmission with slip systems having the same Burgers vector, (b) direct slip transmission, but slip systems have different Burgers vectors, resulting in a residual dislocation in the grain boundary, (c) indirect slip transmission on slip systems that have different Burgers vectors, also leaving a residual boundary dislocation, and (d) no transmission with the impenetrable grain boundaries as predicted by Hall and Petch [23,24]. The ability to predict the outcome consistently is critical and has been the focus of many experimental [25–28] and computational [29–33] works. Indeed, as shown in Figure 1-5 for polycrystals with a
grain size smaller than 70 nm [34], there are other mechanical mechanisms such as
deformation twinning [35], the emission of partial and perfect dislocations [36], and grain
boundary sliding [37]. Except for grain boundary sliding, all of the deformation
mechanisms leading to failure are associated with dislocation – grain boundary
interactions.

1.3 Previous Dislocation Property Studies in FCC Metals

A multiscale approach is required to study dislocations due to its core structure
with atomistic resolution, while its interaction in a network requires significantly larger
space and time domains. Atomistic simulation with its atomic resolution is ideal to study
the dislocation properties and core structure. On the other hand, DDD simulation, in
which the dislocation network is represented as a set of nodes connected by line
segments with distinct Burgers vectors and slip planes [38]. To properly incorporate the
kinematics, kinetics, and interactions of the dislocation network, DDD requires atomistic
dislocation properties such as the dislocation core width, the Peierls stress, and phonon
damping coefficient.

For this work, the focus is on basic dislocation properties such as the core
structures (widths), the Peierls stress, and the mobility of dislocations, which greatly
influence the interaction between a dislocation and itself or other defects [39]. The goal
of this section is to provide an overview of past experimental and computational
attempts to study dislocation properties in FCC metals, especially Al. Due to relatively
low stacking fault energy, dislocations in FCC metals typically dissociate into partial
dislocations on to the \{111\} close-packed planes. Therefore, for FCC metals, the core
structure becomes planar and the main motion of dislocation is the glide of dissociated
dislocations on the \{111\} planes.
1.3.1 The Core Structure and the Peierls Stress of Dislocation in FCC Metals

The Peierls stress is the minimum shear stress to move a dislocation at zero temperature. It can be used as a connection between experiments and simulations when conditions such as thermal vibration and quantum tunneling effects are minimal [39]. Experimentally, there has been a few attempts to study dislocation core structure using high-resolution transmission electron microscopy. Mills and Stadelmann reported a planar dissociated core structure with stacking fault width (SFW) of 0.55 nm for 60° straight dislocations that are part of asymmetric [110] tilt grain boundaries in Al [40]. The core structure of the screw dislocation in nanocrystalline Al has also been found to range from 1.4 – 6.8 nm [41]. Uncertainties come from the curvature of dislocations and the influence of small grain sizes, resulting in high dislocation density. While direct experimental measurements of the Peierls stress for straight dislocations are not yet available, it can be interpreted from the critical resolved shear stress measured by a mechanical deformation test or from the Bordoni internal friction peak [42,43]. For Al, the Peierls stress from the mechanical deformation test ranged from $10^{-4}$ to $10^{-5}$ μ [44], while the estimation from the internal friction measurements ranged from $10^{-2}$ to $10^{-3}$ μ for typical Bordoni peak at 100 to 200 K [45,46] and from $10^{-4}$ to $10^{-5}$ μ for lower temperature [47].

While these experimental works provide some insights on the core structure and the Peierls stress of dislocation, it remains challenging to precisely characterize dislocation core structure and directly measure the Peierls stress due to the atomistic nature of dislocation core [39]. Compared to experiments, computational models of dislocations can be designed to isolate certain dislocation properties or study small
systems of dislocations to gain insight into dislocation interaction mechanisms. For example, atomistic simulations can provide a detailed description of dislocation core structure (cf. [3,48–50]) under the assumption that the interatomic potential provides accurate predictions of the lattice anisotropy and dislocation loop stress field, and can be used to quantify self-interactions or dislocation interactions with grain boundaries [33,51–53]. The Peierls stress of straight dislocations can also be indirectly estimated from the generalized stacking fault energies (GSFE), which can be derived from first-principle calculations or atomistic simulations, based on the framework of the Peierls-Nabarro (PN) model [54,55]. While the PN model is more computationally efficient than atomistic simulations, it still requires the first-principle or atomistic GSFE curve as input. On the other hand, quantum mechanical methods such as density functional theory (DFT) are still computationally expensive for the study of dislocation structures and mobility, and there are often issues with the application of proper boundary conditions. Therefore, atomistic simulation is chosen to study dislocation properties in this work. A more comprehensive description of atomistic simulation is discussed in Chapter 2.

One of the first atomistic simulations to investigate the core structure and the Peierls stress of straight dislocations was Bulatov et al. [48]. Using atomistic simulation with the Ercolessi and Adams potential [56], the effects of pressure normal to the slip plane on the Peierls stress of straight dislocations in Al were investigated and correlated with experimental results of plastic flow pressure dependence [57]. By incrementing the applied shear stress until the dislocation moved, the Peierls stresses of screw and 60° dislocations were found as 82 and 47 MPa, respectively. For both dislocations, the Peierls stresses under positive pressure (compression) increased. This was due to the
interaction between the pressure and the transient change of the dislocation core width. The dislocation core width is transiently expanded when the dislocation moved, as shown in Figure 1-6 where the dislocation core was wider under applied Schmid stress of 0.0007 eV/A³. This transient dislocation core expansion was also consistent with the experimental conclusion that the interaction between the transient expansion of the dislocation core with external pressure caused a pressure-dependent slip in metals [57,58].

This approach was used in subsequent atomistic simulations to study the core structure and the Peierls stress of straight dislocations [3,49,50]. Wang and Fang [50] investigated the core structure and the Peierls stress of the edge dislocation using the Ercolessi and Adams potential [56]. They found the SFW and the Peierls stress of the edge dislocation is about 0.9 nm and 10⁻⁴ μ (about 2.5 MPa, assuming that μ is approximately 25 GPa), respectively. This was in reasonable agreement with the Peierls stress calculated from an experimental deformation test. Pasianot and Moreno-Gobbi focused on the Peierls stress of the screw and 60° straight dislocations using both the Ercolessi and Adams potential [56] and their two developed potentials with the generalized stacking fault (GSF) from first principles calculations [59,60]. Using the Ercolessi and Adams potential [56], the Peierls stress for the screw and 60° straight dislocations were 33.7 – 67.3 MPa and 18.4 – 21.4 MPa, respectively. These values were half of what was reported in previous simulation results by Bulatov et al. [48] using the same interatomic potential because of differences in the boundary conditions. Among the interatomic potentials that they studied, the ones based on the GSF had much less dissociated dislocations. As a result, the Peierls stress for these potentials was approximately an order of magnitude larger. These results from atomistic
Simulations indicated that the core structure and Peierls stress were sensitive to (i) the choice of the boundary conditions and (ii) the accuracy of the semi-empirical many-body interatomic potential.

To systematically account for the image force due to the finite size of the simulation cells, Olmsted et al. proposed a framework to derive the corrections from computing the Peierls stress and the shape of the lattice resistance curve [3]. The differences between uncorrected and corrected simulations were significant, especially for small simulation cells. They also showed that the Peierls stress depended strongly on the dislocation character angle. The Peierls stresses of the screw and 60° dislocations were significantly larger than the edge and 30° dislocations. The accuracy of the semi-empirical EAM potential for Al was compared by Zimmerman and coworkers [61]. In particular, they calculated the GSFE curves for the <112> direction in Al using atomistic simulations with several EAM potentials and compared with DFT results. As shown in Figure 1-7, the GSF curves for various Al EAM potential were different in both the shape and the critical values (intrinsic and unstable stacking fault energies). Interestingly, the Ercolessi and Adams potential [56], which was commonly used for dislocation studies, did not reproduce a sinusoidal curve and reasonable values for the intrinsic and unstable stacking fault energies (γSF and γus, respectively). While the Mishin et al. potential [62] produced results that were closest to the DFT curve, it still underestimated the unstable stacking fault energy, which is critical for dislocation nucleation. Therefore, Zimmerman and collaborators suggested the need for a better EAM potential for Al.
More recent first principle calculations provided two plausible explanations for the wide range of Peierls stresses obtained in simulations and experiments [44,63,64]. Proville et al. showed that a large contribution to the discrepancy between experimental and computational results was the crystal zero-point vibration, which was ignored in atomistic simulation [64]. The kink-pair formation enthalpy was reduced due to the quantization of the crystal vibrational modes. As a result, the flow stress was lower than the classical approximation and in more reasonable agreement with experiments. Moreover, the quantum Peierls stresses using this approach were calculated for straight and kinked dislocations in Fe [63]. Compared to results from atomistic simulation, the quantum Peierls stress was approximately one third for straight dislocations and one half for a kinked dislocation, which was much closer to experimental results.

Shin and Carter showed that the compact core structure of the screw dislocation was another explanation for the discrepancy in the Peierls stress values [44]. As shown in Figure 1-8, a new metastable compact structure for the screw dislocation was found using the orbital-free density functional theory (OFDFT) with the corresponding Peierls stress of $1.1 \times 10^{-2}\mu$, which was in reasonable agreement with typical Bordoni peak measurements (from $10^{-2}$ to $10^{-3}\mu$) [45,46]. On the other hand, the Peierls stresses of the equilibrium dissociated core structure for both the edge and screw dislocations were approximately $10^{-4}$ to $10^{-5}\mu$. These were consistent with experimental results from the mechanical deformation tests and a lower-temperature Bordoni relaxation peak [44]. Depending on the impurities within a crystal, the core structure of screw dislocations could be dissociated or compact, which explained the difference in previous reported Peierls stresses from experiments and simulations.
To understand the role of stress state on the Peierls stress, Liu et al. studied the role of the Escaig stress, which is the shear stress within the slip plane and perpendicular to the Burgers vector, on the Peierls stress of the edge and screw dislocations in Cu using the semi-discrete variational Peierls – Nabarro (SVPN) [65]. As shown in Figure 1-9, the Peierls stress oscillated quasi-periodically and the oscillation gradually decreased with the increase of the Escaig stress. The oscillation in the Peierls stress was due to the variation of the SFW. When the SFW was a multiple of the Peierls period, both partials moved in phase, resulting in the local maximum of the Peierls stress. On the other hand, when the SFW was a half-integral of the Peierls period, the partials moved out of phase, corresponding to the minimum of the Peierls stress. As the distance between the partials increased, their interaction weakened, resulting in the decay of the oscillation. With these characters, the quasi-periodic variation of the Peierls stress under the Escaig stress was mathematically fitted to the combination of a sinusoidal and an exponential function [65].

1.3.2 The Mobility of Dislocations

The mobility of perfectly straight dislocations (periodic along the dislocation core) has been the focus of several prior studies [66–72]. These studies provided mobility laws for straight dislocations, which relate the dislocation velocity to the Schmid stress, which is the shear stress in the Burgers vector direction, and the temperature. Both experiments [66–68] and MD simulations [69,70] found the mobility law to be linear for small dislocation velocities, consistent with theories based on interactions between moving dislocations and thermal lattice vibration, known as the phonon drag mechanism. At high dislocation velocities, MD simulations predicted very different behaviors between edge and screw dislocations. As shown in Figure 1-10, the mobility
of the screw dislocation is significantly reduced compared to the phonon drag regime and can be described by the radiative damping terms proposed by Eshelby [70,73]. On the other hand, the velocity of edge dislocations reached a subsonic plateau velocity that is approximately 80% of the lowest forbidden velocity for Al [70]. For Schmid stresses greater than 500 MPa, the dislocation velocity could jump above the shear wave speed.

The mobility of edge dislocations in Al at high applied shear stresses was further investigated using MD simulations by Vandersall and coworkers [74]. Similar to earlier studies, the subsonic motion of an edge dislocation was observed for shear stresses up to 600 MPa. At slightly higher Schmid stress, the dislocation moved at transonic velocity initially but decelerated to a subsonic saturation velocity because of the interaction with Rayleigh surface waves from the finite simulation model. This transient behavior of the transonic dislocation was speculated to be similar in real crystals where high-stress concentrations typically occur near defects such as dislocations, cracks, or grain boundaries. These defects would serve as barriers similar to the finite-size model encountered in MD simulations. For Schmid stresses higher than 800 MPa, other deformation mechanisms were activated because of the nucleation of dislocation dipoles within the core structure.

To understand the role of dislocation character angle and alloy content on the mobility of dislocations, Marian and Caro studied the mobility law as a function of the Schmid stress, temperature, and alloy composition for edge and screw dislocations in Ni and Ni-Au alloys [75]. Depending on the Schmid stress, the velocity of a dislocation can be categorized into 3 main regimes separated by critical velocities, as shown in Figure
The phonon drag contributed at all velocities but dominated at low velocity due to the lack of contributions from other components. The phonon drag coefficient for Ni-Au alloys was found to be linearly depended on the temperature, the Burgers vector, and the Au concentration. At the velocity of the dislocation increases and reach different phase velocities of particular waves in the crystal, there are instabilities and singularities in the stress necessary to maintain a steady motion of the dislocation. The minimum phase velocity is the smallest possible phase velocity that usually at the Brillouin-zone edge along high symmetry directions in the phonon dispersion curve. The maximum phase velocities, associated with the largest singularity, are typically close to the center of the zone where the phase velocity and the group velocity are equal, also known as the sound velocities. The second component of dislocation velocity, the radiative term, only activated at velocities above a minimum critical velocity \( (v_o) \), which related to the minimum phase velocity \( (v_{p\text{min}}) \). The radiative term was characterized by a power law whose argument was the ratio between the dislocation velocity and \( v_o \). For edge and screw dislocations in Ni and Ni-Au alloys, the exponent was in the range from 1/2 to 1. The third regime corresponds to the singular terms at the maximum phase velocities. The exponents in this regime depended on the dislocation type and varied between 1/2 and 3/2. The mobility of a dislocation depended on the critical wave velocities which are different for different directions of dislocation motion. Therefore, the mobility of dislocation was governed by the direction of motion rather than the core structure.

Similar to the Peierls stress, the dislocation character angle and local stress state strongly influenced the mobility of dislocations. The role of dislocation character angle on the mobility of straight dislocations in Al was investigated by Cho and coworkers [72].
The mobility curves for 8 different dislocation types were fitted to the Eshelby-Olmsted [70,73] phenomenological equation with two regimes separated by the critical velocity. In the phonon drag regime, the dislocation velocity linearly scaled with the Schmid stress. As the applied shear stress increased, the radiative damping due to supersonic wave radiations became dominant. This regime was characterized by the power law derived by Eshelby for a screw dislocation [73]. The damping coefficients in both regimes were influenced by the dislocation character angles. For mixed dislocations, they showed that the correlation between the minimum phase velocity and the critical velocity was invalid. For an arbitrary dislocation where the X, Y, and Z directions of the simulation box did not necessarily align with the axes of the FCC lattice, the periodic length could be large. As a result, the minimum phase velocity became arbitrarily small, which was not the case for the transition velocity. Moreover, the dependence of dislocation mobility on the dislocation character angle was shown to significantly influence the expansion of a dislocation shear loop in discrete dislocation dynamics (DDD) simulations [72]. As shown in Figure 1-12, the geometry of a dislocation shear loop under a constant applied shear stress was altered with different implementations of mobility parameters from MD simulations. Including parameters from all dislocation character angles allowed faceting in the dislocation loop using DDD simulations, which was consistent with experimental observations [76].

To investigate the role of stress state on the mobility of dislocations, Burbery et al. studied the influence of the Escaig stress and Schmid stress on the structure and mobility of 30° dislocations in Cu [77]. Unlike the edge and screw dislocations, the dissociated core of the 30° dislocation was asymmetric, where the structures of the
partials were different. The effect of the Escaig stress was insignificant for straight dislocations in Cu. As shown in Figure 1-13, in order to show the influence on the mobility, the Escaig stress was varied from -1000 to 2000 MPa. As the Escaig stress increased, the dislocation core width reduced, resulting in a reduction in the dislocation mobility shown in Figure 1-13. Moreover, under high Schmid stresses when the dislocation velocity approached the supersonic limit, the asymmetric dislocation core could expand or constrict, depending on the direction of the dislocation motion. This is because of the asymmetric dislocation core structure that provided the different mobility between the leading and trailing partials. The ‘pure screw’ partial had a lower mobility than the 60° partial due to its higher peak Burgers vector density, which is an indication of a more compact dislocation core. When the ‘pure screw’ partial was the leading partial, the SFW became smaller as the Schmid stress increased because the trailing partial moved faster than the leading partial. On the other hand, when the leading partial is the 60° partial, the trailing partial moved slower than the leading partial. As a result, the SFW increased for increasing Schmid stress.

1.3.3 Curved Dislocations and Dislocation Loops

It is challenging for experiments to study dislocation loops at the nanoscale before they interact with themselves or other defects; thus, most studies about properties of the curved dislocation and dislocation shear loop are computational [53,78–80]. In seminal work, de Koning studied the nucleation of dislocation shear loops from a Frank – Read (FR) source in Al using atomistic simulation [78]. The FR source was generated as a rectangular prismatic dislocation loop by removing layers of atoms within the slip plane. As shown in Figure 1-14, the emitted curved dislocations depended on the direction of the applied stress. When the applied stress was parallel to
the Burgers vector of the prismatic dislocation loop, the emitted dislocation shear loop had the same Burgers vector with the FR source. On the other hand, when the applied stress was perpendicular to the Burgers vector of the trailing partials, the emitted dislocation shear loop had different Burgers vector compared with the FR source. This was due to the nonlinear dissociated core structure of dislocations in FCC metals. Using the same approach, Li and Yang found additional non-planar evolutions of curved dislocations emitted from a FR source [80]. In the typical FR source, the edge dislocation dipole served as the pinning points to emit curved dislocations. On the other hand, for the non-planar evolutions, the dislocation dipole glided because of the change in the glide constraint when the segments near two polar nodes come close to the screw orientation.

Xu et al. used concurrent atomistic-continuum (CAC) simulations to investigate the critical shear stress and critical dislocation configuration for the bowing of an edge dislocation segment from a FR source in Cu, Ni, and Al [79]. While the critical stress versus FR source length curve calculated by the CAC simulations had similar shapes with the predictions from a continuum model, the critical stresses from CAC simulations only agreed well for Al, not Cu and Ni. This was due to the larger stacking fault widths and higher elastic anisotropy of dislocations in Cu and Ni compared with Al. The effects of the dislocation dissociation and material anisotropy also appeared in the asymmetric semi-elliptic shape of the critical dislocation segments. As the length of the FR source increased, the axial ratio of the critical geometry decreased and became more semi-circular. For the same FR source length, dislocation segments in Al were consistently the most elliptical among the three.
Bitzek et al. implemented a different approach to create dislocation loops to study dislocation loop – grain boundary interactions in nanocrystals [53]. Their method addressed some of the limitations of commonly used dislocation generation algorithms: (1) restrictive geometries of infinite straight dislocations, and (2) the need to homogenously or heterogeneously [29,52,78] nucleate dislocations under deformation with high applied stresses, resulting in fast-moving dislocations with irregular properties. A circular dislocation loop composed of 8 similar triangles was generated in a preselected grain by applying the linear elastic displacement fields associated with these elemental dislocations [81,82]. This allowed more degrees of freedom for both the dislocation (with specific Burgers vectors and slip systems) and the type of three-dimensional grain boundaries networks. As a result, more complex phenomena such as pinning at grain boundaries and interactions of dislocations with triple junctions between 3 grains could be studied.

