REPORT DOCUMENTATION PAGE

Form Approved OMB NO. 0704-0188

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1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)
16-03-2017	Final Report	21-Sep-2015 - 20-Dec-2016

4. TITLE AND SUBTITLE
Final Report: Virtual Diffraction Techniques Applied to Study Dislocation-Grain Boundary Interactions (9.4 Synthesis and Processing of Materials)

5a. CONTRACT NUMBER
W911NF-15-1-0623

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER
611102

6. AUTHORS
Douglas Spearot, Laurent Capolungo

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAMES AND ADDRESSES
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8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS (ES)
U.S. Army Research Office
P.O. Box 12211
Research Triangle Park, NC 27709-2211

10. SPONSOR/MONITOR'S ACRONYM(S)
ARO

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
68143-MS.4

12. DISTRIBUTION AVAILIBILITY STATEMENT
Approved for Public Release; Distribution Unlimited

13. SUPPLEMENTARY NOTES
The views, opinions and/or findings contained in this report are those of the author(s) and should not contrued as an official Department of the Army position, policy or decision, unless so designated by other documentation.

14. ABSTRACT
The long-range scientific objective of this work is to develop a model of slip transmissibility that is sensitive to dislocation – grain boundary interaction characteristics and is able to capture the complexity resulting from multiple dislocation collisions with grain boundaries. The key idea relies on the use of virtual diffraction techniques as a means to quantify elastic strain energy changes in the microstructure associated with dislocation – grain boundary interactions. Use of diffraction data from atomistic and discrete dislocation dynamics (DDD) simulations for slip transmission criteria validation has not been attempted previously. The limited scope of this one year award was (1)

15. SUBJECT TERMS
Dislocations, Grain Boundaries, Molecular Dynamics Simulations, Discrete Dislocation Dynamics Simulations

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			Douglas Spearot
UU	UU	UU	UU		19b. TELEPHONE NUMBER: 352-392-6747

Report Title

Final Report: Virtual Diffraction Techniques Applied to Study Dislocation-Grain Boundary Interactions (9.4 Synthesis and Processing of Materials)

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The long-range scientific objective of this work is to develop a model of slip transmissibility that is sensitive to dislocation – grain boundary interaction characteristics and is able to capture the complexity resulting from multiple dislocation collisions with grain boundaries. The key idea relies on the use of virtual diffraction techniques as a means to quantify elastic strain energy changes in the microstructure associated with dislocation – grain boundary interactions. Use of diffraction data from atomistic and discrete dislocation dynamics (DDD) simulations for slip transmission criteria validation has not been attempted previously. The limited scope of this one-year award was (1) to develop an atomistic simulation approach capable of modeling dislocation loop – grain boundary interactions without the limitations inherent to existing methods in the literature, and (2) to calibrate DDD simulations of dislocation structure and motion based on the results of atomistic simulations. Atomistic simulations were used to compute the resolved shear stress necessary for dislocation loop stabilization at 0K and finite temperature. This data was used to calibrate dislocation core width and discretization parameters in discrete dislocation dynamics simulations. Preliminary simulations of dislocation – grain boundary interactions are performed using both simulation techniques.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received		Paper
03/16/2017	1	Khanh Dang, Laurent Capolungo, Douglas Spearot. Dislocation Core Structure in Al via Atomistic Simulations for Parameterization of Discrete Dislocation Dynamics Models, Modeling and Simulation in Materials Science and Engineering, ( ): . doi:
		1,034,360.00
TOTAL:	**1**	

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received		Paper
TOTAL:		

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Khanh Dang, Laurent Capolungo, Douglas Spearot, Atomistic Simulation Algorithm for Studying Dislocation Glide Loop – Grain Boundary Interactions in Al, presented at: Society for Engineering Science, October, 2017.

Khanh Dang, Laurent Capolungo, Douglas Spearot, Atomistic Simulation Framework for Studying Dislocation Glide Loop – Grain Boundary Interactions in Aluminum, presented at: TMS Annual Meeting, February, 2017.

Khanh Dang, Laurent Capolungo, Douglas Spearot, Dislocation Core Structure and Mobility in Al via Atomistic Simulations for Parameterization of Discrete Dislocation Dynamics Models, to be presented at: ASME IMECE, November, 2017.

Number of Presentations: 3.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received Paper

TOTAL:

Number of Manuscripts:

Books

Received Book

TOTAL:

Received Book Chapter

TOTAL:

Patents Submitted

None.

Patents Awarded

None.

Awards

None.

Graduate Students

NAME	PERCENT_SUPPORTED	DISCIPLINE
Khanh Dang	100	Mechanical Engineering
Cameron Sobie	33	Mechanical Engineering
FTE Equivalent:	**1.33**	
Total Number:	**2**	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Douglas Spearot	0.04	
Laurent Capolungo	0.02	
FTE Equivalent:	**0.06**	
Total Number:	**2**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:..... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):..... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields: 0.00

Names of Personnel receiving masters degrees

NAME
Total Number:

Names of personnel receiving PHDs

NAME
Total Number:

Names of other research staff

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

1 a. Georgia Institute of Technology 1 b. 225 NORTH AVENUE

ATLANTA GA 303320357

Sub Contractor Numbers (c):
Patent Clause Number (d-1):
Patent Date (d-2):
Work Description (e): Discrete dislocation dynamics simulations aspects of the project.
Sub Contract Award Date (f-1): 9/21/15 12:00AM
Sub Contract Est Completion Date(f-2): 9/20/16 12:00AM

1 a. Georgia Institute of Technology 1 b. 225 NORTH AVENUE

ATLANTA GA 303320357

Sub Contractor Numbers (c):
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Sub Contract Est Completion Date(f-2): 9/20/16 12:00AM

Inventions (DD882)

Scientific Progress

See Attachment.

Technology Transfer

Sandia National Laboratories has provided partial funding for Mr. Khanh Dang during the spring and summer of 2017 to perform additional molecular dynamics simulations of Peierls stress and dislocation mobility in Al. The purpose of these new simulations is conduct uncertainty quantification analysis on the Peierls stress and dislocation mobility results as a function of the parameterization of the embedded-atom method interatomic potential used for Al.

Virtual Diffraction Techniques Applied to Study Dislocation – Grain Boundary Interactions

Final Progress Report
ARO Agreement Number W911NF-15-1-0623
Reporting Dates 09/21/2015 to 12/20/2016

Forward

The following is the Final Progress Report (FPR) for ARO Award W911NF-15-1-0623. This one-year award was provided to Douglas Spearot at the University of Florida, and included a subaward to Laurent Capolungo at the Georgia Institute of Technology. In April of 2016, Dr. Capolungo left Georgia Tech, accepting a Laboratory Scientist position at Los Alamos National Laboratory. Accordingly, the subaward to Georgia Tech was modified such that no ARO funds were provided to Dr. Capolungo directly after the date of his departure from Georgia Tech. Surplus funds were used at the University of Florida to support Mr. Khanh Dang and the atomistic simulation aspects of this work beyond the original end date of the project in August 2016. A no cost extension was provided until December 2016. This report summarizes the major research accomplishments during the project period. Two journal papers are currently being prepared for submission based on the work supported by this ARO award.

1.0 Statement of Problem Studied

The long-range scientific objective of this work is to develop a model of slip transmissibility that is sensitive to dislocation – grain boundary interaction characteristics and is able to capture the complexity resulting from multiple dislocation collisions with grain boundaries. The key idea relies on the use of virtual diffraction techniques [1] as a means to quantify elastic strain energy changes in the microstructure associated with dislocation – grain boundary interactions. Use of diffraction data from atomistic and discrete dislocation dynamics (DDD) simulations for slip transmission criteria validation has not been attempted previously.

The limited scope of this one-year award was (1) to develop an atomistic simulation approach capable of modeling dislocation loop – grain boundary interactions without the limitations inherent to existing methods in the literature, and (2) to calibrate DDD simulations of dislocation structure and motion based on the results of atomistic simulations. Upon completion of these tasks, the longer term objectives are to use recently developed computational methods, capable of producing virtual x-ray 2θ profiles and electron diffraction patterns on-the-fly during an atomistic simulation [1], to study the energetic and structural evolutions resulting from dislocations impinging on a grain boundary. In addition, a systematic investigation of existing dislocation – grain boundary reaction criteria will be performed by means of discrete dislocation dynamics simulations. This numerical technique is capable of modeling bicrystals and generating virtual x-ray diffraction 2θ profiles to be directly compared to both atomistic simulations [2].