1.3.4 Summary of Prior Dislocation Studies

This brief overview of previous atomistic simulations illustrates the effectiveness of using atomistic simulation to study the core structure and mobility of dislocations. Atomistic simulations have not only successfully reproduced similar trends observed in experiments but also provided additional information and insight such as the description of dislocation core structure and different regimes of the mobility law for dislocations under a Schmid stress. However, considering the multiscale nature of the dislocation problem and limitations of current atomistic simulation methods, there are many opportunities to improve. For instance, some of the current problems are limited in the choice of the dislocation (geometry, type, and orientation), high Schmid stresses that result in fast-moving dislocations with irregular properties, and insufficient consideration
for the role of stress state on the core structure and the mobility of dislocations. While previous studies provide fruitful insights into the geometry, structure, and mobility of dislocations, they are restricted to perfectly straight dislocations [69–72]. As mentioned in Section 1.2, nanoscale dislocation shear loops (with diameters less than 100 nm) have been observed experimentally using transmission electron microscopy (TEM) and studied computationally using molecular dynamics simulations [7–9,14,15,83–85]. Even though their role in plasticity is recognized to be important, an understanding of the structure and mobility of nanoscale dislocation shear loops remains limited. Previous simulations typically focused on the nucleation of curved dislocations and dislocation loops from FR source [78–80]. This is originated from the lack of an effective atomistic framework to generate curved or loop dislocations that required reasonable driving stress and is frame invariant to allow more degree of freedoms for different types of dislocations.

1.4 Goals and Objectives

The goal of this dissertation is to study the properties of dislocations and the role of stress state on dislocation properties. Chapters 4 and 5 will focus on the effect of stress state on the Peierls stress and mobility of straight dislocations. In particular, the effect of pressure applied normal to the (111) slip plane on the Peierls stress in Al will be shown in Chapter 4. Edge, screw, 30°, and 60° straight dislocations are created using the Volterra displacement fields for isotropic elasticity. For each dislocation character angle, the Peierls stress is calculated based on the change of Gibbs free energy, which is an invariant measure of the dislocation driving force. Both the Peierls stress and the dislocation core structure are validated by comparing to previous experimental and simulation results. To study the effects of <111> pressure, the Peierls
stress is computed under pressures that range from -750 to 750 MPa. Variation in the Peierls stress due to pressure is understood by analyzing the dislocation core structures via parameters such as the interatomic spacing between atoms along the dislocation core and the SFW.

Moreover, the mobility of straight dislocations in Al with a particular focus on the combined effects of the Escaig stress and pressure applied normal to the (111) slip plane will be presented in Chapter 5. First, the phonon drag part of the mobility law for straight dislocations with different dislocation character angles is determined from MD simulations. Second, the radiative damping part of the mobility law is studied for different dislocation character angles. This provides insight on how dislocations move differently at high applied Schmid stresses, especially for mixed dislocations. For each dislocation character angle, the effects of pressure applied normal to the (111) slip plane and the Escaig stress on the phonon drag of dislocations are considered. The role of Al interatomic potential on the mobility of dislocations is also discussed.

Finally, Chapter 6 will discuss the geometry, resolved Schmid stress necessary for equilibrium, and mobility of nanoscale dislocation shear loops in Al. A frame invariant atomistic simulation algorithm to generate stable dislocation loops at 0 K and finite temperatures is developed. This is coupled with a bisection algorithm to systematically determine the fundamental properties of nanoscale dislocation shear loops in Al, such as geometry and the resolved Schmid stress necessary for equilibrium at 0 K of nanoscale dislocation shear loops, including the influence of loop radius and temperature. Al is selected as the material of interest as it is computationally tractable for both atomistic and DDD simulations. Al is also relatively isotropic, which prevents the
irregular “corners” in dislocation loops that were seen in anisotropic material such as BCC Fe [17]. The role of Al interatomic potential on static equilibrium properties is also discussed. For finite temperature studies, the minimum Schmid stress required to open a dislocation loop is computed. This provides a mean to compute the effective lattice friction stress as a function of temperature. A critical dislocation loop size is identified above which the effective lattice friction stress is size independent. Moreover, the expansion of the dislocation loop is also investigated to understand how the difference in mobility between segments of the dislocation loop influences the overall geometry of the dislocation loop.

Figure 1-1. TEM micrograph showing the microstructure of Fe-20Mn-1.3C-3Cu steel at a true strain of 0.02 [86].
Figure 1-2. The stacking sequence of crystalline planes demonstrating prismatic dislocation loops formed from the clustering of the disc-shaped platelets [87].

Figure 1-3. Schematic of a dislocation shear loop [88].
Figure 1-4. Bright field TEM images of a UO$_2$ polycrystalline thin foil with marked prismatic dislocation loops [89].

Figure 1-5. Deformation mechanism map of Al with a wide grain size range [34].
Figure 1-6. View along the dislocation line of the core structure of the 60° dislocation. A) View along the dislocation line of the core structure of the 60° dislocation at equilibrium. B) View along the dislocation line of the core structure of the 60° dislocation at equilibrium under applied Schmid stress of 0.0007 eV/A³ [48].

Figure 1-7. GSF energy curves for Al using EAM potentials compared to DFT results [61].
Figure 1-8. Variation of the relative dislocation core energies for dissociated and undissociated screw dislocations as a function of normalized displacement traveled by the dislocation core. Insets show corresponding atomic configurations of the undissociated (upper inset) and the dissociated (lower inset) screw dislocation along the MEP [44].
Figure 1-9. Variation of the Peierls stress with increasing Escaig stress for a screw dislocation in Cu. Predictions by the improved SVFN model and MD are fitted and shown using dashed curves [65].

Figure 1-10. Al screw dislocation velocity as a function of the applied shear stress [70].
Figure 1-11. Schematic of the three dynamic regimes observed in simulations of dislocation mobility [75].

Figure 1-12. Snapshots of dislocation loop dynamics at 0, 2.5, 5 and 10ps with three different dislocation mobility laws. A) A linear relation between dislocation velocity and shear loading is considered and interpolated linearly from edge to screw segments. B) The linear and supersonic asymptotic regimes are considered for edge (90 °) and screw (0 °) dislocations. Intermediate angles are interpolated linearly from edge to screw. C) The new mobility law proposed by Cho et al., which accounts for the linear and supersonic regimes and a total of 8 character angles [72].
Figure 1-13. Influence of Escaig stress effect on the velocity versus the Schmid stress for screw dislocations in Cu [77].

Figure 1-14. FR source operation using the Ercolessi-Adams Al EAM potential. Only atoms in the dislocation cores and ISF areas are shown. The orientation of applied stress and dislocation line senses (curved arrows) are also indicated. A) Relaxed prismatic loop configuration at zero stress. B) The (111) face of the Thompson tetrahedron (viewed from outside). C) Conventional multiplication. D) Anomalous multiplication [78].
CHAPTER 2
THEORY OF ATOMISTIC SIMULATION

2.1 Atomistic Simulations

Atomistic simulation is a computational modeling technique that allows for the analysis of properties of materials at the atomic level [90–92]. As mentioned in Section 1.3, while it is possible for experiments to view dislocations, it still remains challenging to fully characterize them in details such as their core structure, mobility, and initiation. Therefore, the atomic details that atomistic simulations provide can be used to gain insight into the properties of dislocations. In atomistic simulation, each atom is treated as a particle with mass, \( m \). This reduces the computational cost associated with the motion of individual electrons and interactions between electrons. As a result, a larger system composed up to 10s of millions of atoms can be studied. This is important because the stress fields of a straight dislocation, which will be discussed in Chapter 3, decays with \( 1/r \), where \( r \) is the distance from the dislocation core. Therefore, the simulation domain necessary to study dislocations is required to be large enough to capture the full stress field of a dislocation.

Atomistic simulations can be categorized into three different simulation techniques: Monte Carlo, molecular statics, and MD simulations. In this dissertation, only the latter two methods are utilized. Molecular statics simulation is used to obtain the equilibrium structure of dislocation loops in Chapter 4 and straight dislocations in Chapter 5, while MD simulation is used to study the mobility of dislocations at finite temperature in Chapter 6. Section 2.2 and 2.3 will briefly discuss the concepts of both of these techniques. Comprehensive discussions about the Monte Carlo method can be found in references [90–95].
Since every atom is modeled as a point mass without the explicit consideration of electrons and their interactions in classical atomistic simulations, it is necessary to describe interaction energy between atoms based solely on atom positions. This relationship is captured via an interatomic potential function (simply referred as an interatomic potential), $U$. The force acting on atom $i$ due to the neighboring atoms is then determined as the negative gradient of this potential function as shown in Equation (2-1).

$$\vec{F}_i = -\frac{\partial U}{\partial \vec{r}_i}$$ (2-1)

Here, $\vec{r}_i$ is the generalized displacement vector of the $i$th atom from its neighbors. The accuracy of the interatomic potential significantly influences the result of the simulations. Therefore, it is essential to choose an appropriate interatomic potential depending on the application of the simulations. Details about the interatomic potential, especially the embedded atom method (EAM), will be discussed in Section 2.4.

Depending on the complexity of the interatomic potential as well as the time and length scale of the simulation, atomistic simulations can easily model up to 10s of millions of atoms. This is tiny compared to the number of atoms in macroscale materials. Therefore, it is often essential to eliminate the free surface effect and imitate a bulk environment to properly calculate material properties. One popular method is to apply periodic boundary conditions (PBCs), which is a computational trick to replicate a material domain. Figure 2-1 demonstrates periodic boundary conditions for a two-dimensional simulation box with 4 atoms. The simulation box containing 4 “real” atoms,
drawn by solid lines, is surrounded by its replicated images with “ghost” atoms, with identical properties to the “real” atoms (shown by dashed lines). As shown by the red arrows in Figure 2-1, all “ghost” atoms move exactly the same way the “real” atoms in the simulation cell. If an atom leaves the simulation cell through a boundary, one of its images will enter the simulation cell through the opposite boundary. The atoms that are close to the boundary of the simulation cell can potentially interact with “ghost” atoms in the image cell, eliminating the free surface effect.

However, there are two issues that need to be considered when using periodic boundary conditions [90–92]. First, the size of the simulation cell must be at least two times larger than the cut-off distance for the interatomic potential to avoid interaction between atoms and their own images. Second, for simulations studying defects such as dislocations, periodic boundary conditions also replicate the dislocation in the simulation cell, whose stress field may interact with itself through the periodic boundary. In order to minimize and eliminate the effects of these artifacts, the simulation cell size should be carefully chosen to be large enough so that atoms at the boundary, away from the dislocations, do not feel the presence of the dislocation. Details about the dimensions of the simulation cell for each dislocation will be provided in Chapters 4 and 5.

The atomistic simulations in this dissertation are performed using the classical molecular dynamics code, LAMMPS, which has been developed and distributed by Sandia National Laboratories [96]. The current version of LAMMPS is written in C++, which allows the implementation of new functions and variables. The displacement field of both straight dislocations and dislocation loops, which will be discussed in Chapter 3, are implemented by modifying a set of commands within LAMMPS, thereby extending
the capability of the atomistic simulation code. Results from LAMMPS are output as dump files that contain atomistic information such as index number, the position of atoms, and the potential energy of each atom.

2.2 Molecular Statics

Molecular statics simulation (also known as energy minimization) is a branch of atomistic simulation that focuses on determining the lowest energy configuration of a system of atoms at zero temperature. Therefore, the goal of energy minimization is to numerically find the configuration with the minimum potential energy starting from a given initial configuration [97]. It is also possible to apply an external pressure to the simulation cell during an energy minimization. In particular, the size and shape of the simulation cell are modified during the energy minimization, as additional degrees of freedom, so that the final configuration will be at equilibrium and under an externally applied state of stress. This feature is important for this work, especially for the dislocation loop study, since the dislocation loop under no applied Schmid stress will collapse due to the self-interaction between dislocation segments. Including pressure control, the overall objective function to minimize is

\[ E = U + P_t (V - V_o) + E_{strain} \]  \hspace{1cm} (2-2)

where \( U \) is the system potential energy from the interatomic potential, \( P_t \) is the desired hydrostatic pressure, \( V \) and \( V_o \) are the system current and reference volumes, and \( E_{strain} \) is the strain energy proposed by Parrinello and Rahman [98]. When \( E \) reaches the minimum, the global system stress tensor \( P \) will satisfy the following relation:

\[ P = P_t I + S_i \left( h_o^{-1} \right)^T h_o d \]  \hspace{1cm} (2-3)
In Equation (2-3), I is the identity matrix, $h_0$ is the box dimension tensor of the reference cell, $h_{0d}$ is the diagonal part of $h_0$, and $S_t$ is a symmetric stress tensor such that the upper triangular components of $P$ equal the target stress tensor. To find the minimum of the objective function (with or without the externally applied stress), there are five energy minimization methods implemented in LAMMPS, such as conjugate gradient, Hessian-free truncated Newton, steepest descent, quickmin, and FIRE [96]. The first three methods are mostly based on some approximations for the Hessian matrix, while the last two are damped dynamics methods that take dynamical steps during the minimization [99,100]. For this dissertation, preliminary simulations show that the conjugate gradient method converges with the least number of iterations. Therefore, all energy minimization to find equilibrium dislocation core structures, which will be presented in Chapters 4 and 6, are performed using the conjugate gradient method.

The remainder of this section provides an overview of the steepest descent and conjugate gradient methods. A more comprehensive overview of other methods is provided in Sheppard et al. [100].

As mentioned earlier, energy minimization is the process of finding the configuration of atoms (x) from an initial configuration ($x_o$) that corresponds to the minimum of the potential energy function, $U(x)$ [97]. For methods based on the Hessian matrix such as steepest descent and conjugate gradient methods, there are two components of the search: the searching direction ($d$) and the step size ($\alpha$). The step size, which determines how far to move in a specific direction, and its calculation is similar between the two methods. Once the direction of the search is determined, the new configuration is updated via the following equation:
where \( x_{(i)}, x_{(i+1)} \) are the configurations at step \( i \) and \( i+1 \), \( d_{(i)} \) is the searching line unit vector at step \( i \), \( \alpha \) is the distance travel along the force vector \( d_i \). The step size is determined to minimize the potential energy along the search direction via a line search algorithm. Choosing the step size in this way results in the gradient direction of the next step \( (i+1) \) to be orthogonal to the search direction of the previous step \( (i) \). Currently, there are three line search methods implemented in LAMMPS: backtracking, quadratic, and forcezero [96]. The default option is the quadratic method, which is more efficient than the backtracking method for highly converged relaxations.

The difference between steepest descent and conjugate gradient methods is the direction of the search [97]. For the steepest descent method, the direction of the search is always in the negative of the gradient (referred as negative gradient) of the potential energy function because the negative of the gradient of any function always points in the direction that steepest decrease of that function. Moreover, the negative gradient of the potential energy function is the force vector, \( f \). Therefore, Equation (2-4) can be rewritten as

\[
x_{i+1} = x_i + \alpha_if_i
\]

(2-5)

where \( f_{(i)} \) is the force unit vector at step \( i \). The problem with the steepest descent is the lack of passing information from previous steps in determining the new searching direction. As a result, as shown in Figure 2-2A, for ill-conditioned systems the steepest descent method converges slowly with multiple steps moving in the same directions. On
the other hand, the conjugate gradient method utilizes the orthogonality properties between the previous step and the gradient of the next step to avoid the repetition in the search direction. While the first step of the conjugate gradient method is identical to the steepest descent, the next searching direction is constructed in a way that it is conjugate with the previous searching direction:

$$d_{i+1} = f_{i+1} + \beta_{i+1}d_i$$  \hspace{1cm} (2-6)

with $\beta_{i+1}$ is the scaling parameter at step $i$ to ensure conjugation between all of the search directions, as shown in Figure 2-2B. For nonlinear conjugate gradient problems, there are four best-known formulas to calculate $\beta_{i+1}$, which are the Fletcher-Reeves, Polak-Ribiere, Hestenes-Stiefel, and Dai-Yuan formulas. Among them, the Polak-Ribiere formula is the current method implemented in LAMMPS to find $\beta_{i+1}$:

$$\beta_{i+1} = f_{i+1} \cdot (f_{i+1} - f_i) / |f_i|^2$$  \hspace{1cm} (2-7)

It is worth noting that for complex potential energy functions, in which many local minima exist, no method is guaranteed to converge to the global energy minimum. Since the line search algorithm to calculate the step size is dependent on the starting point, it is possible for any algorithm to get stuck in a local minimum and never escape to find the absolute minimum. One way to increase the probability for the algorithm to not get trapped at local minima is to run multiple energy minimizations with multiple starting points on the potential energy surface.
2.3 Molecular Dynamics Simulation

Molecular dynamics simulation is another branch of classical atomistic simulation that solves the time evolution (trajectories) of a system of particles (atoms, molecules, or united atoms) under a set of boundary conditions by numerically integrating their equations of motions [90–95]. In this work, the particles of interest are atoms, while two sets of boundary conditions are implemented corresponding to the microcanonical (NVE) and the isothermal-isobaric (NPT) ensembles in statistical mechanics. In a standard molecular dynamics simulation, the macroscopic properties of the system such as pressure, temperature, kinetic energy, and potential energy fluctuate around their corresponding average values, which can be extracted using thermodynamic averaging. The remainder of the section will provide a brief overview of molecular dynamics simulation and how it is employed in this research via LAMMPS. A more comprehensive review of molecular dynamics simulation can be found in references [90–95].

2.3.1 The Microcanonical (NVE) Ensemble

In molecular dynamics simulations of atoms in an isolated environment, the goal is to solve Newton’s 2nd law of motion for the N-body system where N is the number of atoms [94].

\[
\dot{r}_i = \frac{p_i}{m_i} \quad \text{and} \quad \dot{p}_i = F_i \quad (2-8)
\]

In Equation (2-8), \(r_i, p_i,\) and \(m_i\) are the position, momentum, and mass of atom \(i,\) respectively. The dot indicates the first derivative with respect to time. \(F_i\) is the sum of forces acting on atom \(i\) contributed from interactions with neighboring atoms and external forces. However, it is important to recognize that the coupled first order
ordinary differential equations in Equation (2-8) only describe a system of atoms that is isolated from the environment, corresponding to the microcanonical (NVE) ensemble in statistical mechanics. In this setting, the number of atoms, the shape, the volume, and the total energy of the simulation cell remains constant throughout the simulation. The characteristic of the NVE ensemble is the lack of temperature control. One way to address this is to rescale the velocity of atoms in the system to reset the system temperature to a target value, which results in a system that no longer in NVE ensemble:

\[ u_i^{\text{new}} = \sqrt{\frac{T_0}{T}} u_i \]  \hspace{1cm} (2-9)

with

\[ T(t) = \frac{2K(t)}{3NK_b} \]  \hspace{1cm} (2-10)

where \( T_0 \) is the desired temperature, \( T(t) \) is the instantaneous temperature, \( N \) is the number of atoms within the system, \( K(t) \) is the kinetic energy of the system, and \( k_B \) is the Boltzmann constant. Once the system temperature reaches equilibrium at the target temperature, the velocity rescaling should be turned off before taking statistical averages, which are still in the NVE ensemble. While the velocity rescaling technique allows the temperature to be controlled, it is not equivalent to performing MD simulations in a constant temperature ensemble.

2.3.2 The Canonical (NVT) and the Isothermal-Isobaric (NPT) Ensembles

To impose more realistic boundary conditions, it is necessary to use other ensembles in statistical mechanics such as the canonical (NVT) and the isothermal-isobaric (NPT) ensembles [94]. The NVT ensemble represents the possible states of a
simulation cell with a heat bath at a fixed temperature. In particular, the volume of the simulation cell is constant, while energy is exchanged with the environment through the boundaries of the simulation cell to maintain thermal equilibrium. This is accomplished by introducing a new thermal friction coefficient, $\zeta$, which connects the system to a target temperature. This idea was implemented in the Nosé-Hoover thermostat that was originally developed by Nosé [101] and further improved for easier implementation in molecular dynamics simulation by Hoover [102],

$$
\dot{r}_i = \frac{p_i}{m_i},
$$

$$
\dot{p}_i = F_i - \zeta p_i,
$$

$$
\dot{\zeta} = \nu_T^2 \left( \frac{T}{T_o} - 1 \right)
$$

where $\nu_T$ is the thermostat rate. As seen in Equation (2-11), the thermal friction coefficient dynamically modifies the momentum of each atom in order to drive the system temperature toward the desired one.