2.0 Summary of the Most Important Results

2.1 Material Selection and Interatomic Potential Analysis

Aluminum is selected in this work as it is relevant as a lightweight structural material in many applications and computationally tractable for both atomistic and DDD simulations. Aluminum has a relatively high intrinsic stacking fault energy (~140 mJ/m^2 [3]) which prevents significant

spreading of the Shockley partial dislocation cores; thus, DDD simulations can be conducted by approximating the dislocation loop as a single discretized core [4]. Metals like Cu or Au have much lower intrinsic stacking fault energies, which allows significant spreading between partial dislocations. To model these metals, larger atomistic simulation cells would be required to avoid periodic boundary condition effects, and the partial dislocations would need to be modeled explicitly in the DDD simulations, increasing computational cost.

The embedded-atom method (EAM) interatomic potential [5] is used to model Al in the atomistic simulations. Several Al EAM potentials exist (cf. [3,6–8]) and a critical first step in this work is to evaluate their ability to capture (1) the ideal shear strength of Al, (2) the distortion fields caused by edge and screw components of an Al dislocation loop, and (3) the temperature dependence of the elastic constants. Although the Mishin et al. potential [3] does an excellent job predicting unstable and intrinsic stacking fault energies, Boyer et al. [9] reported that this potential does not capture atomic plane relaxations during the shearing process (compared to DFT calculations). Further, Winey et al. [7] showed that the Mishin et al. potential does not provide an accurate description of the temperature dependence of the elastic constants, as shown in Fig. 1(a) (MFMP data). More recent EAM potentials for Al [6–8] include data from the phonon dispersion curve in the fitting procedure, and thus these potentials provide a better description of the temperature dependence of the elastic constants, as shown in Fig. 1(a). Recently, Soleymani et al. [10] assessed the ability of different Al EAM potentials to describe the stress field around a disassociated edge dislocation in Al, via comparison to the anisotropic elasticity solution. An example of their results is shown in Fig. 1(b). They reported that the Sheng et al. [8] and the Zope and Mishin [6] EAM potentials did an acceptable job describing stress components of the edge dislocation stress field. Thus, the Zope and Mishin Al potential is selected at the primary potential of use in this work, but several interatomic potentials are tested at each stage of the research.

As an example of impact of early results in this project, Sandia National Laboratories has provided partial funding for Mr. Khanh Dang during the spring and summer of 2017 to perform additional atomistic simulations of dislocation properties in Al. The purpose of these new simulations is to conduct uncertainty quantification analysis on the dislocation loop stabilizing stress (Sections 2.2 and 2.3) and the Peierls stress for different dislocation characters (Section 3.0) as a function of the parameterization of the embedded-atom method interatomic potentials. The algorithms developed by Mr. Dang and discussed in the sections below will be employed in this new research project.

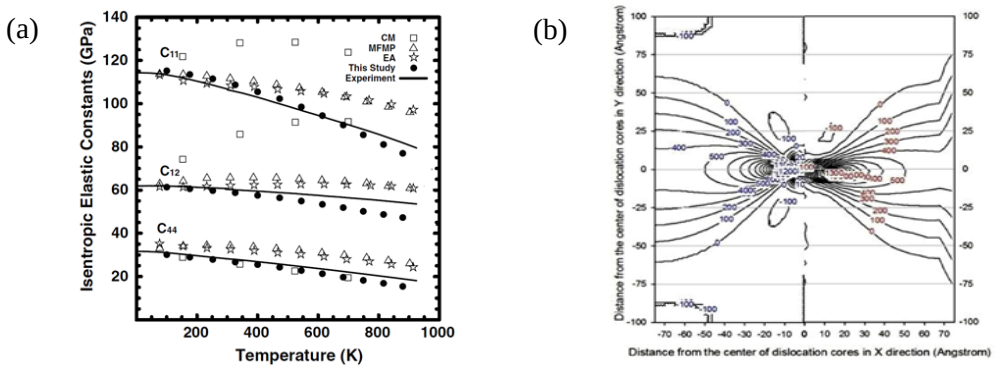


Figure 1. (a) Temperature dependence of the elastic constants for different Al potentials [7], (b) Distribution of the shear stress around an edge dislocation core in Al using the Sheng et al. EAM potential [10].