On the other hand, the NPT ensemble represents the possible states of a simulation cell under a fixed pressure and temperature, which is another experimental setting. To achieve this, a number of methods have been developed such as those proposed by Parrinello and Rahman [98], Nosé [101], Hoover [102], and Melchionna et al. [103]. The general idea of these methods is to allow isotropic or anisotropic changes in the dimensions and shape of the simulation cell under external work or pressure. This is accomplished by incorporating an isobaric friction coefficient, which is similar to the thermal friction coefficient in the Nose-Hoover temperature-controlled algorithm. The Hoover improvement to the NPT ensemble allows easy implementation into a molecular dynamics code. However, Melchionna et al. argued that the Hoover isothermal-isobaric
equations of motion do not properly sample the NPT ensemble, due to the rescaling of
the coordinates with a new volume of the simulation cell at each step [103]. Instead,
Melchionna et al. shifted the system by the center of mass:

\[ \dot{r}_i = \frac{p_i}{m_i} + \eta (r_i - R_0) \]
\[ \dot{p}_i = F_i - (\eta + \zeta I) p_i \]
\[ \dot{\zeta} = \nu^2 \left( \frac{T}{T_0} - 1 \right) \]
\[ \dot{\eta} = \frac{\nu^2}{Nk_B T_0} V (\sigma - P_0) \]
\[ V = \eta V \]

(2-12)

where \( \eta \) is the frictional parameter to couple the ensemble of atoms to a desired
pressure bath, \( \nu \) is the damping coefficients to modify the rate of convergence to a
desired pressure, \( R_0 \) is the center of mass of the system, \( P_0 \) is the target pressure, and
\( \sigma \) is the internal stress that calculated using the virial definition, which will be discussed
in Section 2.3.4.

2.3.3 Molecular Dynamics Integration Algorithm and Initial Conditions

Regardless of the ensemble, the method to solve Equations (2-8), (2-11), and (2-12) is identical. To solve these ordinary differential equations, it is necessary to (1) set
up the initial conditions such as initial positions and velocities, (2) implement an efficient
integration algorithm, and (3) calculate the forces acting on each atom via Equation (2-1).
First, initial conditions such as the initial positions and velocities for atoms in the
system are required. For modeling the thermodynamics of crystalline solids, the initial
atom positions are specified on a lattice with the primitive unit cell and basis. The initial
velocities are randomly assigned consistent with a desired temperature such that the
net velocity is zero. There are two distributions implemented into LAMMPS, the uniform
and Gaussian distribution for the initial velocities of atoms. All simulations in this work are performed with Gaussian distributed initial velocities. Simulation results are required to be averaged for different starting velocities to understand the error in the simulation results due to thermal oscillations and variance. This will be further discussed in more detail in Chapters 5 and 6 for mobility of straight dislocations and dislocation loops, respectively. Second, while there are many numerical integration techniques to solve 1st order ordinary differential equations such as the 4th order Runge-Kutta method, the Verlet algorithm, and the leapfrog method, the velocity Verlet finite difference algorithm is the most popular in molecular dynamics simulations. It is also the only one implemented into LAMMPS due to its efficiency. For the NVE ensemble,

\[
\begin{align*}
\mathbf{r}_i(t + \Delta t) &= \mathbf{r}_i + \Delta t \mathbf{v}_i(t) + \frac{1}{2}(\Delta t)^2 \mathbf{a}_i(t) \\
\mathbf{v}_i(t + \Delta t) &= \mathbf{v}_i + \frac{1}{2} \Delta t [\mathbf{a}_i(t) + \mathbf{a}_i(t + \Delta t)]
\end{align*}
\] (2-13)

where \(\mathbf{v}_i\) and \(\mathbf{a}_i\) are the velocity, acceleration of atom \(i\), which correspond to the momentum and force \((p_i\) and \(F_i\)). The velocity Verlet algorithm is preferred in molecular dynamics simulations since it requires only 1 force calculation each iteration and the error term is proportional to \((\Delta t)^2\) for the velocities and \((\Delta t)^4\) for the positions [94]. Moreover, it automatically calculates the velocity of each atom at every time step without additional calculations. Third, given the positions of each atom, the forces acting on each atom are calculated using the interatomic potential.

### 2.3.4 Virial Stress

The concept of stress in a system of interacting particles is essential to connect results from atomistic simulations to analysis at the continuum scale. As explained above, the internal stress used in Equation (2-12) is calculated using the virial definition
first proposed by Clausius [104] and given in [105] for pair potentials and EAM potentials:

\[
\sigma = \frac{1}{V} \sum_{i \in \Omega} \left[ \frac{1}{2} \sum_{j \in \Omega} \left( r_i - r_j \right) \otimes f_{ij} - m_i \nu_i \otimes \nu_i \right]
\]  

(2-14)

where \( V \) is the system volume, \( \Omega \) denotes the set of all indices for the system, and \( f_{ij} \) is the force exerted from atom \( j \) on atom \( i \). For inhomogeneous and non-equilibrium systems, Irving and Kirkwood [106] proposed a procedure to calculate stress which was later generalized by Hardy [107]. The validity of virial stress as an atomistic stress equivalent representative to the continuum Cauchy stress and its form has been an ongoing controversial topic [108–114]. Zhou demonstrated that the point-wise measure of stress using the virial definition in Equation (2-14) violated the classical conservation of linear momentum [111]. Moreover, he argued that in a dynamic system of discrete particles, the stress should be a function of only the interaction between atoms instead of both the potential energy due to atomic interactions and the kinetic energy shown in Equation (2-14).

It is important to understand that the stress in atomistic simulation must be spatially and temporally averaged in a Eulerian reference frame and represents the force per unit area on the surface of a defined volume containing interacting particles. While it is mathematically feasible to decompose the expression in Equation (2-14) to calculate the point-wise measure of stress around an atom, it has no physical meaning at finite temperature. This was proved by Zimmerman and coworkers in the comparison between the continuum mechanical stress in atomistic systems derived by Hardy [107] and the atomic stress taken from the virial theorem. For the small spatially averaging region, there was a discrepancy between the Hardy’s stress and the virial stress. As the
spatially averaging region became larger, the discrepancy between those stresses decreased. Moreover, the time averaging of the stress further improved the convergence between the two stress expressions. Therefore, Zimmerman et al. proposed to extend Hardy’s spatial averaging technique to include temporal averaging for finite temperature systems.

Further discussion of stress calculations in atomistic systems is beyond the scope of this dissertation. A more comprehensive review of this discussion can be found in Zhou [111], Subramaniyan and Sun [113], and Zhang et al. [114]. In this work, the definition of the virial stress with both the potential and kinetic contributions is used. It is worth noting that the kinetic energy term was shown to be much smaller compared to the atomic interaction term for solids [111]. At low temperatures (from 0K to 400K) and subjected to an external deformation, the contribution from the kinetic energy is largely insignificant. The majority of this dissertation considers stress or pressure as the spatial and temporal average over the whole system at thermodynamic equilibrium. The only point-wise measure of stress around an atom is performed in Chapter 6 to show the effect of externally applied Schmid stress on the core structure of dislocation loops. This is performed at zero temperature with no contribution from the kinetic part.

2.4 Interatomic Potential

2.4.1 Overview

As defined in Section 2.1, for atomistic simulation, electrons and the nucleus of an atom are combined and modeled as a point mass. Therefore, it is necessary to quantify the interactions between atoms based on the atom configuration. This is accomplished by utilizing an interatomic potential, which provides the potential energy given the position of every atom within the system. As a result, interatomic potentials
significant influences the result of atomistic simulations [115]. There are three essential features in choosing an interatomic potential for an arbitrary application: accuracy, transferability, and computational cost. Depending on the intended application, the focus will be a shift from one feature to the other. In other words, there is no good or bad interatomic potential, just appropriate or inappropriate for a particular application. For instance, simulations in Computational Chemistry typically require high accuracy, while the ones in Material Science for larger problems focus more on the efficiency and computational cost. In this work, it is essential to simulate large systems to properly model the large stress/displacement field of a dislocation. Therefore, there is a balance in choosing a potential that satisfies both accuracy and efficiency.

Given a particular system, there are different forms for an interatomic potential ranging from analytical forms inherited from quantum-mechanical arguments to purely empirical functions. Many interatomic potentials are semi-empirical including guidance from quantum-mechanical equations but with simplification to fit experiments. Some example potentials of this type are the EAM potentials [116], the glue model by Ercolessi et al. [56], or the bond order potentials [117,118]. As shown in Figure 2-3, interatomic potentials can be categorized based on the level of complexity into 4 different types: pair potentials, cluster potentials, pair functionals, and cluster functionals [115]. In the simplest form, the pair potentials consider only interactions between 2 atoms and ignore the influence of many-body interactions, such as the bond angles between triplet atoms or the environment generated by neighboring atoms. On the other hand of the spectrum, the cluster functionals incorporate both the many-body interactions and the local environment.
As mentioned earlier, the study of dislocations in FCC metals via atomistic simulations requires a balanced interatomic potential with both accuracy and computational time. Therefore, it is desired to choose interatomic potentials with a simpler form. However, the simplest form, the pair potentials, is unsuitable to simulate metals or problems of crystalline defects such as dislocations. First, pair potentials typically overestimate the vacancy formation energy and underestimate the cohesive energy of metals due to its lack of consideration for the local environment [119]. Moreover, the local environmental independence of the pair potentials does not allow it to differentiate between bulk atoms and atoms near surfaces or crystalline defects. Therefore, it is essential to choose an interatomic potential form that includes the local environment for this dissertation. A simple yet efficient way to accomplish this is to include an extra function in the potential energy that accounts for the local electron density. One of the most popular families of potentials using this idea is the EAM potential, which will be discussed in Section 2.4.2. A more comprehensive review of other interatomic potentials and their applications can be found in Carlsson [115].

### 2.4.2 The Embedded-Atom Method

The EAM is the most well-known method in a class of interatomic potentials (such as the glue [56] and the Finnis-Sinclair potentials [120]) that include both the cohesive functional of pair interactions and the pair potentials in the total internal energy [116,121]. In the EAM potential, the internal energy is given by:

\[
U = \frac{1}{2} \sum_{i,j \neq i} \phi_{\alpha \beta}(r_{ij}) + \sum_i G_{\alpha}(\bar{\rho}_i) \quad (2-15)
\]

where \(\phi_{\alpha \beta}\) is the pair-wise potential function of atom i (type \(\alpha\)) and atom j (type \(\beta\)), \(r_{ij}\) is the distance between atom i and atom j, \(G_{\alpha}\) is the embedding energy function of atom i,
and $\bar{\rho}_i$ is the spherically averaged background electron density ($\bar{\rho}_i$) due to neighbors of atom i. The first term in Equation (2-15) includes all the pair interactions between atoms, while the second term describes the many-body effects by using the embedding energy that depends on the local background electron density. The background electron density is given by the sum:

$$\bar{\rho}_i = \sum_{j \neq i} \rho_{ji}(r_{ij}) \quad (2-16)$$

where $\rho_{ji}$ is the electron density assigned to atom j. Both summations in Equations (2-15) and (2-16) are performed over a region defined by a cut-off distance. Typically, the cut-off distance is chosen to include at least the first and second nearest neighbors. With this local environment information, the functional part in Equation (2-15) provides (in an average manner) the many-body interaction between atoms so that the force exerted by one atom on another depends on the neighboring atoms of both. This allows the EAM potential to examine crystalline defects such as dislocations, free surfaces, and grain boundaries.

While the original forms were motivated by the effective medium theory [122] and the tight-binding theory [120], all functions of the EAM potential have semi-empirical expressions with adjustable parameters to match material properties from experimental measurements and ab initio calculations [123]. Some of the common material properties are the lattice constant, atomic volume, bulk modulus, elastic constants, vacancy formation energy and free energy. Depending on a particular application, additional properties can be included. For instance, the melting temperature, change in enthalpy and volume upon melting, and liquid density are additional fitting targets for crystallization kinetics problems in Al and Cu [124]. For the study of dislocations,
stacking fault energies are essential to capture the proper dislocation core structure. The process of choosing an appropriate EAM potential is discussed further in Chapters 4, 5, and 6.

While the EAM potential incorporates local environment that contains many-body interactions implicitly, it lacks explicit 3- or higher-body interaction terms to account for the angle between triplets. As a result, it fails to describe the directional bonding in covalent bonded solids, significant charge transfer, or handle the Fermi-surface effects [121]. While these conditions are unimportant for FCC metals with nearly empty or nearly full d-bands [125], it is challenging to use EAM potentials to describe other crystalline structures such as BCC, HCP, and nonmetallic metals. To describe the directionality of bonding, Baskes added a degree of angular dependence that influences the electron density [126,127]. The modified embedded-atom method (MEAM) potential has shown the capability to describe different types of bonding, so it can apply to a wide variety of crystalline structures such as FCC, BCC, and nonmetallic systems.
Figure 2-1. Schematic of 2-D periodic boundary conditions in atomistic simulations.
Figure 2-2. Graphical illustration of methods for energy minimization calculations. A) Steepest descent method. B) Conjugate gradient method [97].
Figure 2-3. Diagram of types of interatomic potentials. Arrows point in the direction of increasing complexity.
CHAPTER 3
THEORY OF DISLOCATIONS

3.1 The Volterra Displacement Field of Infinitely Straight Dislocations

The Volterra displacement field of an infinitely straight dislocation in an isotropic medium is commonly used to generate a dislocation in atomistic simulations (cf. [78,128]). As shown in Figure 3-1, the displacement field around an infinitely straight right-handed screw dislocation can be determined by considering a cylinder of elastic material deformed as defined by the Volterra deformation mode [1]. For a screw dislocation, whose dislocation axis (Z-axis) is parallel to the Burgers vector direction, the displacement field has only one nonzero component along the Z-axis:

\[ u_z = \frac{b \theta}{2\pi} = \frac{b}{2\pi} \tan^{-1}\left(\frac{y}{x}\right) \]  

where \( b \) is the Burgers vector, \( \theta \) is the angle with respect to the X-axis that goes from 0 to \( 2\pi \), resulting in a displacement that varies from 0 to \( b \). Similarly, the stress field of a screw dislocation in polar coordinates also has only one nonzero component:

\[ \sigma_{\theta z} = \frac{\mu b}{2\pi r} \]  

On the other hand, the displacement field around an infinitely straight edge dislocation is more complex. As shown in Figure 3-2, an edge dislocation produces zero displacement and strains in the Z-axis. The stress field is then derived using an Airy stress function and appropriate boundary conditions at \( \theta = -\frac{\pi}{2}, \frac{\pi}{2} \). In polar coordinates, the stress field of a straight dislocation is:
\[
\sigma_{rr} = \sigma_{\theta\theta} = -\frac{\mu b \sin \theta}{2\pi (1-\nu) r} \\
\sigma_{zz} = -\frac{\mu b \nu \sin \theta}{\pi (1-\nu) r} \\
\sigma_{rz} = \sigma_{\theta z}
\] (3-3)

Complete details of the derivation of the stress field can be found in Hirth and Lothe [1]. Ultimately, the displacement field can be derived by integration of the stress field:

\[
u_x = \frac{b}{2\pi} \left[ \tan^{-1} \left( \frac{y}{x} \right) + \frac{xy}{2(1-\nu) \left( x^2 + y^2 \right)} \right]
\] (3-4)

\[
u_y = -\frac{b}{2\pi} \left[ \frac{1-\nu}{4(1-\nu)} \ln \left( x^2 + y^2 \right) + \frac{x^2 - y^2}{4(1-\nu) \left( x^2 + y^2 \right)} \right]
\] (3-5)

where \(\nu\) is the Poisson’s ratio, \(b\) is the Burgers vector, and \(\theta\) is the angle with respect to the X-axis that goes from 0 to \(2\pi\). While the Volterra displacement field for a straight dislocation is simple to implement, there are limitations that need to be addressed. As shown in Equations (3-2) and (3-3), the stress fields are proportional to \(1/r\), which results in unrealistic displacements near the core region. Thus, the Volterra displacement field cannot capture properly the deformation near the dislocation core (and hence the structure of the core). In this work, the displacement field near the dislocation core is resolved by coupling the Volterra displacements from linear elasticity theory with an energy minimization procedure in atomistic simulations (as discussed in Chapter 2). Moreover, to generate straight mixed dislocations with arbitrary dislocation
character angles, a linear superposition approach that includes the displacement fields of both the edge and the screw dislocations is presented in Chapter 4.

**3.2 The Displacement Field of a Triangular Dislocation Loop**

Based on early work on line tension proposed by Lothe [129], Brown showed that it is possible to compute the stress and strain fields of a planar dislocation loop configuration based on the knowledge of infinitely straight dislocations [130]. Details of this proof can be found in Hirth and Lothe [1]. Based on this, Hirth and Lothe also proposed a displacement field for a triangular dislocation loop in an infinite isotropic medium. This elemental dislocation loop is simpler and more efficient to use compared to the analytical solution of a dislocation loop with a particular geometry such as a circle (cf. [131,132]) or a rectangle.

However, it is complex and inefficient to numerically implement the displacement fields of a triangular dislocation loop presented in [1]. In particular, the displacement field contains the total solid angle that is the sum of individual segment solid angles. Moreover, the calculation of this solid angle involves the unconventional choice of inverse trigonometric functions. These were addressed and improved in Barnett [81,82] resulting in the following equation for the displacement field of a triangular dislocation.

\[
\begin{align*}
    u(P) &= -\frac{b\Omega}{4\pi} + \frac{(1-2\nu)}{8\pi(1-\nu)}[f_{AB} + f_{BC} + f_{CA}] + \frac{1}{8\pi(1-\nu)}[g_{AB} + g_{BC} + g_{CA}]
\end{align*}
\]

(3-6)

In Equation 3-6, \( \Omega \) is the solid angle associated with the triangle ABC, as seen by an observer at point P. \( b \) and \( \nu \) are the Burgers vector and Poisson’s ratio, respectively. \( f_{AB}, f_{BC}, f_{CA} \) and \( g_{AB}, g_{BC}, g_{CA} \) are positional vectors, related to the relative...
position between the point of the observer and the edges of the triangle ABC. For example, $f_{AB}$ and $g_{AB}$ can be calculated as [81,82]:

$$f_{AB} = (b \wedge t_{AB}) \ln \left( \frac{R_B}{R_A} \cdot \frac{1 + \lambda_B \cdot t_{AB}}{1 + \lambda_A \cdot t_{AB}} \right) \quad (3-7)$$

$$g_{AB} = \left[ b(\lambda_A \wedge \lambda_B) \right] \left( \lambda_A + \lambda_B \right) \frac{1}{1 + \lambda_A \cdot \lambda_B} \quad (3-8)$$

where $t_{AB}$, $t_{BC}$, and $t_{CA}$ are the unit tangents along the directed segments AB, BC, and CA, as shown in Figure 3-3, respectively. $\lambda_A$, $\lambda_B$, and $\lambda_C$ are the unit vectors along $R_A$, $R_B$, and $R_C$, respectively. $R_A$, $R_B$, and $R_C$ are vectors from P to the vertices A, B, and C. The remaining f and g terms are obtained by cyclic interchange of indices.

The solid angle is defined as the projection of triangle ABC onto the unit sphere, so that, $\Omega = S$, where S is the area of the spherical triangle A'B'C', as shown in Figure 3-4. The area of the spherical triangle A'B'C', S, is equal to the excess (in radians) of the spherical triangle, which can be calculated using L'Huillier's theorem:

$$\tan^2 \frac{E}{4} = \tan \left( \frac{s}{2} \right) \tan \left( \frac{s-a}{2} \right) \tan \left( \frac{s-b}{2} \right) \tan \left( \frac{s-c}{2} \right) \quad (3-9)$$

where $s = \frac{(a + b + c)}{2}$ and a, b, c are the sides of the spherical triangle A'B'C', which can be calculated using the cosine rule in a triangle. For example, B'C' can be calculated as:

$$a = \|B'C'\| = \cos^{-1} (\lambda_B \wedge \lambda_C) \quad (3-10)$$

Depending on the side of the observer (above or below the plane that contains the triangular dislocation loop), the solid angle can be negative or positive:

$$\Omega = -\text{sign}(\lambda \cdot t_n) E \quad (3-11)$$
where \( \lambda \) can be either \( \lambda_A, \lambda_B \), or \( \lambda_C \), \( t_n \) is the unit normal to the plane ABC such that one traverses the triangular boundary from A to B to C counterclockwise, and \( E \) is given by Equation (3-9).

Since the displacement field is derived from linear elasticity, the principle of superposition is applicable, allowing addition and subtraction of triangular dislocation displacement fields to create more complex polygons. As mentioned earlier, the polygon approximation is an efficient method to study complex configurations of dislocation loops. As shown in Figure 3-5, dislocations with more complex geometry can be generated by adding the displacement field of the blue triangular dislocation loops and subtracting the displacement field of the red triangular dislocation loops [133]. In this work, the focus is on dislocation shear loops, whose configurations are purely planar. Indeed, Bitzek and collaborators have utilized this approach to generate an initial octagonal dislocation loop by adding 8 similar elemental dislocation loops. Chapter 6 will provide a more systematic approach to study dislocation shear loops approximated as polygons, which includes details such as stabilized Schmid stress, number of elemental triangular dislocation loops, and dislocation loop geometry.

### 3.3 Dislocation Core Structure of FCC Metals

While the displacement fields of straight dislocations and dislocation loops derived from linear elastic theory are valid far away from the dislocation cores, they are incapable of capturing the structures of the dislocation core. The goal of this section is to provide an overview of the core structure of dislocations in FCC metals, which plays a major role in dislocation properties as shown by previous studies discussed in Section 1.3. In FCC metals, perfect \( \frac{1}{6} <110> \) dislocations typically dissociate into two partial
dislocations that are separated by the stacking fault (SF) area [39]. For example, the
dissociation of the perfect $\gamma [110]$ dislocations can be written as:

$$\frac{a}{2}[110] = \frac{a}{6}[21 \overline{1}] + SF + \frac{a}{6}[121]$$

(3-12)

This reaction occurs due to the reduction in energy and the existence of stable
low-energy stacking faults on the \{111\} planes in FCC metals [39]. Based on the Frank’s
energy criterion, the energy state of the LHS of the reaction is proportional to $\frac{\Delta \gamma}{2}$, which
is greater than the energy state of the RHS, which is proportional to $\frac{\Delta \gamma}{6}$. The existence
of the stable SF on the \{111\} planes for FCC metals is due to their inherent atom
arrangements. As shown in the top view normal to the \{111\} planes of Figure 3-6, there
are three atomic layers, denoted as A, B, and C, that are $\gamma <111>$ apart along the plane
normal and repeat periodically with the period of $<111>$. These layers are stacked in a
way that the position of any atom type is at the center of the triangle formed by either
one of the other two types. For example in Figure 3-6, atoms in the A layers are at the
center of either triangle that forms by nearby B or C atoms. This stacking sequence
allows the intrinsic stacking fault that forms when one layer shifted into the ‘wrong’
triangles to be relatively low energy since the shift does not influence the relative
distances to the first and second nearest neighbors in the FCC lattice [39].

Due to this reaction, the core structure of a dislocation in FCC metals composed
of two Shockley partials and a SF area. The width of the SF area can be calculated
based on the forces acting on each partial [77]:

$$\begin{cases}
\tau_s b_\parallel + \tau_s b_\perp - F(R_p) - \gamma - B_\nu = 0 \\
\tau_s b_\parallel - \tau_s b_\perp + F(R_p) - \gamma - B_\nu = 0
\end{cases}$$

(3-12)
where $\tau_s$ is the Schmid stress, $\tau_e$ is the Escaig stress. The sign of the Escaig stress is defined such that a positive $\tau_e$ increases the SFW \cite{134,135}. $b_\parallel$ and $b_\perp$ is the components of the partial dislocation Burgers vectors that are parallel and perpendicular to the full Burgers vector, respectively. $F(R_p)$ is the elastic repulsive force between the two partials that is a function of the distance between the two partials, while $\gamma$ is the intrinsic stacking fault energy. $B_1\nu$ and $B_2\nu$ are the phonon friction forces acting on the leading and trailing partials, respectively. Subtracting the equations in Equation 3-12 gives the force balance that can be used to calculate $F(R_p)$, which allows the calculation of the distance between the partials, known as SFW.

$$F(R_p) = \tau_e b_\perp + \gamma - \frac{B_1 - B_2}{2} \nu$$

(3-13)

From Equation 3-13, the dislocation core structure depends on three parameters: the Escaig stress, the stacking fault energy, and the difference in the phonon drag between the Shockley partials. For edge and screw dislocations, the last term is zero since the structure of the dislocation core is symmetric. On the other hand, for mixed dislocations with arbitrary dislocation character angles, the structures of the dislocation core are asymmetric. Therefore, all parameters will affect the dislocation core structure. Chapter 4 and 5 will provide details computed from MD simulations regarding how each parameter influences the dislocation core structure and, as a result, the dislocation properties.
Figure 3-1. Volterra displacement field of a right-handed screw dislocation [1].

Figure 3-2. Volterra displacement field of an edge dislocation [1].
Figure 3-3. Geometry associated with a triangular dislocation loop [81,82].

Figure 3-4. The plane triangle ABC and its projection, the spherical triangle A'B'C', on the unit sphere [81,82].
Figure 3-5. Construction of a dislocation loop with complex geometry via addition and subtraction of triangular displacement fields [133].

Figure 3-6. Stacking faults in FCC metals. A) Plane-on view of the \{111\} plane in a FCC lattice. B) Perfect Burgers vectors \(b_{1,2,3}\) and partial Burgers vectors \(b_{p1,p2,p3}\) on the \{111\} plane. C) A perfect dislocation loop with Burgers vector \(b_3\), formed by first shifting the lattice by \(b_{p2}\) in the outer loop, and then shifting the lattice by \(b_{p1}\) in the inner loop, eliminating the stacking fault [39].
4.1 Background

The Peierls stress is the minimum required Schmid stress in the Burgers vector direction to move a dislocation [1]. According to Schmid’s law, the Schmid stress is the only stress component that influences dislocation motion [135]. As discussed in Section 1.3.1, the Peierls stress has been shown to be affected by other components of the local stress state [48,63,65,136–138]. For example, the Peierls stress is influenced by the Escaig stress [63,65,136], which is the shear stress within the slip plane perpendicular to the Burgers vector. Liu et al. used both MD and a semi-discrete variational Peierls-Nabarro approach to study the variation in the Peierls stress of straight edge and screw dislocations in Cu under different Escaig stresses [65]. In particular, under positive or negative Escaig stresses, the dislocation core could expand or constrict, resulting in a change in the Peierls stress for the dislocation. Dislocations with different character angles showed a different dependence on the Escaig stress since each dislocation has a unique core structure.

The Peierls stress is also influenced by pressure applied normal the (111) slip plane, $\sigma_n$ [48,137,138]. Using atomistic simulations, Bulatov et al. [48] studied the pressure dependence of the Peierls stress for screw and 60° straight dislocations in Al. For positive (compressive) pressure, the Peierls stress for both dislocations increased monotonically. While these studies provide insights into the pressure dependence of the Peierls stress, they are limited to certain types of dislocations (screw and 60°
dislocations) and only positive pressures (compression). This limited scope is relevant for understanding macroscopic plasticity since screw and 60° dislocations have lower mobility compared to other dislocations.

However, for the study of microscopic properties and mechanisms, such as the motion of dislocation loops [139] and their interaction with other defects [53], a more comprehensive understanding of the pressure dependence of the Peierls stress is essential. Thus, the goal of this chapter is to determine effects of pressure applied normal the (111) slip plane on the Peierls stress of straight dislocations in Al with different dislocation character angles. The character angle is defined as the angle between the dislocation core axis and the Burgers vector. First, for each dislocation character angle, the Peierls stress under a traction-free condition is calculated. The Peierls stress at 0K is calculated based on the change of the internal energy, which is an invariant measure of the dislocation driving force. Both the Peierls stress and the dislocation core structure are validated by comparing to previous experimental and simulation results. To study the effects of the <111> pressure, the Peierls stress is computed under pressures that range from -750 to 750 MPa. Variation in the Peierls stress due to pressure is understood by analyzing the dislocation core structures via parameters such as the interatomic spacing between atoms along the dislocation core and the SFW.

4.2 Simulation Methods

Mendelev et al. [124] and Mishin et al. [62] EAM interatomic potentials for Al (denoted as Mendelev potential and Mishin potential) are used to evaluate the role of interatomic potential on the pressure dependence of the Peierls stress. The simulation cell is oriented such that the dislocation line is along the X direction, while the normal
vector to the slip plane is along the Y direction. This allows the dislocation movement to be consistently in the Z direction. PBCs are implemented in the X and Z directions. The orientation and size of the simulation cell for each dislocation character angle, in term of the fundamental repeating unit in each direction, is shown in Table 4-1. The Burgers vector, \( \mathbf{b} \), is oriented along the [\( \overline{1}01 \)] direction in the (111) slip plane, which is an arbitrary choice.

To generate dislocations with different character angles, a superposition of the Volterra displacement fields for edge and screw dislocations is utilized [1,140]:

\[
\mathbf{u}(z,y) = \left[ u_x^0(z,y) \cos \phi, u_y^0(z,y) \sin \phi, u_z^0(z,y) \sin \phi \right]
\] (4-1)

and from Chapter 3,

\[
u_x^0(z,y) = b \frac{\theta}{2\pi}
\] (4-2)

\[
u_y^0(z,y) = -\frac{b}{2\pi} \left[ \frac{1-2\nu}{4(1-\nu)} \ln(z^2 + y^2) + \frac{z^2 - y^2}{4(1-\nu)(z^2 + y^2)} \right]
\] (4-3)

\[
u_z^0(z,y) = \frac{b}{2\pi} \left[ \theta + \frac{zy}{2(1-\nu)(z^2 + y^2)} \right]
\] (4-4)

where \( \theta \) varies from 0 to \( 2\pi \) about the X-axis, \( u_x^0 \) is the Volterra displacement field for a screw dislocation, \( u_y^0 \) and \( u_z^0 \) are the Volterra displacement fields for an edge dislocation, and \( \phi \) is the dislocation character angle. The origin of the dislocation is imposed at the center of the simulation cell. As shown in Figure 4-1, the simulation cell before imposing the modified Volterra displacement field is denoted by blue lines, respectively. While this displacement field successfully generates a straight dislocation at the center, the periodic boundary conditions along X and Z directions are violated.
The edge component of the Volterra solution creates an atomic step on the boundary in the positive Z direction, while the screw component causes an incompatibility between atoms along the Z direction. These artifacts are corrected by removing extra planes of atoms at the step and tilting the simulation cell about the Z axis a distance of \((-b/2)\cos\phi\) in the X direction.

Since the Volterra displacements are nonlinear at the Y positions associated with the top and bottom surfaces, when one surface moves relative to the other, the stress acting on the dislocation is biased by the initial position of the dislocation. To have an invariant effect on the dislocation, it is necessary to impose instead linear X and Z displacement fields on the boundary atoms:

\[
\begin{align*}
    u_x^{\text{boundary}}(z, y) &= -\frac{\text{sgn}(y) b \cos\phi}{2L_z} \left( z + \frac{L_z}{2} \right) + \frac{b \cos\phi}{2} & (4-5) \\
    u_y^{\text{boundary}}(z, y) &= 0 & (4-6) \\
    u_z^{\text{boundary}}(z, y) &= -\frac{\text{sgn}(y) b \sin\phi}{2L_z} \left( z + \frac{L_z}{2} \right) + \frac{b \sin\phi}{2} & (4-7)
\end{align*}
\]

After the imposition of the displacement fields, energy minimization is performed to resolve the proper atomic displacements around the dislocation core. For each character angle, the Peierls stress is then calculated based on the change in the internal energy, which is an invariant measure of the dislocation driving force, as the system is quasi-statically loaded [141,142]. Specifically, the top surface atoms are translated along the Burgers vector direction in increments of \(10^{-7}\) nm, while the bottom atoms are fixed. This increment size is necessary to capture the energy drop associated
with small Peierls barriers. The energy of the system is minimized and monitored after each translation. The Peierls stress of the dislocation is then computed via [142]:

$$\sigma_p = \frac{\Delta E_{ave}}{bh_x L_x}$$  

where $\Delta E_{ave}$ is the average energy released as the dislocation jumps to new locations, $h_z$ is the displacement of the dislocation in Z direction corresponding to one Burgers slip (also known as the Peierls period and shown in Table 4-1), and $L_x$ is the X-length of the simulation cell. To verify the results, the Peierls stresses are compared with previous atomistic simulations [48,143] and density functional theory (DFT) calculations [44].

To study the effects of $\sigma_n$, the Peierls stress under $\sigma_n$ that range from -750 (tension) to 750 (compression) MPa is computed. $\sigma_n$ is imposed by adjusting the Y position of the top boundary with a fixed bottom boundary. The dislocation core structures are measured using the OVITO visualization software [144]. Specifically, the interatomic spacing is defined as the average X-distance between atoms along the dislocation core. The SFW is defined as the Z-distance between two Shockley partial dislocations identified by the Dislocation Extraction Algorithm (DXA) in OVITO [145]. For each dislocation, the SFW is normalized by the corresponding Peierls period ($h_z$).

**4.3 Results and Analysis**

Figure 4-2 shows the variation in total potential energy as the top surface is shifted in the Burgers vector direction for screw and 60° dislocations. For each simulation, the potential energy drops when the dislocation abruptly jumps $h_z$ distance due to the imposed shear. Using Equation 4-8, the Peierls stress of the screw, 30°, 60°, and edge dislocations are shown in Table 4-2, with a comparison to previous atomistic
simulation results [48,143]. The Peierls stress of edge and screw dislocations using the Mishin potential (1.34 and 30.5 MPa) is in better agreement with DFT calculations [44] (1.6 and 9.9 MPa) compared to the Mendelev potential (6.36 and 86.3 MPa) probably because the Mishin potential includes the intrinsic stacking fault energy in the fitting database.

Figure 4-3 shows the dependence of the Peierls stress on $\sigma_n$ for both Mendelev and Mishin potentials. For the Mendelev potential, the Peierls stresses of the edge and $30^\circ$ dislocations decrease with increasing $\sigma_n$ from tension to compression. The ratios between the largest and smallest Peierls stress, $\frac{\sigma_{p,\text{max}}}{\sigma_{p,\text{min}}}$, for the edge and $30^\circ$ dislocations are 11.3 and 4.88, respectively. For the screw and $60^\circ$ dislocations, these ratios are much smaller: 1.14 and 1.44, respectively. The Peierls stresses for the screw and $60^\circ$ dislocations reach maximum values (87.8 and 49.4 MPa) at 450 MPa (compression) and -150 MPa (tension), respectively. This is consistent with the reported Peierls stress of 86 MPa for a screw dislocation at 340 MPa in Bulatov et al. [48]. However, their reported Peierls stress of 50 MPa for the $60^\circ$ dislocation at 340 MPa does not match the trend reported in this study. This is likely due to differences in the simulation geometry, specifically the use of a dislocation dipole model, and their use of the Ercolessi and Adams Al potential [56]. For the Mishin potential, the Peierls stress of edge and $30^\circ$ dislocations under tension are relatively constant. Under compression, the Peierls stress of the edge dislocation decreases slightly, while the Peierls stress of the $30^\circ$ dislocation increases with increasing $\sigma_n$. While the overall trends are similar to the Mendelev potential, the Peierls stresses of the screw and $60^\circ$ dislocations using the Mishin potential are more sensitive to $\sigma_n$. For the screw dislocation, the ratio between
the largest (at 150 MPa) and smallest Peierls stress (at 750 MPa) is 1.87, compared to 1.14 for the Mendelev potential. Moreover, the core structure of the Mishin 60° dislocation under compressive $\sigma$, greater than 300 MPa becomes nonplanar and thus is not analyzed here. More detail regarding this observation is provided in Chapter 5.

To understand the observed effects of $\sigma$ on the Peierls stress in Al, the $\sigma$ dependence of the SFW and the interatomic spacing between atoms along the dislocation core are analyzed. As shown by Liu et al., the Peierls stress is at a local maximum or minimum when the SFW is equal to a multiple or half-multiple of the Peierls period ($h_z$), respectively, due to the in-phase or anti-phase movement of the Shockley partials [65]. The deviation of the SFWs from multiples of $h_z$, denoted as $\phi_n$, is calculated by:

$$\phi_n = \frac{d_{\text{width}}}{h_z} - n_{\text{common}}$$  \hspace{1cm} (4-9)

where $d_{\text{width}}$ is the SFW and $n_{\text{common}}$ is a common integer that is unique for each character angle. As shown in Figure 4-4A, the $\phi_n$ of the screw and 60° dislocations for the Mendelev potential is relatively constant, consistent with the small ratio between the largest and smallest Peierls stress. Moreover, the SFWs of the screw and 60° dislocations at 450 and -150 MPa, respectively, deviate the most from a half-multiple of the Peierls period, resulting in the highest Peierls stress at these $\sigma$, in Figure 4-3A. On the other hand, the $\phi_n$ of the screw and 60° dislocation for the Mishin potential varies significantly as $\sigma$ increases from tension to compression. This is consistent with the $\sigma$ dependent behavior of each potential shown in Figure 4-3. For the Mendelev edge
and 30° dislocations, as $\sigma_n$ increases from tension to compression, the $\phi_n$ deviates away from zero, which is consistent with the constant decrease in the Peierls stress. On the other hand, Figure 4-4B shows a consistent reduction in the SFW for the edge and 30° dislocation for the Mishin potential, which is consistent with the higher unstable stacking fault energy for increasing $\sigma_n$ in Al [146]. The reduction in SFW and change in $\phi_n$ increase the Peierls stress for the 30° dislocation under compressive $\sigma_n$ as shown in Figure 4-3B.

The reduction in Peierls stress under compression for both potentials is associated with a linear increase in interatomic spacing along the dislocation core for each dislocation. As $\sigma_n$ increases from tension to compression, atoms within the slip planes are separated due to the Poisson effect. Moreover, due to the directional bonding in Al, the bottom atoms contract in the dislocation axis direction when the top atom hop to the next location, similar to the “hinged rod” model [147]. Thus, if atoms within the slip plane are wider spaced along the dislocation core, it is easier to move a dislocation in the Burgers vector direction, resulting in a reduction in the Peierls stress.

4.4 Summary

The $\sigma_n$ dependence of the Peierls stress for straight dislocations in Al is studied via atomistic simulations. The Peierls stresses for screw, 30°, 60°, and edge straight dislocations in a stress-free condition are in the same general range as previous atomistic simulations and DFT calculations. The Peierls stress calculated from the Mishin potential is more sensitive to the change in $\sigma_n$. For the screw and 60° dislocations, the Peierls stress versus $\sigma_n$ relationship shows maximums associated with SFWs that are multiple of the Peierls period. For the edge dislocation, the Peierls
stress decreases with increasing \( \sigma_n \). For the Mishin potential, the core structure of the 60° dislocation under compressive \( \sigma_n \) greater than 300 MPa becomes nonplanar.

Results from this chapter provide insight into improving DDD models. For systems with high dislocation density, the stress field generated by neighboring dislocations influences both the force and the mobility of dislocations. While the force on each dislocation is captured by the Peach-Koehler equation, the influence of the local stress field on dislocation mobility has not been incorporated within DDD simulations.