2.2 Dislocation Loop Structure and Stabilizing Stress at 0K

One of the deficiencies of prior atomistic simulations efforts focused on dislocation – grain boundary interactions is that it is common for researchers to model infinitely straight dislocations due to the enforcement of periodic boundary conditions. Thus, the reaction that takes place at the grain boundary is between an infinitely straight dislocation over an infinite grain boundary area, which likely leads to unrealistic energetic barriers for dislocation reactions. It is more realistic to consider the interaction between a curved dislocation and a localized area of the grain boundary, such as done recently by Xu et al. [11]. In this work, a dislocation loop construction algorithm is used, building upon prior work by Barnett [12,13] and Bitzek et al. [14], and a new algorithm is developed to compute the resolved shear stress in the Burger's vector direction necessary to stabilize the dislocation loop.

Specifically, dislocation loops are constructed on any {111}<110> slip system at any arbitrary lattice orientation via superposition of the displacement fields, $\mathbf{u}$, associated with triangular dislocation loops [12,13],

$$\mathbf{u} = -\frac{\mathbf{b}\Omega}{4\pi} - \frac{1-2\upsilon}{8\pi(1-\upsilon)}\left[\mathbf{f}_{AB} + \mathbf{f}_{BC} + \mathbf{f}_{CA}\right] + \frac{1}{8\pi(1-\upsilon)}\left[\mathbf{g}_{AB} + \mathbf{g}_{BC} + \mathbf{g}_{CA}\right] \tag{1}$$

where,

$$\mathbf{f}_{AB} = \left(\mathbf{b} \wedge \mathbf{t}_{AB}\right)\ln\left(\frac{R_B}{R_A} \cdot \frac{1+\boldsymbol{\lambda}_B \cdot \mathbf{t}_{AB}}{1+\boldsymbol{\lambda}_A \cdot \mathbf{t}_{AB}}\right) \tag{2}$$

and

$$\mathbf{g}_{AB} = \frac{\left[\mathbf{b} \cdot \left(\boldsymbol{\lambda}_A \wedge \boldsymbol{\lambda}_B\right)\right]\left(\boldsymbol{\lambda}_A + \boldsymbol{\lambda}_B\right)}{1+\boldsymbol{\lambda}_A \cdot \boldsymbol{\lambda}_B} \tag{3}$$

The vector functions $\mathbf{f}_{AB}$ and $\mathbf{g}_{AB}$ depend on the Burgers vector of the dislocation, $\mathbf{b}$, the unit tangent vectors describing the shape of each triangle, $\mathbf{t}$, and unit vectors, $\boldsymbol{\lambda}$, that describe the position of a general point in space (such as the position of an atom) relative to each triangle vertex. The superposition of the displacement fields from eight triangular dislocations creates an octagon-shaped dislocation loop.

Equations (1) – (3) do not describe the atom displacements close to the dislocation core; thus, energy minimization (via the conjugate gradient method [15]) is performed after the insertion of the octagonal dislocation loop. Unfortunately, if the atomistic simulation cell is stress free, the energy minimization procedure will cause the dislocation loop to disappear since the minimum energy configuration of the system is that of a perfect lattice. To stabilize the dislocation loop structure, the energy of the system must be minimized under an appropriate state of stress. To determine the stress necessary to stabilize the dislocation loop, the bisection algorithm presented in Fig. 2 is developed. Briefly, the bisection algorithm iterates over different values of resolved shear stress (which are applied via a three-dimensional state of stress acting on the simulation cell according to the anisotropic elastic constants of the Al lattice) and performs multiple energy minimizations to determine the resolved shear stress necessary for dislocation loop equilibrium. Collapse or expansion of the dislocation loop is determined by monitoring the number of atoms