Table 4-1. Dislocation character angle, lattice orientations and sizes for each simulation model.

<table>
<thead>
<tr>
<th>( \theta ) (°)</th>
<th>X-axis</th>
<th>Y-axis</th>
<th>Z-axis</th>
<th>( h_z )</th>
<th>Size</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 (Screw)</td>
<td>[(\bar{1}01)]</td>
<td>[111]</td>
<td>[(\bar{1}2\bar{1})]</td>
<td>( b\sqrt{3}/2 )</td>
<td>10x20x60</td>
</tr>
<tr>
<td>30</td>
<td>[(\bar{1}12)]</td>
<td>[111]</td>
<td>[(\bar{1}10)]</td>
<td>( b/2 )</td>
<td>6x20x120</td>
</tr>
<tr>
<td>60</td>
<td>[0(\bar{1}1)]</td>
<td>[111]</td>
<td>[(\bar{2}11)]</td>
<td>( b\sqrt{3}/2 )</td>
<td>10x20x60</td>
</tr>
<tr>
<td>90 (Edge)</td>
<td>[1(\bar{2}1)]</td>
<td>[111]</td>
<td>[(101)]</td>
<td>( b/2 )</td>
<td>6x20x120</td>
</tr>
</tbody>
</table>

Table 4-2. Peierls Stress (MPa) for each dislocation character angle.

<table>
<thead>
<tr>
<th>( \theta ) (°)</th>
<th>Mendelev</th>
<th>Mishin</th>
<th>Previous studies</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 (Screw)</td>
<td>86.3</td>
<td>30.5</td>
<td>39 [143], 82 [48], 6.2,9.9 [44]</td>
</tr>
<tr>
<td>30</td>
<td>6.49</td>
<td>0.709</td>
<td></td>
</tr>
<tr>
<td>60</td>
<td>48.0</td>
<td>9.25</td>
<td>47 [48]</td>
</tr>
<tr>
<td>90 (Edge)</td>
<td>6.36</td>
<td>1.343</td>
<td>1.75 [143],1.6 [44]</td>
</tr>
</tbody>
</table>
Figure 4-1. Simulation cell after imposing the modified Volterra fields. A) View along the dislocation axis. B) View normal to the slip plane.
Figure 4-2. Energy variation versus top layer displacement in the Burgers vector direction. Energy variation is computed relative to the original energy of the dislocation model.
Figure 4-3. Peierls stress for screw, $30^\circ$, $60^\circ$, and edge dislocations using different EAM potentials. A) Mendelev potential [124]. B) Mishin potential [62].
Figure 4-4. Deviation of the SFWs from integral multiples of the Peierls period for different EAM potentials. A) Mendelev potential [124]. B) Mishin potential [62].
CHAPTER 5
STRESS STATE DEPENDENCE OF THE MOBILITY LAW IN ALUMINUM

5.1 Background

Since plastic deformation is governed by the motion of dislocations, the mobility of a dislocation has a great influence on mechanical strength and failure mechanisms. The mobility of perfectly straight dislocations (periodic along the dislocation core) has been the focus of several prior studies as shown in Section 1.3.2 [66–72]. For straight dislocations moving at the subsonic speed in Al, the mobility curve between the dislocation velocity and the applied Schmid stress contains a linear damping regime and a nonlinear radiative damping regime. Both of these regimes vary for each of the dislocation character angle. It is found that a simple interpolation function between the mobility of edge and screw dislocations is insufficient [71,72], which has been the conventional assumption used in DDD simulations [75,148]. Moreover, the mobility law of straight dislocations was reported to be dependent on the local stress state [65,77,149–151]. For example, Burbery et al. found that the phonon drag coefficient of the 30° dislocation depended on the imposed Escaig stress due to its influence on the dislocation core structure. While these studies have provided insights on the mobility of dislocation, combined effects of both pressure normal to the (111) slip plane and the Escaig stress have not been studied.

Therefore, the objective of this chapter is to study the mobility of straight dislocations in Al with a particular focus on the effects of local stress state in both the phonon drag and the radiative damping regime. First, the phonon drag part of the mobility law for straight dislocations with different dislocation character angles is determined from MD simulations. For each dislocation character angle, the separate
and combined effects of pressure normal to the (111) slip plane and the Escaig stress on the mobility of dislocations are considered. In addition, the radiative damping regime of the mobility curve at higher applied Schmid stress is also studied. In particular, the role of both dislocation character angle and the local stress state on the damping parameters and the critical velocity, which separates the linear phonon damping regime from the nonlinear regime at the higher Schmid stress, are investigated.

5.2 Simulation Methods

5.2.1 Simulation Code and Interatomic Potential

Al is chosen due to its high intrinsic stacking fault energy (~140 mJ/m²) and low elastic anisotropy. This prevents the Shockley partial dislocation cores from spreading significant distances and avoids the formation of irregular corners in dislocation loops characteristic of elastically anisotropic materials [152]. To show the role of interatomic potential on mobility in the phonon drag regime, typical EAM potentials used to study dislocation mobility in Al are investigated [124,153–155]. Note, in the Liu et al. potential for Al-Mg [155], the Al only part is identical to the glue potential by Ercolessi and Adams [56]. The phonon damping coefficient \( B^* \) is calculated by using a linear regression model for the Schmid stress range from 0 to 15 MPa. The comparisons between different EAM potentials in this chapter are performed by an undergraduate student as part of the University of Florida University Scholars program under the supervision of myself.

5.2.2 Mobility of Straight Dislocation and the Role of Stress State

To investigate the mobility of straight dislocations, edge, screw, 30°, and 60° dislocations are generated at the center of a simulation cell (shown in Figure 5-1) using the Volterra displacement fields [1]. PBCs are implemented in the X and Z directions,
which are the dislocation line (core) and gliding directions, respectively, while a mixed boundary condition is applied in the Y direction. Specifically, atoms in the top layers are restricted to move rigidly in the XZ plane, while atoms in the bottom layers are fixed in all directions. This boundary condition has been previously used to study the mobility of straight dislocations [70,72]. The lengths of the simulation cell in X, Y, and Z directions are approximately 6.0 x 18.0 x 60.0 nm, resulting in approximately 400,000 atoms. The Y and Z lengths are sufficient to minimize the image force effects from the free surface and the periodic boundary on the simulation results. The slip system is chosen arbitrarily as the [\( \bar{1}01 \)] Burgers direction within the (111) slip plane. Further details about the method to generate straight dislocations and lattice orientations for each dislocation are discussed in Section 4.2 and Table 4-1. After inserting the dislocation, energy minimization is performed via a nonlinear conjugate gradient method to resolve the dislocation core structure. The system is then brought to thermodynamic equilibrium at 100K using the Nosé-Hoover thermostat [103]. The Y position of the top boundary is manually adjusted using an iterative technique to relieve the pressure due to the lattice thermal expansion at 100K.

To move the dislocation, a Schmid stress (denoted as \( \tau_s \)) is imposed by applying a constant force on each atom in the top boundary. The force applied to each atom in the global Cartesian coordinate system is calculated via,

\[
F_g = (F_x, F_y, F_z)_g = (\tau_s \cos \phi, 0, \tau_s \sin \phi) A / N
\]  

(5-1)

where \( \phi \) is the dislocation character angle between the dislocation line and the Burgers vector, \( A \) is the XZ surface area subjected to the applied shear force, and \( N \) is the number of atoms in the top boundary. The range of the Schmid stress is limited from 5
to 500 MPa since the focus of this chapter is on the phonon drag and radiative damping portions of the dislocation mobility curve. As shown in Figure 5-1, thermostat regions, using the Nosé-Hoover thermostat [103], are implemented near the boundary in a region separated from the dislocation core to limit the effects of artificial frictional forces on dislocation mobility. The positions and velocities of atoms in the non-thermostated regions are updated using equations of motion associated with the microcanonical ensemble (Chapter 2).

For each simulation, the position of the dislocation core is tracked via the DXA in OVITO [145]. The velocity of the dislocation under an applied Schmid stress is then calculated by a forward finite difference formula and averaged over 100 ps once the dislocation velocity reaches steady state. The velocity versus Schmid stress curves are then fitted to this data using the function [70,73,75]:

$$\sigma = \begin{cases} 
B\nu & \text{if } \nu \leq \nu_o \\
B\nu + D(\nu - \nu_o)^a & \text{if } \nu > \nu_o 
\end{cases} \quad (5\text{-}2)$$

where B is the phonon drag coefficient, D is the radiative damping coefficient, $\nu_o$ is the critical velocity, $\nu$ is the velocity of the dislocation, and $a$ is the power of the radiative damping regime. The piecewise form of Equation (5-2) is necessary to capture both the linear phonon damping and the nonlinear radiative damping regimes of the dislocation mobility curve. This form has been previously derived [73] and used in fitting mobility curve in MD simulations [3,72] with the power, $a$, of 1.5 for screw dislocation. Here, the power is considered as a variable to capture the mobility law of other non-screw dislocations. Each mobility curve is fitted using the damped least-squares method with
the constraint that the power is the smallest while maintaining the coefficient of
determination of at least 0.9999.

To understand the effect of local stress state on dislocation mobility, the mobility
of straight dislocations under pressure normal to the (111) slip plane, $\sigma_n$, and the
Escaig stress, $\tau_e$, is studied. The pressure normal to the (111) plane is imposed by
displacing the Y position of the top boundary relative to the bottom boundary. The
Escaig stress is imposed by applying a constant force to every atom within the top
boundary using,

$$F_e = (F_x, F_y, F_z)_e = (\tau_e \sin \phi, 0, -\tau_e \cos \phi) A / N \quad (5-3)$$

This chapter considers $\sigma_n$ from -500 MPa (tension) to 500 MPa (compression),
and $\tau_e$ from -250 to 250 MPa. These values are reasonable for the local stress state
commonly encountered within metals [68,156]. In addition, preliminary simulation results
show that the dislocation core may cross-slip or become nonplanar for the screw and
60° dislocations under Escaig stresses greater than the range examined in this work.

5.3 Results and Analysis

5.3.1 The Role of Interatomic Potential on the Mobility of Straight Dislocations

Figure 5-2 shows the velocities of edge and screw dislocations under Schmid
stresses from 5 to 100 MPa for different EAM interatomic potentials [124,153–155].
Overall, all interatomic potentials predict that the mobility law for edge and screw
dislocations consists of two regimes, which is consistent with previous studies about the
mobility of straight dislocations in Al [69,70,72]. The first regime shows a linear
relationship between dislocation velocity and Schmid stress, corresponding to the
phonon drag mechanism. The second regime, which is associated with an additional
damping mechanism (radiative damping), is nonlinear and has a much lower mobility compared to the phonon drag regime. The critical velocity that separates the two regimes varies from 15 to 50 MPa for different EAM potentials. Using the Schmid stress range from 0 to 15 MPa, the phonon drag coefficient, $B^*$, for edge dislocations is consistently smaller than for screw dislocations for all potentials, which indicates that edge dislocations have higher mobility. This is consistent with known behavior regarding the mobility of straight edge and screw dislocations [70,72].

Figure 5-2 shows that different EAM potentials can predict different mobility relationships. For both edge and screw dislocations, the phonon drag coefficient is highest for the Ercolessi and Adams style glue potential and lowest for the Mendelev potential. This can be explained by the difference in the dislocation core widths bounded by two Shockley partial dislocations that are predicted by each potential, as shown in Table 5-1. The core width predicted by the Mendelev potential is consistently the lowest among the four EAM potential studied. On the other hand, the equilibrium structure of the dislocation core using the glue potential shows the most dissociation. Since dislocation mobility increases with increasing core width, the trend observed in Figure 5-2 with the highest mobility for the glue potential and lowest mobility for the Mendelev potential is reasonable. The variance in the dislocation core structure predicted by EAM potentials is caused by the difference in both the intrinsic and unstable stacking fault energies [157]. An increase of either the intrinsic or unstable stacking fault energy results in a shorter stacking fault width. The dislocation core structure is the most compact for the smallest product of the stacking fault energies.
For the remainder of this chapter, the Zope and Mishin EAM potential [153] for Al is used for all simulations. First, it predicts reasonable B* at 100K (4.47 and 8.56 x10^{-6} Pa-s for edge and screw dislocations, respectively) when compared to experimental ranges from 1.8 to 7.0 x10^{-6} Pa-s, which are reported without identifying the dislocation character angle [158,159]. Compared to previous MD simulations, Cho et al. [72] reported phonon drag coefficients of approximately 3.25 and 4.0 x10^{-6} Pa-s for edge and screw dislocations, respectively, using the Mendelev potential [124]. Using the Ercolessi-Adams potential [56], the phonon drag coefficients were found to be 3.7 and 6.0 x10^{-6} Pa-s for edge and screw dislocations [70]. Based on the results of each potential in Figure 5-2, the slope using the Zope and Mishin potential should be in between the Mendelev [124] and Ercolessi-Adams potentials [56]. While it is possible to reproduce Olmsted et al. results [70] for the Ercolessi-Adams potential [56], the phonon drag coefficients for the Mendelev potential [124] calculated in this study are 8.41 and 10.6 x10^{-6} Pa-s for edge and screw dislocations, respectively. The difference between these values and reported results in [72] for the same potential is due to the lack of specification for the range of values that were used to fit the phonon drag coefficient in [72]. Furthermore, the Zope and Mishin potential has reasonable unstable and intrinsic stacking fault energies (151 and 115 mJ/m², respectively) compared to DFT calculation by Hartford et al. [59,61,140]. Finally, it properly accounts for the lattice softening effects with increasing temperature and produces a smooth shape for a dislocation shear loop at static equilibrium, which will be shown in Chapter 6 [139]. This is essential to capture the expansion of dislocation loop at finite temperature.
5.3.2 Phonon Drag of Straight Dislocation and the Role of Stress State

Figure 5-3 shows a sample data for dislocation velocity versus time for an edge dislocation under a Schmid stress of 100 MPa. As mentioned in Section 5.2, each data point is calculated by a forward finite difference formula using the position of the dislocation extracted from DXA. The position of the dislocation is extracted every 1 ps, so the number of DXA calculations for each simulation is 300. For each simulation, an average velocity is calculated using data between 200 and 300 ps. Figure 5-4 shows phonon drag coefficients under pure Schmid stress for edge, screw, 30°, and 60° dislocations at 100K, as well as comparisons to previous simulation results [72] and common interpolations that are used in DDD simulations [148]. Under pure Schmid stress, the drag coefficient of the 60° dislocation is approximately equal to that of the screw dislocation. Compared to the edge and 30° dislocations, the drag coefficients of the screw and 60° dislocations are larger indicating a higher phonon damping. These results are in agreement with results from Cho et al. [72] using the Mendelev potential [124]. Note, a common interpolation used in DDD simulations for the phonon drag coefficient of different dislocation character angles fails to capture the general trend.

\[
B(\phi) = B_{\text{edge}} \sin^2 \phi + B_{\text{screw}} \cos^2 \phi
\]  

(5-4)

In Equation (5-3), \(B_{\text{edge}}\) and \(B_{\text{screw}}\) are the phonon drag coefficients of the straight edge and screw dislocations, respectively. Compared to atomistic results for the two mixed dislocations, the approximation in Equation (5-4) is even worse than the simple linear interpolation between the phonon drag coefficients of the edge and screw dislocations. This indicates that it is necessary to improve the interpolation function.
implemented in DDD simulations to include more information about the mobility of mixed dislocations.

Figure 5-5 illustrates the role of stress state on the phonon damping of edge, screw, 30°, and 60° dislocations. In particular, Figure 5-5A shows the phonon drag coefficients of each dislocation under $\tau_e=0$ and different values of $\sigma_n$. For each dislocation, increasing $\sigma_n$ from tension to compression increase the phonon drag coefficient. This is analogous to the increase in the Peierls stress, as discussed in Chapter 4, for dislocations under compressive stress [48,149]. In addition, the effect of $\sigma_n$ depends significantly on the dislocation character angle. Compared to the edge and 30° dislocations, the phonon damping of the screw and 60° dislocations are more sensitive to changes in $\sigma_n$. The ratios between the maximum and minimum phonon drag coefficients of the screw and 60° dislocations for different $\sigma_n$ are approximately 132 and 251 %, respectively. The corresponding ratios for the edge and 30° dislocations are 112 and 107 %, respectively. Among the dislocations studied in this work, the 60° dislocation is the most sensitive to the change in $\sigma_n$. Moreover, the increase in B due to compressive $\sigma_n$ is more significant than the decrease in B due to tensile $\sigma_n$.

The Escaig stress, $\tau_e$, also influences the phonon damping coefficient of dislocations, as shown in Figure 5-5B. For each dislocation, increasing $\tau_e$ from negative to positive decreases the phonon drag coefficient. This trend is in agreement with previous MD study of Escaig stress effects on the Peierls stress of edge and screw dislocations in Cu [65]. However, it contradicts the influence of Escaig stress effects on
the mobility of a 30° dislocation in Cu [77]. This disagreement is due to the difference in the definition of the sign of the Escaig stress, which is defined in this work so that a positive Escaig stress increases the SFW between two Shockley partial dislocations. The influence of the Escaig stress is also greater for the screw and 60° dislocations compared to the edge and 30° dislocations. For instance, under $\tau_e = 250$ MPa, the reductions in the phonon drag coefficients of the screw and 60° dislocations compared to $\tau_e = 0$ are about 6.22 and 21.4 %, respectively. On the other hand, the corresponding reductions for the edge and 30° dislocations are 2.93 and 1.09 %, respectively. Moreover, the increase in the phonon damping coefficient due to $\tau_e < 0$ is also greater than the decrease due to $\tau_e > 0$.

In Figure 5-5B, the data for the 60° dislocation under $\tau_e = -250$ MPa is incomplete because the combined stress state causes a nonplanar dislocation core structure. The generation of this nonplanar core structure is similar to the Fleischer mechanism for screw dislocation cross-slip. Compared to other FCC metals, cross-slip of screw dislocations in Al is more probable due to its relatively high stacking fault energy and thus narrow dislocation core [160]. If the dislocation core is further constricted, cross-slip becomes a more viable mechanism. Indeed, cross-slip of the screw dislocations via Fleischer mechanism has been observed in Al dislocations near defects with high local stress such as nanovoids [161] or grain boundaries [162]. In the Fleischer model, the leading 30° partial dislocation of the screw dislocation splits into the Shockley partial of the cross-slip plane and a stair-rod dislocation. The trailing 30° partial is then recombined with this stair-rod dislocation to form another Shockley partial of the cross-slip plane. This completes the cross-slip process and the new pair of
Shockley partials continue the motion on the cross-slip plane. Figure 5-6A shows the asymmetric core structure of the 60° dislocations, which composed of a 30° and a 90° partial. Due to its asymmetric core structure, only half of the reaction in the Fleischer mechanism can happen, which is a splitting reaction from a 30° dislocation into a new partial dislocation in the cross-slip plane and a stair-rod dislocation. Indeed, as shown in Figure 5-6B, the nonplanar core structure under $\tau_e = -250$ MPa composed of the original 90° partial dislocation and a new 30° dislocation partial in the cross-slip plane. Dislocation analysis via DXA implemented in OVITO [145] confirms that there is a stair-rod dislocation in this nonplanar dislocation core structure.

Figure 5-7 accumulates the phonon drag coefficients for each dislocation character angle under all possible combinations of local stress state considered in this research. The nonplanar dislocation core structure of the 60° dislocation is also encountered in other combinations of local stress, which are omitted from Figure 5-7. For each dislocation, increasing the $\tau_e$ or $\sigma_n$ from tension to compression increases the phonon drag coefficient. In addition, the effects of both $\tau_e$ and $\sigma_n$ vary for different character angles. The phonon damping of the screw and 60° dislocations are highly sensitive to the stress state with ratios between the maximum and minimum phonon drag coefficients of approximately 218 and 268 %, respectively. On the other hand, the changes in the phonon drag coefficients are smaller for both the edge and 30° dislocations with the corresponding ratios of approximately 128 %. Moreover, compression/tension asymmetry effects are also observed where the increase in B is more significant than the decrease in B under the combined state of stress. This
indicates that it is easier for local stress state to decrease than increase the mobility of a dislocation.

The role of stress state observed in Figures 5-5 and 5-7 can be explained by the influence of local stress state on the dislocation core structure. In particular, the phonon drag coefficients and the average stacking fault widths (over the Schmid ranges of 0 – 15 MPa) of each combination of the stress state are shown in Figure 5-8. From Figure 5-8, it is clear that the phonon drag coefficients for edge and 30° dislocations are less sensitive to the dislocation core structure compared to screw and 60° dislocations. This is consistent with previous simulation results by Marian and Caro [75], which suggested that the direction of motion also influenced the mobility of a dislocation, in addition to the dislocation core structure. Although the core structure of the 30° dislocation is more compact compared to the 60° dislocation, the mobility of the 30° dislocation is much higher than the 60° dislocation. In fact, the phonon drag coefficients of the edge and 30° dislocations, which move in the <121> directions, are similar to each other and much smaller than the screw and 60° dislocations, which move in the <101> directions.

The data in Figure 5-8A and 5-8B are colored differently to investigate the role of each component of the stress state on the dislocation core structure. Figure 5-8A focuses on the role of σ_n on the dislocation core. Data from the state of stress with positive (compressive), negative (tensile), and zero pressure is colored by blue, red, and green, respectively. On the other hand, Figure 5-8B emphasizes on the role of τ_e with similar coloring scheme for the data from negative to positive τ_e. For each dislocation in Figure 5-8B, increasing τ_e increases the stacking fault width resulting in a lower dislocation drag coefficient and thus higher mobility, as shown in Figures 5-5B
and 5-6. On the other hand, while decreasing $\sigma_n$ (from compression to tension) also increases the stacking fault width, the reduction in the dislocation core is less significant compared to the reduction due to $\tau_e$. Therefore, the influence of $\sigma_n$ on the mobility of a dislocation can be associated with another crystallographic effect in addition to the effect on the dislocation core. Indeed, as $\sigma_n$ increases from tension to compression, the interatomic spacing along the dislocation core for each dislocation decreases. With less space between the (111) planes, it is harder to move a dislocation in the Burgers vector direction at finite temperature, resulting in a reduction in the mobility of a dislocation. This is consistent with the increase in ideal shear strength under compressive stress from DFT calculations in Al [163].

5.3.3 Radiative Damping of Straight Dislocation and the Role of Stress State

Figure 5-9 shows the dislocation mobility data and the fitted curves using Equation (5-2) for different dislocation character angles. The power for the screw dislocation is found to be 1.8, which is greater than the 1.5 in the phenomenological form proposed by Olmsted et al. [70]. This power of 1.5 is inspired by the proportional relationship between the applied Schmid stress and $(\Delta \nu / \nu_m)^{1.5}$ for screw dislocations moving with supersonic speed ($> \nu_m$) by Eshelby [73]. Since the range of the Schmid stress considered in this work is from 0 to 500 MPa, which is reasonable for larger scale modeling of dislocations in DDD simulations, all dislocations move at subsonic speeds. Therefore, it is plausible that the 1.5 power does not apply in this study. Moreover, Equation 5-2 with the power 1.5 has been shown to be phenomenological since the critical velocity that it predicted for the screw dislocation was not correlated to any physical velocities. For instance, fitted critical velocity ($\nu_o$) from the MD simulations
using this phenomenological equation with power 1.5 were approximately 1.40 nm/ps [3,72], which is not related to the velocities of any relevant phonon modes. On the other hand, as shown in Figure 5-10, \( v_o \) for each dislocation in this study is in reasonable agreement with the minimum phase velocity, which is the velocity when the dispersion is introduced.

Figure 5-9 also captures the differences in the mobility of each dislocation character angle between the phonon and radiative damping regimes. Unlike the phonon damping regime where the mobility of the dislocation pairs (such as the screw and 60° dislocation pair or the edge and 30° dislocation pair) have similar damping coefficients, the mobility of dislocations in the nonlinear radiative damping regime varies significantly for different dislocation character angles. For instance, the 60° dislocation transitions from similar mobility to the screw dislocation in the phonon damping regime to significantly higher mobility for Schmid stresses greater than 100 MPa. This results in differences in \( v_o \) and the power law exponent between the screw and the 60° dislocations, presented in Table 5-2. Since \( v_o \) of the 60° dislocation is lower than the screw dislocation, it moves into the radiative damping regime at a lower Schmid stress. As a result, the velocity of the 60° dislocation increases at a faster rate than the screw dislocation as the Schmid stress increases. Moreover, the combination of low radiative damping parameter (D) and high power law exponent captures the faster rate of change in the mobility of 60° dislocation with increasing Schmid stress compared to the screw dislocation.

Figures 5-11 through 5-14 show the effects of \( \sigma_n \) on the radiative damping portion of the mobility curve of the screw, 30°, 60°, and edge dislocations, respectively. While
the mobility of the dislocation is generally decreased when the pressure is increased from tension to compression, each dislocation has a distinct behavior, especially in the radiative damping regime. Figure 5-12 illustrates that the 30° dislocation continues to be insensitive with the change in \( \sigma_n \), which is consistent with the phonon damping regime. On the other hand, the other three dislocations behave differently when they transition to the radiative damping regime. For the screw dislocation, the radiative damping coefficient increases and \( \nu_0 \) decreases, while the power law coefficient is relatively constant (as shown in Figure 5-15) as \( \sigma_n \) increases from tension to compression. This results in a higher mobility for dislocations than that under tensile \( \sigma_n \) since the dislocation stays longer in the phonon damping regime. Moreover, the change in the radiative damping coefficient due to \( \sigma_n \) is less than 7%, which results in parallel mobility curves in the radiative damping regime, as shown in Figure 5-11. In contrast, for the edge dislocations, both the radiative damping coefficient, the power law exponent, and \( \nu_0 \) increase with increasing \( \sigma_n \) from tension to compression. The change in \( \nu_0 \) is less significant for the edge dislocation compared to the screw dislocation. This results in the same mobility for different \( \sigma_n \) until the dislocation velocity reaches \( \nu_0 \) and transitions to the radiative damping regime, where the difference between mobility becomes more visible, as shown in Figure 5-14. For the 60° dislocation, which is the most sensitive to \( \sigma_n \) in the phonon damping regime, the mobility becomes less sensitive to \( \sigma_n \) in the radiative damping regime. This is captured in the decrease in the power (shown in Figure 5-16) and the increase in \( \nu_0 \), as \( \sigma_n \) changes from tensile to compressive pressure.
On the other hand, the influence of $\tau_e$ on the radiative damping portion of the mobility curve of screw, $30^\circ$, $60^\circ$, and edge dislocations are shown in Figures 5-16 through 5-19, respectively. Generally, dislocations under positive $\tau_e$ are more mobile than the ones under negative $\tau_e$ in the radiative damping regime. However, similar to $\sigma_n$, the influence of $\tau_e$ on the mobility of each dislocation character angle in the radiative damping regime varies. For the screw dislocation, the radiative damping coefficient decreases and $\nu_0$ increases as $\tau_e$ increases from negative to positive values. As a result, shown in Figure 5-16, screw dislocations under positive $\tau_e$ consistently move faster than the ones under negative $\tau_e$. Moreover, the mobility curves of screw dislocations under different $\tau_e$ in the radiative damping regime are parallel, quantified via a computed change in the radiative damping coefficient due to $\tau_e$ of less than 16%. This also shown in the constant power law coefficient for screw dislocations in Figure 5-20. Figure 5-17 shows that the mobility of the $30^\circ$ dislocation is slightly sensitive to $\tau_e$ at the beginning of the radiative damping regime and become less sensitive to $\tau_e$ as it moves faster. This is reflected in an increase in the power law exponent of the fitted mobility curve as $\tau_e$ increases. Similarly, the mobility of the $60^\circ$ dislocation also becomes less sensitive to $\tau_e$ at higher velocities at higher applied Schmid stresses, as presented in Figure 5-18. However, since the mobility of the $60^\circ$ dislocation is highly sensitive to the $\tau_e$ in the phonon regime, the power law exponent is increased (as shown in Figure 5-20) and $\nu_0$ is decreased as $\tau_e$ increases. The mobility of the edge dislocation in Figure 5-19 shows the asymmetric effects of $\tau_e$. While negative $\tau_e$ has
little influence on the mobility in both the phonon and radiative damping regimes, positive $\tau_e$ has a noticeable effect on the mobility of the edge dislocation at the beginning of the radiative damping regimes and decays as the dislocation moves faster. As a result, the power law exponent of the mobility curves for edge dislocations under positive $\tau_e$ is higher than the ones under $\tau_e \leq 0$.

As shown in a few previous studies and discussed in Chapter 1, the mobility of dislocations depends on both the dislocation core structure and the direction of dislocation motion [72,75]. Figures 5-21 and 5-22 show the dislocation core widths for screw, 30°, 60°, and edge dislocations for different combinations of Schmid stress, Escaig stress ($\tau_e$), and pressure normal to the (111) slip plane ($\sigma_n$). For screw, 30°, and edge dislocations, the dislocation core contracts as the dislocation moves faster. This is consistent with results for screw dislocation in Cu moving at subsonic velocity assuming that the trailing and leading partials have the same mobility [164]. On the other hand, the core width of the 60° dislocation remains relatively constant at higher velocities. This is due to the higher mobility of the 90° leading partial compared to the 30° trailing partial for the 60° dislocation, which expands the dislocation core width. As a result, these two effects cancel each other out resulting in a relatively constant dislocation core width for 60° dislocations at higher velocities. This special behavior of the 60° dislocation core also explains the less damped radiative regime compared to the other three dislocations shown in Figure 5-9. Since the core widths of the screw, 30°, and edge dislocations reduce significantly at higher velocities, their mobilities are reduced significantly in the radiative damping regime. On the other hand, the relatively constant dislocation core structure of the 60° dislocation allows for a lesser damped mobility in the radiative
damping regime. Figures 5-21 and 5-22 also show the dependence of the local stress state on the dislocation core structure in the radiative damping regime, which is consistent with the phonon damping regime. Specifically, compressive $\sigma_n$ or $\tau_e < 0$ increases the SFWs, while tensile $\sigma_n$ or $\tau_e > 0$ increases the SFWs of the dislocation. The effects of $\tau_e$ on the dislocation core structure are more significant than $\sigma_n$.

Another important aspect of the mobility of a dislocation is the direction of dislocation motion, which influences the minimum phase velocity. This minimum phase velocity has been shown to be related to the critical velocity that separates the phonon damping and the radiative damping regimes [75]. The minimum phase velocity is calculated using the phonon dispersion curve, which was shown to be dependent on the stress state for dislocations in Al [165]. In particular, from Clatterbuck et al. data for the dispersion curves, the minimum phase velocity for an edge dislocation, which moves in the $<110>$ direction, under tensile $\sigma_n$ is expected to decrease. This is consistent with the reduction in the critical velocity ($v_o$) for the edge dislocation in this study.

5.4 Summary

The mobility of straight dislocations at a finite temperature under a range of Escaig stress, $\tau_e$, and pressure applied normal to the (111) slip plane, $\sigma_n$, is investigated. The phonon drag coefficients of the screw, 30°, 60°, and edge straight dislocations under pure Schmid stresses are consistent with previous atomistic simulations [70,72] and experiments [158,159]. Moreover, the critical velocities of the screw, 30°, 60°, and edge straight dislocations under pure Schmid stress are also in agreement with the minimum phase velocities from previous MD simulations [72]. The effects of $\tau_e$ and $\sigma_n$ on the mobility of each dislocation in the phonon and radiative
damping regimes are different and are captured through modification to traditional methods to describe the dislocation mobility curve.

For each dislocation, decreasing $\tau_e$ or the pressure normal to the (111) slip plane from tension to compression increases the phonon drag coefficient. In addition, the effects of both $\tau_e$ and $\sigma_n$ vary for different character angles. Compared to the edge and 30° dislocations, the phonon damping of the screw and 60° dislocations are more sensitive to the stress state. For the 60° dislocations under $\tau_e = 250$ MPa, the dislocation core structure becomes nonplanar due to the cross-slip of the 30° partial dislocation similar to the Fleischer cross-slip mechanism in screw dislocations. Moreover, the magnitude of the increase in the phonon damping coefficient due to either compressive $\sigma_n$ or negative $\tau_e$ is larger than the opposite effects, which indicates that it is easier to decrease than increase the mobility of a dislocation.

In the radiative damping regime, the influence of $\sigma_n$ or $\tau_e$ on each dislocation character angle varies. For the screw dislocation, either compressive $\sigma_n$ or negative $\tau_e$ decreases dislocation mobility, while the opposite state of stress increases dislocation mobility. This is due to the influence of the stress state on the critical velocity of a screw dislocation. On the other hand, the 60° dislocation becomes less sensitive to the stress state as it moves faster under higher applied Schmid stresses. The mobility of the edge and 30° dislocations are most sensitive to $\tau_e$ at the beginning of the radiative damping regime. In contrast, the mobility of the edge dislocation in the radiative damping regime is sensitive to $\sigma_n$, while the mobility of the 30° dislocation is insensitive to $\sigma_n$. The change in dislocation core structure for each dislocation in the radiative damping regime
explains the difference in the mobility between different dislocations. Moreover, the role of stress state on the dislocation mobility is due to its influences on both the dislocation core structure and the direction of motion.

Table 5-1. Dislocation core width and stacking fault energies for different EAM potentials.

<table>
<thead>
<tr>
<th></th>
<th>EAM1</th>
<th>EAM2</th>
<th>EAM3</th>
<th>EAM4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dislocation Core Width (nm)</td>
<td>1.22/0.54</td>
<td>1.78/1.10</td>
<td>1.51/1.02</td>
<td>1.40/0.71</td>
</tr>
<tr>
<td>(Edge/Screw)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Intrinsic Stacking Fault Energy (mJ/m²)</td>
<td>129 [140]</td>
<td>103 [56]</td>
<td>128 [154]</td>
<td>115 [153]</td>
</tr>
<tr>
<td>Unstable Stacking Fault Energy (mJ/m²)</td>
<td>243 [140]</td>
<td>124 [56]</td>
<td>163 [154]</td>
<td>151 [153]</td>
</tr>
<tr>
<td>Product of Unstable and Intrinsic Stacking Fault Energy (mJ²/m⁴)</td>
<td>31347</td>
<td>12772</td>
<td>20864</td>
<td>17365</td>
</tr>
</tbody>
</table>

Table 5-2. Damping parameters for different dislocation character angle under pure Schmid stress

<table>
<thead>
<tr>
<th>θ (°)</th>
<th>B</th>
<th>b</th>
<th>a</th>
<th>ν₀ (nm/ps)</th>
<th>D (MPa ps⁻¹ nm⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 (Screw)</td>
<td>8.56</td>
<td>2.0</td>
<td>0.773</td>
<td>450</td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>4.27</td>
<td>2.7</td>
<td>1.63</td>
<td>850</td>
<td></td>
</tr>
<tr>
<td>60</td>
<td>9.28</td>
<td>2.5</td>
<td>0.483</td>
<td>95</td>
<td></td>
</tr>
<tr>
<td>90 (Edge)</td>
<td>4.47</td>
<td>2.0</td>
<td>1.71</td>
<td>1291</td>
<td></td>
</tr>
</tbody>
</table>

Figure 5-1. Simulation cell with a straight dislocation has 3 different regions. Blue: boundary region, yellow: thermostat region, and green: mid region. The dislocation core structure is colored red.
Figure 5-2. Dislocation velocity versus Schmid stress for different EAM potentials. A) Edge dislocation. B) Screw dislocation.
Figure 5-3. Example dislocation velocity versus time for an edge dislocation under a Schmid stress of 100 MPa.
Figure 5-4. Phonon drag coefficients for edge, screw, 30°, and 60° dislocations at 100K compared to Cho et al. [72] and interpolation functions in DDD simulations.
Figure 5-5. Phonon drag coefficients for the edge, screw, 30°, and 60° dislocations at 100K. A) Under different pressure and zero Escaig stress, B) Under different Escaig stress and zero pressure.
Figure 5-6. Dislocation core structure of the 60° dislocation. A) At equilibrium. B) Under the Escaig stress of 250 MPa.

Figure 5-7. Phonon drag coefficients for edge (black), screw (blue), 30° (red), and 60° (green) dislocations at 100K.
Figure 5-9. Mobility data and curves for different dislocation character angles under pure Schmid stress.
Figure 5-10. Comparison between critical velocities and the minimum phase velocities for different dislocation character angles under pure Schmid stress.
Figure 5-11. Mobility data and curves for screw dislocations under different pressures normal to the (111) slip plane and Schmid stresses.
Figure 5.12. Mobility data and curves for 30° dislocations under different pressures normal to the (111) slip plane and Schmid stresses.
Figure 5-13. Mobility data and curves for 60° dislocations under different pressures normal to the (111) slip plane and Schmid stresses.
Figure 5-14. Mobility data and curves for edge dislocations under different pressures normal to the (111) slip plane and Schmid stresses.
Figure 5-15. Power law exponent for screw and $60^\circ$ dislocations under different pressures normal to the (111) slip plane and Schmid stresses.
Figure 5-16. Mobility data and curves for screw dislocations under different Escaig and Schmid stresses.
Figure 5-17. Mobility data and curves for 30° dislocations under different Escaig and Schmid stresses.
Figure 5-18. Mobility data and curves for 60° dislocations under different Escaig and Schmid stresses.
Figure 5-19. Mobility data and curves for edge dislocations under different Escaig and Schmid stresses.
Figure 5-20. Power law exponent for screw and $60^\circ$ dislocations under different Escaig and Schmid stresses.
Figure 5.21. Dislocation core widths of edge and 30° dislocations under different combinations of Schmid stress, Escaig stress, and pressure normal to the (111) slip plane.
Figure 5-22. Dislocation core widths of screw and 60° dislocations under different combinations of Schmid stress, Escaig stress, and pressure normal to the (111) slip plane.
6.1 Background

The geometry of a dislocation loop in equilibrium with an externally applied Schmid stress has been the focus of multiple experimental and analytical studies over the last half century. In seminal work, deWit and Koehler [166] computed the shape of a dislocation loop in an anisotropic crystal under an externally applied Schmid stress, using the elastic energy per unit length of an infinitely straight dislocation. This approach ignored the influence of the dislocation loop elastic field on itself [130], and thus predicted that the elliptical shape of a dislocation loop is independent of size. Scattergood and Bacon [167] proposed a different approach to compute the size and shape of a dislocation loop, via force equilibrium applied to nodal points that discretize the loop. They showed that dislocation loops become more elongated (elliptical) as the size of the dislocation loop decreases. A more generalized way to compute the self-stress was proposed by Gavazza and Barnett [168]. Later work by Schmid and Kirchner [169] provided the opposite conclusion using a different approach to compute the dislocation loop self-stress, showing that the inclusion of a dislocation core tension term [170] caused dislocation loops to become more circular as the size of the dislocation loop decreases. This conclusion was supported by Mughrabi [171] through measurement of dislocation line curvatures in Cu in the TEM. However, Brown [172] argued that dislocation loops in stable equilibrium (without an externally applied stress)

within a TEM foil must be supported by internal stress fields, and he showed that such fields could cause the dislocation loop to be circular.

Determining the properties of dislocation loops quantitatively from TEM experiments remains challenging, representing an ideal opportunity for atomistic and DDD simulations to verify proposed theories. Compared to experiments, computational models of dislocations can be designed to isolate certain dislocation properties or study small systems of dislocations to gain insight into dislocation interaction mechanisms. For example, atomistic simulations can provide a detailed description of dislocation core structure (cf. [50,173]) under the assumption that the interatomic potential provides accurate predictions of the lattice anisotropy and dislocation loop stress field, and can be used to quantify self-interactions or dislocation interactions with other defects [51,53,174,175], which are essential inputs for DDD simulations. Aubry et al. [152] performed DDD simulations with estimates of the dislocation core energy from atomistic simulations and concluded that the Bacon and Scattergood approach to approximate crystal anisotropy was appropriate to model irregular “corners” in dislocation loops in α-Fe. They also concluded that the dislocation core energy term had a negligible effect on the dislocation loop shape, for loops with 50 nm radius. Together, atomistic and DDD simulations provide powerful tools to address the size and shape of nanoscale dislocation loops subjected to a Schmid stress, which is an important first step for studies of dislocation loop interactions with other defects.

To date, atomistic simulation has not been used to compute systematically the stability and geometry of nanoscale dislocation shear loops at static equilibrium and finite temperature. Thus, the objective of this chapter is to determine the geometry and
the resolved Schmid stress necessary for equilibrium of nanoscale dislocation shear loops in Al, including the influence of loop radius and temperature, using atomistic simulations. Furthermore, this chapter presents a direct approach to extract lattice friction stress including temperature dependence from atomistic simulations. The scope of this chapter is limited to nanoscale dislocation shear loops, which will be referred to simply as dislocation loops, with initial radii less than 24.3 nm, due to the computational cost of the atomistic simulations. Dislocation loops of this size are observed in several applications, such as in metals subjected to irradiation [176–178]. A frame invariant computational algorithm to generate stable dislocation loops at 0 K and finite temperatures is developed and presented. The geometry of dislocation loops at 0 K, the structure of the core and the resolved Schmid stress necessary for dislocation loop equilibrium provide validation of trends presented by Scattergood and Bacon [167]. The role of Al interatomic potential on static equilibrium properties is also discussed. For finite temperature studies, the minimum Schmid stress required to open a dislocation loop is computed. This provides a means to compute the effective lattice friction stress as a function of temperature. A critical dislocation loop size is identified above which the effective lattice friction stress is size independent. Finally, the expansion of the dislocation loop is also investigated to understand how the difference in mobility between segments of the dislocation loop influences the overall geometry of the dislocation loop.

6.2 Simulation Methods

EAM potentials for Al parameterized by Mishin et al. [62], Zope and Mishin [153], Liu et al. [154], Winey et al. [179] and Sheng et al. [180] are used to show the effect of
different interatomic potentials on the resolved Schmid stress necessary for dislocation loop equilibrium.

6.2.1 Dislocation Shear Loop Algorithm

Three methods are commonly used to introduce curved dislocation segments or dislocation loops in atomistic simulations. First, self-interstitial-atom (SIA) dislocation loops can be constructed by inserting extra atomic planes into the lattice [181]. However, the atom insertion process requires a certain global orientation of the simulation cell to satisfy PBCs. This limits application of this method in dislocation – grain boundary interaction problems where different grain boundaries require different lattice orientations. Second, dislocation shear loops can be generated via a Frank-Read source within a periodic simulation cell [80,182]. The use of a Frank-Read source requires large simulation cells to avoid periodic boundary conditions and often restricts the lattice orientations that can be studied. Third, dislocations can be homogenously [183,184] or heterogeneously [52,185] nucleated during deformation. This often generates dislocations that form and move at GPa level stresses, which may influence the structure and behavior of the dislocation core [74]. While these methods have shown some success in the investigation of dislocation loops and their interaction with other defects, they have clear drawbacks.

A different approach is implemented in this chapter. Figure 6-1 shows the atomistic simulation framework developed to compute the resolved Schmid stress necessary for dislocation loop equilibrium. To introduce a dislocation loop, the loop is divided into $N_{tri}$ triangles arranged to form circular or elliptical geometries. The displacement fields associated with the triangular dislocations, derived by Barnett and coworkers using linear elasticity [81,82], are summed considering a common origin. The
number of triangles employed, $N_{\text{tri}}$, is taken as a multiple of 8 so that edge and screw dislocation segments are easily aligned with the boundaries of the initial dislocation loop structure. This approach was used by Bitzek et al. [53] to construct a dislocation loop within a nanocrystalline Al grain to study dislocation – grain boundary interactions. However, since the focus of their work was to study only the interaction between an expanding dislocation loop and a general grain boundary in nanocrystalline Al, it was not necessary for Bitzek et al. to compute a precise value for the resolved Schmid stress required for equilibrium of a dislocation loop with a given radius. Those details, including the role of interatomic potential, are investigated in this paper. Furthermore, the effect of the triangulation on the resolved Schmid stress necessary for equilibrium is discussed briefly in Section 3.1.

The equations derived by Barnett et al. do not consider atomic displacements near the core of a triangular dislocation loop; thus, energy minimization calculations are necessary to resolve these atomic displacements. In this work, the nonlinear CG energy minimization method is employed. If the atomistic simulation cell is stress-free, the energy minimization procedure will cause the dislocation loop to disappear. Therefore, before applying the displacement field solutions from Barnett et al., the atomistic model is pre-stressed to avoid the collapse of the dislocation loop due to self-interactions. As shown in Figure 6-1, the energy minimization process is performed first without adjusting the dimensions/tilt of the simulation cell. Then, a final minimization using CG allowing dimensional and tilt changes in accordance with the requisite stress tensor is performed. The displacement field of the energy minimized dislocation loop is then stored to use in the finite temperature simulations.
For each dislocation loop, the applied Schmid stress required for dislocation loop equilibrium, so that it neither expands nor collapses during the energy minimization process, is denoted as \( \tau_{ss} \). This value is obtained via a bisection method with the initial interval \([0, \tau_{theory}]\), where \( \tau_{theory} \) is the shear stress necessary to balance self-interactions in a circular dislocation loop of radius \( R_{loop} \) [167],

\[
\tau_{theory} = \frac{G_A b}{2\pi 2R_{loop}} \left( \ln \frac{2R_{loop}}{r_0} + 1.56 \right) \quad (6-1)
\]

with,

\[
G_A = \frac{4\pi E_s}{b^2} \quad . \quad (6-2)
\]

Here, \( G_A \) accounts for the anisotropic nature of the lattice and is 25.9 GPa for Al using the prelogarithmic part of the energy per unit length of a screw dislocation, \( E_s \) [167,186]. In Equation (6-1), \( r_0 \) is the dislocation core radius, which is taken to be equal to the Burger’s vector magnitude, \( b \). At least 15 iterations are used in the bisection method to provide a theoretical error of \( 2 \tau_{theory} / 2^{15} \), which is \( \approx 0.05 \) MPa for the smallest dislocation loops considered in this study.

Figure 6-2 shows the algorithm developed to compute the minimum resolved Schmid stress necessary to expand a dislocation loop at a desired temperature. Different temperatures are considered in this work ranging from 100 to 400 K. Before applying the displacement field obtained via energy minimization calculations for a given dislocation loop radius, determined by the bisection algorithm in Figure 6-1, the simulation box is pre-stressed and equilibrated to a desired temperature via Nosé-Hoover thermostat and barostat [102]. The minimum applied Schmid stress required to
expand the dislocation loop at a given size and temperature, denoted as $\tau_{sd}$, is obtained via a bisection method with the initial interval specified as $[0.5 \tau_{ss}, 1.5 \tau_{ss}]$. The results presented for each dislocation loop radius and temperature are averaged over five independent simulations.

6.2.2 Simulation Cell Geometries

Two different simulation cell geometries are considered in this work to illustrate the frame-invariance of the proposed bisection algorithm. In both models, PBCs are implemented in all directions. The first simulation cell, denoted as “box” geometry, is cubic with side lengths of 28.35 nm and X, Y, and Z axes aligned along [100], [010], and [001] crystal orientations. It contains 1,332,800 atoms and is used to calculate the resolved Schmid stress necessary to stabilize the dislocation loop at 0 K using different Al interatomic potentials. In addition, simulations are performed using the box geometry to study the effect of the number of triangles used to construct the initial dislocation loops. Dislocation loops are created on the (111) slip plane with a Burgers vector of $[\bar{1}01]$, which is an arbitrary choice. To study the role of dislocation loop size, which influences the magnitude of self-interactions, dislocation loops with radii of 4.05, 4.86, 5.67, 6.48, 7.29, and 8.10 nm are constructed.

As shown in Figure 6-3, the second simulation cell, denoted as “plate” geometry, resembles a two-dimensional plate with lattice rotated so that the $[\bar{1}01]$, $[1\bar{2}1]$ and [111] crystal orientations are aligned with the X, Y, and Z axes, respectively, of the simulation cell. The purpose of this geometry is to allow sufficient length in the X and Y axes to study larger dislocation loops with minimal and controllable effect of image forces on the simulation results. The plate simulation cell is used to calculate the
resolved Schmid stress necessary for dislocation loop equilibrium at 0 K and at finite
temperature, using the algorithms presented in Sections 6.2.1. The dislocation loop is
then expanded to study the role of the mobility of individual dislocation segments on the
mobility of a dislocation loop. For the minimum Schmid stress at finite temperature,
dislocation loops with radii 4.05, 8.10, 12.15, 16.2, 20.25, and 24.3 nm are constructed.
For dislocation loop equilibrium at 0 K, initial dislocation loop semimajor/semiminor axial
ratios of 1, 1.2, 1.4, and 1.6 (with the same semimajor axis) are used to evaluate the
sensitivity of equilibrated dislocation loop geometries to the initial dislocation loop
shape.

The Z dimension of the plate model is 28 nm, while the plate dimensions in X and
Y directions are proportional to dislocation loop radii. For finite circular dislocation loops,
as the distance from the dislocation loop core is greater than 2r, the long-range stress
field converges to the stress field of the infinitesimal loop, which decreases as 1/r^3 [1].
Thus, a minimum ratio of at least 6:1 between the X and Y simulation box dimensions
and the loop radii is implied. Preliminary studies of simulation box size show that a ratio
7.41:1 provides a relative error in the 0 K resolved Schmid stress of less than 1%,
meaning that image forces do not play a major role in the presented results. With this
ratio, the number of atoms in the plate simulation cell varies from 1,497,600 to
54,259,200 atoms for simulations with initial dislocation loop radii of 4.05 to 24.3 nm,
respectively.

For the expansion of the dislocation loop, a constant Schmid stress of 380 MPa
is applied for a dislocation loop with radius 12.15 nm. The plate geometry is utilized with
the same Z dimension of 28 nm, but much larger dimensions in X and Y directions of
182 nm. As a result, the ratio between the X and Y simulation box dimensions and the loop radii for the dislocation loop expansion study is 15:1. Moreover, results are obtained before the expanded dislocation loop reaches the ratio that is greater than 7.41:1. This ensures that image forces from PBCs have minimal effect as the dislocation loop becomes larger. Different local stress states are imposed on the dislocation loop to study the role of stress state on the mobility of the dislocation loop. Similar to the study of straight dislocations in Chapter 5, Escaig stresses of -250 and 250 MPa as well as pressures normal to the (111) slip plane of -500 and 500 MPa are used as these are the extremes of the behavior observed in Chapter 5.

Table 6-1 shows the state of stress applied to each simulation cell, in terms of the Schmid stress in Burgers vector direction within the dislocation slip plane. For the box model with the chosen lattice orientation, the complete state of stress is specified so that it resolves using the anisotropic elastic constants into a single Schmid stress matching the state of stress used in the plate model. The positions of the edge and screw components of the expanding dislocation loop are tracked via filtering out atoms with centrosymmetry values less than 2.0 Å² and averaging the position of the leading and trailing partials. Due to the continuous nature of the dislocation loop, it is necessary to define rules for locating the edge and screw components. The screw components are defined as dislocation segments whose averaged X distance from the center of the loop is the largest. The distance between the screw segments of the dislocation loop is denoted as \( l_s \), to match the notation of Scattergood and Bacon. On the other hand, the edge components are defined as dislocation segments whose averaged Y distance from the center of the loop is the largest. Data from this approach is verified by
comparing the dislocation loop perimeters to OVITO analysis via DXA algorithm, which automatically identifies dislocations via a discrete Burgers circuit integral over the elastic displacement field [145].

6.3 Results and Analysis

6.3.1 Static Equilibrium Size and Shape of Dislocation Loops

Figure 6-4 presents the static (0 K) Schmid stress necessary for dislocation loop equilibrium for each of the interatomic potentials employed using the box geometry. The triangulation approach successfully generates an initial octagonal dislocation loop. However, depending on the employed interatomic potential, different results are attained for the dislocation loop shape and the details of the relationship between the dislocation loop size and the resolved Schmid stress necessary for loop equilibrium. For interatomic potentials denoted with solid lines in Figure 6-4, the energy minimization procedure is capable of resolving a smooth dissociated dislocation core structure, properly capturing partial dislocation separation distances between edge and screw segments. For example, the Mishin et al. potential [62] predicts partial edge and screw segment separations of $1.239 \pm 0.104$ nm and $0.732 \pm 0.118$ nm, respectively, which are consistent with previous results for edge [187] and screw [157] dislocation simulations. For interatomic potentials denoted with dashed lines, energy minimization is not able to resolve a smooth dislocation loop structure for all dislocation loop radii studied.

Figure 6-4 also shows that the Al EAM potential selected can influence the magnitude of the equilibrium Schmid stress at 0 K. Compared to the Scattergood and Bacon equation [167], the Winey et al. and Sheng et al. potentials provide a different curvature. Moreover, these potentials do not consistently predict a smooth shape for the dissociated dislocation loop after energy minimization, as discussed above, indicating
that they may not properly account for the stress field around all segments of the dislocation loop. On the other hand, the Mishin et al., Zope and Mishin, and Liu et al. potentials have similar curvatures to the relationship proposed by Scattergood and Bacon. Also, as discussed above, these potentials provide an elliptical shape to the resolved dislocation loop structure, which is consistent with previous atomistic simulation results [53].

Among the three successful Al EAM potentials, only the Zope and Mishin potential predicts a consistent decreasing relationship between elastic constants and temperature, as shown in Figure 6-5A. Both the Mishin et al. and Liu et al. potentials predict that the material becomes more stiff as the temperature increases, which is contradictory to experimental observations and data [188,189]. On the other hand, the Zope and Mishin potential provides data in reasonable agreement with experiment, especially for the anisotropic shear modulus, $C_{44}$. This improved performance is a consequence of including linear thermal expansion factors at several temperatures in the parameterization of the potential [153]. The Zener anisotropy ratio, $\frac{2C_{44}}{C_{11}-C_{12}}$, for each potential is also plotted in Figure 6-5B. Only the Zope and Mishin potential reproduces the Al anisotropy ratio temperature dependence similar to experiments. Thus, the Zope and Mishin potential is employed for static and finite temperature stability calculations using the plate geometry.

A supplemental study of the number of elemental triangular dislocations used to construct the initial dislocation loop shows that N=16 edges is appropriate, with relative errors in the resolved Schmid stress between 16 and 32 edges less than 2%, for all dislocation loop sizes considered. Figure 6-6A shows results using the Zope and Mishin
potential and both simulation cell geometries with initial hexadecagon (N=16 edge) dislocation loops. The resolved Schmid stress for equilibrium at 0 K and the dislocation loop geometry are generally consistent (between the box and plate models) validating the frame invariant nature of the dislocation loop algorithm. Minor differences for the largest dislocation loop in the box model are apparent since the box model does not abide by the ratio 7.41:1 deemed necessary to minimize image force effects. When the resolved Schmid stress necessary for equilibrium is normalized similarly to Scattergood and Bacon ($\tau_{ss} \ell / G A b$) and plotted against $\ell$ on a semi-log scale, the atomistic simulation data is linear ($R^2 = 0.97$) within the range of dislocation loop sizes considered. However, the slope of the normalized atomistic simulation data is larger than that derived in [167], indicating the effect of anisotropic elasticity and the dislocation core on the Schmid stress required for equilibrium.

For the plate simulation cell, Figure 6-6B shows the axial ratio of the equilibrated elliptical dislocation loops for different initial dislocation loop sizes and geometries. The calculated perimeters based on extracted semimajor and semiminor axes are in very good agreement with DXA calculations. The relative error is less than 1%, except for the dislocation loop with a semimajor axis of 4.05 nm, which is 2.25%. This is due to the slightly skewed shape of the equilibrium dislocation loop geometry, as shown in Figure 6-6B. This is caused by the competing effects of the large required Schmid stress for dislocation loop equilibrium and the overlapping stress fields associated with the smallest dislocation loop. Overall, for each initial dislocation loop size (semimajor axis), the final elliptical ratio is reasonably consistent for different initial dislocation loop shapes, although some scatter is apparent for larger dislocation loops. This is due to the
decreasing influence of interactions between dislocation segments at distances across the dislocation loop. This confirms the ability of the energy minimization process to find the proper dislocation loop equilibrium shape under an applied Schmid stress regardless of starting configuration. Overall, the range of axial ratios between 1.2 and 1.5 is in agreement with Scattergood and Bacon for different materials [167]. Furthermore, as the dislocation loop becomes larger, the equilibrated dislocation loop becomes more circular, which is consistent with Scattergood and Bacon [167] and contrary to Schmid and Kirchner [170]. However, the difference in the axial ratio between 4.05 and 24.3 nm radius dislocation loops is smaller in Scattergood and Bacon than computed here using atomistic simulation.

6.3.2 Temperature Dependence of the Effective Lattice Friction Stress

Figure 6-7A shows the effect of temperature on the resolved Schmid stress necessary for dislocation loop stability. Specifically, Figure 6-7A shows the smallest value of the resolved Schmid stress that causes the dislocation loop to open, within MD time scales. This resolved Schmid stress overcomes the sum of the dislocation loop self-stress and the effective lattice friction stress. Here, the effective lattice friction stress is defined as a mean resistant stress that prevents the expansion of a dislocation loop. Each data point in Figure 6-7A is the average of five independent simulations with different initial random velocities applied to the atoms in each model. The standard deviation between each of these runs is less than 10 MPa.

It is clear in Figure 6-7A that temperature lowers the minimum resolved Schmid stress necessary to open the dislocation loop. Thermal vibrations act as a source of energy for the dislocation loop to escape its 0 K energy minimum structure. This is in agreement with results for straight edge dislocations where the dislocation energy
increases at higher temperatures [190]. Figure 6-7A also shows that the differential between resolved Schmid stresses at a given dislocation loop size becomes smaller with increasing temperature. This provides a measurement of the decay in the effective lattice friction stress as a function of temperature. Furthermore, Figure 6-7A shows that the difference in resolved Schmid stresses between any two temperatures decreases with increasing dislocation loop size. This is an indication that below a critical dislocation loop size, the self-interaction stress influences the calculation of the effective lattice friction stress.

To better elucidate these observations, a calculation of the effective lattice friction stress from molecular dynamics is proposed. At equilibrium, the externally imposed Schmid stress is balanced by the sum of the dislocation loop self-stress and the effective lattice friction stress at a given temperature. Under the notion that the effective lattice friction stress at 400 K is negligible (supplemental simulations at 500 K show that this assumption is valid), the effective lattice friction stress can be computed via,

\[
\tau_{\text{friction}} = \tau_{sd,T} - \frac{G_T}{G_{400K}} \tau_{sd,400K},
\]

(6-3)

where \( \tau_{sd,T} \) is the minimum required Schmid stress to open a dislocation loop at a given temperature (Figure 6-7A), \( G_T \) is the shear modulus at a given temperature and \( G_{400K} \) is the shear modulus at 400 K (Figure 6-5). Since the self-stress of the dislocation loop is proportional to the temperature dependent elastic moduli, the Schmid stress at 400 K is normalized by \( G_T/G_{400K} \). A similar approach, without considering temperature dependence, is typically used in the analysis of TEM images of dislocation loop geometry and motion [191]. Figure 6-7B shows, as expected, that the effective lattice
friction stress decreases as a function of temperature for all dislocation loop sizes.

Importantly, the decay in the effective lattice friction is not directly proportional to the decrease in the anisotropic shear modulus as a function of temperature shown in Figure 6-5. In addition, a dislocation loop size dependence is apparent, which is prominent for dislocation loops smaller than 16.2 nm in radius. Specifically, the slope reduces as dislocation loop size increases and converges to a constant value with less than 10% relative error for dislocation loops larger than 16.2 nm. The dependence of the effective lattice friction stress on dislocation loop size is a consequence of different dislocation loop shapes, as presented in Figure 6-6B, which is driven by the different shear stress fields inside of each dislocation loop.

To illustrate the differences in the shear stress field, Figure 6-8 shows the normalized atomic Schmid stress, $r_{xz}$, computed using the virial definition [192,193] at 0 K. The atomic volume per atom is computed using a Voronoi tessellation approach [194]. Note, the calculation of per-atom stress is for illustrative purposes of the distortion field and the individual atomic stress magnitudes may not be directly comparable to continuum concepts of stress. The Schmid stress $r_{xz}$ in Figure 6-8 is normalized by the equilibrium Schmid stress at 0 K for each loop size. Figures 6-8A and 6-8B show the atomic shear stress field around the screw segments of the dislocation loop in the YZ plane. Clearly, compared to the 24.3 nm dislocation loop, the stress state inside of the 4.05 nm radius dislocation loop is more influenced by the overlapping distortion fields associated with the dislocation loop segments. Specifically, for the 4.05 nm radius dislocation loop (Figure 6-8A), there is a continuous negative shear stress (pull-back stress) between the screw dislocation segments, whereas for the 24.3 nm dislocation
(Figure 6-8B), the dislocation loop is sufficiently large so that the shear stress field decays towards that of the externally applied Schmid stress. Thus, the screw dislocation cores in the 4.05 nm dislocation loop experience a larger pull-back stress resulting from all segments of the dislocation loop. Similar conclusions can be made considering the stress field around the edge segments of the dislocation loop as shown in Figures 6-8C and 6-8D. Note, some features of the atomic shear stress field around the dislocation loop in the 4.05 nm model are not apparent due to the consistent scale bar used in Figure 6-8, which is chosen to clearly present the differences in the shear stress field on the interior of the dislocation loop.

6.3.3 Expansion of the Dislocation Shear Loop under a Constant Schmid stress

Figure 6-9 shows snapshots of a 12.15 nm radius dislocation shear loop at different time steps under a pure Schmid stress of 380 MPa at 100 K. The dislocation loop expands since this Schmid stress is greater than the minimum Schmid stress to open the 12.15 nm dislocation loop of 360 MPa at 100 K shown in Figure 6-7. The Schmid stress and dislocation loop size are chosen so that the net Schmid stress (defined as the difference between applied Schmid stress and the minimum Schmid stress to open a dislocation loop) is always smaller than 380 MPa. This prevents the dislocation from transonic and supersonic velocities as shown in Chapter 5. Moreover, with the initial net Schmid stress of 20 MPa, it is possible to differentiate the influence between dislocation mobility in the phonon and radiative damping regimes. As the dislocation loop expands, the self-stress between segments of the dislocation loops reduces, resulting in a higher net stress even though the applied Schmid stress remains constant. As shown in Figure 6-9, the expanded dislocation loop becomes faceted in the screw and 60° segments. This is in reasonable agreement with results from DDD
simulations [72], which use mobility laws of straight dislocation with different character angles derived from atomistic simulations, and experiments [76] for dislocation loops in Al. The facets in the screw and 60° segments of the expanding dislocation loop are associated with the much higher Peierls stresses and lower mobilities of these two dislocation characters compared to the edge and 30° dislocations discussed in Chapters 4 and 5. Moreover, as shown in Figure 6-9, the dislocation loop expands asymmetrically along the X direction, and this asymmetry is more apparent as the loop enlarges. Additional MD simulations of the mobility of straight dislocations are performed to understand this phenomenon. It is found that the loop asymmetry is due to the difference in mobility between the 60° types of dislocations (which are 60° and 120° dislocations) that are initially symmetrically positioned about the X axis. As shown in Figure 6-10, the mobility of the 60° dislocation is significantly higher than the mobility of the 120° dislocation in the radiative damping regime. Recall, as a dislocation loop becomes larger, the minimum Schmid stress required to stabilize the loop reduces (Figure 6-7). Thus, the net Schmid stress increases, driving the dislocation segments to move with velocities in the radiative damping regime. Here, the difference in mobility between the 60° and 120° dislocations becomes critically important, resulting in an asymmetric expansion of the dislocation loop shown in Figure 6-9.

Figures 6-11 and 6-12 capture the effects of pressure normal to the (111) slip plane ($\sigma_n$) on the expansion of a dislocation loop. For instance, compared to dislocation loop expansion under a pure Schmid stress, the mobility of the dislocation loop under a compressive $\sigma_n$ of 500 MPa decreases, as presented in Figure 6-11. In particular, the size of the dislocation loop under compressive $\sigma_n$ is consistently smaller than the size
of the dislocation loop under a Schmid stress only. On the other hand, the mobility of the dislocation loop increases when under a tensile $\sigma_n$ of -500 MPa normal to the slip plane, as shown in Figure 6-12. In this case, the size of the dislocation loop under this tensile $\sigma_n$ is consistently larger than the size of the dislocation loop under a pure Schmid stress. These effects on the mobility of the dislocation loop are in agreement with the increase/reduction in the Peierls stress and mobility for the screw, 30°, 60°, and edge straight dislocations under compressive/tensile $\sigma_n$ normal to the (111) slip plane, as discussed in Chapters 4 and 5. Similarly, Figures 6-13 and 6-14 show the influence of the Escaig stress ($\tau_e$) on the mobility of a dislocation loop. Specifically, as shown in Figure 6-13, under the same applied Schmid stress of 380 MPa, the dislocation loop under the $\tau_e$ of -250 MPa expands slower than the dislocation loop under $\tau_e = 0$. This indicates that negative $\tau_e$ reduces the mobility of the dislocation loop. On the other hand, Figure 6-14 shows the increase in mobility of the dislocation loop under positive $\tau_e$. Similar to $\sigma_n$, the effects of $\tau_e$ on the expansion of the dislocation loop are in agreement with the effects of $\tau_e$ on the mobility of straight dislocations discussed in Chapter 5.

The role of stress state on the expansion of the dislocation loop observed in Figures 6-11 through 6-14 can be explained by the influence of local stress state on the core structure of the dislocation loop. Specifically, the core widths at different angular locations on the dislocation loop are presented for different $\sigma_n$ and $\tau_e$ in Figure 6-15 and 6-16, respectively. As shown in Figure 6-15, the dislocation core structures of the dislocation loops under compressive or tensile $\sigma_n$ are relatively similar. This is in
agreement with observation for straight dislocations in Chapter 5, where the effect of $\sigma_n$ on dislocation mobility was concluded to be due to its effects on the interatomic spacing perpendicular to the dislocation core for each dislocation rather than due to changes in the dislocation core width. With less space between the (111) planes, it is harder for each segment of the dislocation loop to move, resulting in a reduction in the overall mobility of the dislocation loop. On the other hand, Figure 6-16 shows the role of $\tau_e$ on the dislocation core widths along the dislocation loop. The dislocation loop under positive $\tau_e$ has a wider dislocation core structure compared to the one with zero or negative $\tau_e$, which is in agreement with results from Chapter 5 for straight dislocations. This leads to a higher mobility for every segment of the dislocation loop, resulting in the faster expansion of a dislocation loop under positive $\tau_e$ as shown in Figure 6-14.

### 6.4 Summary

The stability of dislocation shear loops at 0 K and finite temperature is studied using atomistic simulations. An algorithm to introduce dislocation loops in atomistic simulation and precisely determine the resolved Schmid stress necessary for static equilibrium and thermal stability is developed. This algorithm is frame invariant so that it can be used later for more complicated dislocation – grain boundary interaction problems, as will be discussed in Chapter 7. Schmid stresses associated with static equilibrium and dislocation loop geometries are obtained for different loop sizes. As the dislocation loops become larger, both the resolved Schmid stress necessary for equilibrium and the axial ratio of the dislocation loop decreases. This is in agreement with conclusions made by Scattergood and Bacon [167]. The finite temperature study provides a calculation of the temperature dependence of the effective lattice friction
stress in Al. Importantly, for dislocation loops smaller than 16.2 nm in radius, the overlapping self-stress field of the dislocation loop affects the calculation of the effective lattice friction stress such that a loop size dependence is observed.

In addition, the mobility of a dislocation loop under different stress states is investigated via MD simulations. For the dislocation loop under pure Schmid stress, the ellipsoidal dislocation loop becomes faceted in the screw and 60° segments due to the higher Peierls stress barrier and much lower mobility of these two dislocation character angles. This is consistent with experimental [76] and DDD simulation results [72] for faceting dislocation loops in Al. Moreover, the asymmetric expansion of the dislocation loop, particularly noticeable in the radiative damping regime, can be explained by the difference in the mobility of 60° type dislocations (60° and 120°) that are originally positioned symmetrically about the X axis. The role of stress state, such as pressure normal to the (111) slip plane and the Escaig stress ($\sigma_n$ and $\tau_e$), is studied by comparing the expansions of the dislocation loops under different stress combinations. A compressive $\sigma_n$ decreases the mobility of the dislocation loop, while a tensile $\sigma_n$ to the slip plane increases the mobility of the dislocation loop. Similarly, negative $\tau_e$ decreases the mobility of the dislocation loop while positive $\tau_e$ increases the mobility of the dislocation loop. While the effects of $\tau_e$ on the mobility of the dislocation loop are related to its influences on the dislocation core structures, the effects of $\sigma_n$ is caused by the change in the interatomic spacing along the dislocation core. Overall, the effects of the local stress state on the structure and mobility of the dislocation loops are consistent with the straight dislocations discussed in Chapter 4 and 5.
Table 6-1. Stress tensor required to generate a state of pure Schmid stress in the dislocation loop slip plane [139].

<table>
<thead>
<tr>
<th>Orientation</th>
<th>$\sigma_{XX}$</th>
<th>$\sigma_{YY}$</th>
<th>$\sigma_{ZZ}$</th>
<th>$\tau_{YZ}$</th>
<th>$\tau_{XZ}$</th>
<th>$\tau_{XY}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Box</td>
<td>-0.816$\tau_s$</td>
<td>0</td>
<td>0.816$\tau_s$</td>
<td>0.408$\tau_s$</td>
<td>0</td>
<td>-0.408$\tau_s$</td>
</tr>
<tr>
<td>Plate</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>$\tau$</td>
<td>0</td>
</tr>
</tbody>
</table>

Figure 6-1. Bisection algorithm to determine the resolved Schmid stress necessary for dislocation loop equilibrium at 0 K [139].
Figure 6.2. Bisection algorithm to determine the minimum resolved Schmid stress necessary to expand each dislocation loop at finite temperature [139].

Figure 6.3. Schematic of the “plate” simulation cell with a dislocation loop.
Figure 6-4. Equilibrium resolved Schmid stress for different loop radii and different Al EAM potentials. Solid curves and box indicate potentials that provided successful relaxation. Dashed curves and box indicate potentials that provided unsuccessful relaxation. Only atoms with centrosymmetry values higher than 2.0 Å² are shown [139].
Figure 6-5. Temperature dependence of elastic properties in Al predicted by different EAM potentials. A) Elastic constants. B) Anisotropy ratio.
Figure 6-6. Statics properties of dislocation loops in Al. A) Resolved Schmid stress for equilibrium versus initial dislocation loop radius for different simulation cell geometries. B) Axial ratio of equilibrium elliptical dislocation loop versus initial semimajor axis for different starting axial ratio. Equilibrium dislocation loops with a semimajor axis of (bottom left) 4.05 nm and (upper right) 24.3 nm and initial ratio of 1.6. Only atoms with centrosymmetry values higher than 2.0 Å² are shown [139].
Figure 6-7. Temperature effects on different stress for different starting dislocation loop radius in Al. A) Minimum Schmid stress to open dislocation. B) Effective lattice friction stress [139].
Figure 6-8. Normalized stress field with $r_{ss}$ around edge and screw segments of dislocation loop with different dislocation loop radius. A) Screw segment of a 4.05 nm dislocation loop. B) Screw segment of a 24.3 nm dislocation loop. C) Edge segment of a 4.05 nm dislocation loop. D) Edge segment of a 24.3 nm dislocation loop [139].
Figure 6-9. Snapshots of dislocation shear loop under pure Schmid stress of 380 MPa at different time steps. The locations of dislocation segments are marked as red.
Figure 6-10. Dislocation velocity versus Schmid stress for 60° types of dislocations using the Zope and Mishin potential. A) 60° dislocation. B) 120° dislocation.
Figure 6-11. Snapshots of dislocation shear loop under the Schmid stress of 380 MPa and compressive pressure normal to the (111) slip plane of 500 MPa at 100 K and different time steps.
Figure 6-12. Snapshots of dislocation shear loop under the Schmid stress of 380 MPa and tensile pressure normal to the (111) slip plane of -500 MPa at 100 K and different time steps.
Figure 6-13. Snapshots of dislocation shear loop under the Schmid stress of 380 MPa and the Escaig stress of -250 MPa at 100 K and different time steps.
Figure 6-14. Snapshots of dislocation shear loop under the Schmid stress of 380 MPa and the Escaig stress of 250 MPa at 100 K and different time steps.
Figure 6-15. Dislocation core widths at different locations on the dislocation loops under different pressures normal to the (111) slip plane at different time. A) 0 ps. B) 12 ps.
Figure 6-16. Dislocation core widths at different locations on the dislocation loops under different Escaig stress at different time. A) 0 ps. B) 12 ps.
CHAPTER 7
CONCLUSIONS

7.1 General Implications

This dissertation has provided insights on properties of straight dislocations and dislocation loops in Al as well as the role of local stress state on these properties using atomistic simulations. Chapters 4 and 5 study the mobility of straight dislocations with a focus on the role of stress state. In Chapter 4, the role of $\sigma_n$ on the Peierls stress for screw, $30^\circ$, $60^\circ$, and edge dislocations is investigated, which can be associated with its influence on the dislocation core structure. For instance, the Peierls stresses of screw and $60^\circ$ dislocations reach maximum values when the SFWs are multiples of the Peierls period. The effects of $\sigma_n$ on the Peierls stress are also sensitive to the choice of the interatomic potential.

In addition, the focus of Chapter 5 is on the mobility of straight dislocations at finite temperature and the effects of both $\tau_e$ and $\sigma_n$. The velocities of screw, $30^\circ$, $60^\circ$, and edge dislocations under different combinations of stress state are calculated. In general, $\tau_e > 0$ or tensile $\sigma_n$ increase the mobility of the dislocation, while $\tau_e < 0$ or compressive $\sigma_n$ decrease the mobility of the dislocation. However, the influence of the local stress state varies for different character angles and damping regimes. These differences can be associated with the change in the dislocation core structure under different combinations of stress state, and are sensitive to the direction of dislocation motion for mixed dislocations.

Increasing the complexity of the problem, Chapter 6 explores the stability and mobility of dislocation shear loops at 0 K and finite temperature. For larger dislocation
loops, both the resolved Schmid stress necessary for equilibrium and the axial ratio of
the dislocation loop decrease, which is in agreement with Scattergood and Bacon [167].
A new formula to calculate the effective lattice friction stress in Al for different
temperature is presented. For dislocation loops smaller than 16.2 nm in radius, this
calculation of the effective lattice friction stress shows a loop size dependence due to
the overlapping self-stress field of smaller dislocation loops. In addition, the expansion
of a dislocation loop under different stress state is investigated. For a dislocation loop
under pure Schmid stress, the ellipsoidal dislocation loop shows faceting in the screw
and 60° segments as well as an asymmetry in the 60° and 120° segments, which are
caused by the mobilities of these dislocations. The role of stress state, such as $\sigma_n$ and
$\tau_e$, on the core structure and the mobility of dislocation is also shown to be consistent
with observations for straight dislocations discussed in Chapters 4 and 5.

**7.2 Impact and Future Works**

As mentioned in Chapter 1, a multiscale approach is required to study dislocation
properties due to their atomic core structure but complex network system. Therefore,
atomistic results from this work provide essential insights into improving larger scale
models such as DDD simulations [39]. In particular, the study of the role of dislocation
center angle and local stress state on the Peierls stress and the mobility of
dislocations in Chapter 4 and 5 improves the mobility law used in DDD simulations. The
current interpolated mobility law for mixed dislocations does not capture the mobility of
the 30° and 60° dislocations. Moreover, for systems with high dislocation density, the
stress field generated by neighboring dislocations influences both the force and the
mobility of dislocations. While the force on each dislocation is captured by the Peach-
Koehler equation, the influence of the local stress field on dislocation mobility has not been incorporated within DDD simulations.

The static behavior and mobility of nanoscale dislocation shear loops understood from atomistic simulations discussed in Chapter 6 can be used to parameterize DDD simulations. Specifically, the temperature dependence of the effective lattice friction stress and the shear modulus are used to determine the core width parameters in DDD simulations that best match the Schmid stress required for dislocation loop stability at 300 and 400 K [139]. An optimal core width parameter of \( a = 0.6 \) lattice spacings is selected for 300 K, while \( a = 0.8 \) lattice spacings provides the best match to the atomistic data at 400 K. As shown in Figure 7-1, an excellent fit is attained for dislocation loops above the critical radius of 16.2 nm, below which atomistic simulation data begins to show size dependencies. The core width parameter could be reduced in magnitude to fit to the lower temperature data similarly [139].

The algorithm to generate a dislocation shear loop in Chapter 6 can be used for different material systems and more complex simulation settings. For instance, this algorithm is currently being used to study the interaction between a dislocation shear loop and the \( \{10\bar{1}2\} \) reflection twin boundary in Mg which has HCP crystalline structure. In particular, the dislocation loop algorithm is superimposed onto the \( \{10\bar{1}2\} \) reflection twin boundary and characterized after static and dynamic relaxation. Characterization of this defect shows many low-energy interfaces: the \( \{10\bar{1}2\} \) reflection twin, prismatic/basal (PB) and twist pyramidal/pyramidal (PP) interfaces.

Finally, since the dislocation loop algorithm is frame invariant, it can be used in more complicated systems composed of multiple types of crystallographic defects such
as dislocations and grain boundaries. An example of a potential application is shown in Figure 7-2 where a dislocation shear loop is inserted between two Σ3(112) grain boundaries. This model can be used to study the interaction between dislocations and grain boundaries under reasonable dislocation velocities.

Figure 7-1. Comparison between MD and DDD data at 300 and 400 K. The core width parameter in DDD is tuned to match the MD data using the temperature dependence of the elastic moduli and friction stress extracted from MD [139].
Figure 7-2. Simulation setting of a system with a dislocation loop and two Σ3(112) grain boundaries. Only atoms with the centrosymmetry values greater than 2 Å² are shown.
LIST OF REFERENCES


BIOGRAPHICAL SKETCH

Khanh Dang was born and raised in the Ho Chi Minh City, Vietnam. After high school, he moved to Fayetteville to attend the University of Arkansas (UARK). In May 2012, he graduated from UARK with a B.S. in mechanical engineering. He started his master’s study at UARK in August 2012 with Prof. Douglas E. Spearot. His master’s research focuses on the mechanical properties and the role of defects in molybdenum disulfide (MoS$_2$), which is a 2-D material that can substitute for silicon semiconductors. After graduating from UARK with a M.S. in mechanical engineering in May 2014, he was accepted into the doctoral program in mechanical engineering at UARK, working with Prof. Douglas E. Spearot in a new project. In May 2015, he decided to transfer to the University of Florida (UF) to continue working in the same project with Prof. Douglas E. Spearot. His Ph.D. project focuses on the unexplored properties of an isolated dislocation and the role of stress states on these properties using atomistic simulations. These atomic details can be used to parameterize larger scale models such as discrete dislocation dynamics (DDD) simulations. He graduated from UF with a Ph.D. in mechanical engineering in August 2018.