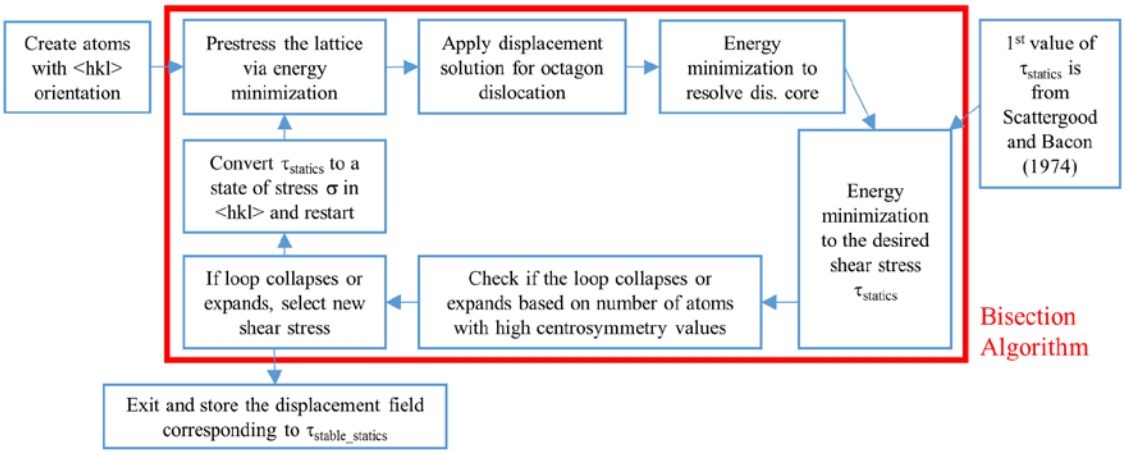
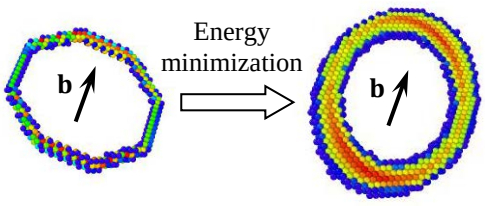


Figure 2. Energy minimization algorithm to resolve the size and shape of the dislocation loop and atomic displacements in the neighborhood of the dislocation core under an applied shear stress.

with nonzero values of the centrosymmetry parameter [16]. This algorithm runs until convergence is attained within +/- 2 MPa.

Figure 3 shows simulation results illustrating the success of this algorithm for a dislocation loop in the $(111)[\bar{1}01]$ slip system in Al. The energy minimization procedure is capable of resolving the dissociated dislocation core structure, as shown in Fig. 3(a), properly accounting for partial dislocation spreading differences between edge and screw segments. The resolved shear stress necessary to stabilize the dislocation loop computed using the bisection algorithm is shown in Fig. 3(b) for different loop radii and lattice orientations. First, it is clear that the algorithm is frame invariant as results for <100>, <210> and <310> oriented lattices (relative to the global X direction of the simulation cell) provide the same solution. This is important, as this aspect of the algorithm will allow for the study of dislocation – grain boundary interactions at any lattice orientation, which is a major limitation of prior approaches that employ infinitely straight dislocations with periodic boundary conditions. Second, the computed resolved shear stresses are in general agreement with the theoretical solution derived by Scattergood and Bacon [17] for different loop radii, which

(a)



(b)

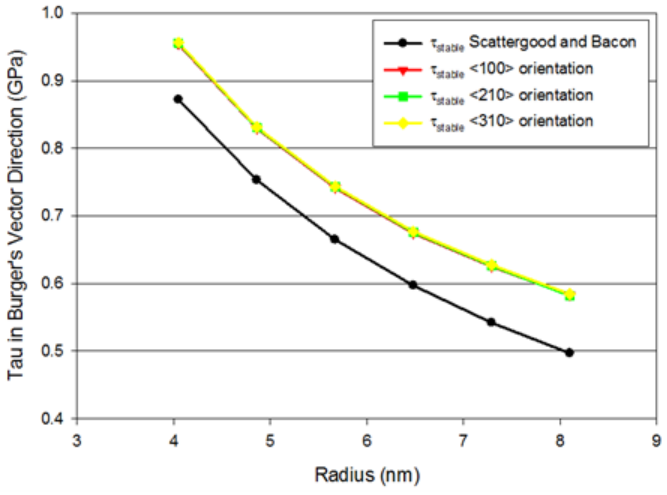


Figure 3. (a) Energy minimization of an octagonal dislocation loop showing the resolved dislocation core structure. (b) Computed resolved shear stress necessary to stabilize the dislocation loop.

considers crystal anisotropy and dislocation self-interactions. Differences between the MD results and the Scattergood-Bacon theory are likely caused by dislocation core effects, which are not considered in the theoretical solution.

Figure 4 shows the sensitivity of the results to different EAM potentials for Al. The Mishin et al. [3] and Zope and Mishin [6] potentials are very similar. Both potentials provide an elliptical shape to the dislocation loop structure. On the other hand, the Winey et al. [7] and Sheng et al. [8] potentials for Al provide a different curvature to the relationship between the stabilizing shear stress and the dislocation loop radius. These potentials do not consistently predict an elliptical shape for the dislocation loop after energy minimization, as a function of loop radius, indicating that they may not properly account for the stress field around different segments of the dislocation loop.

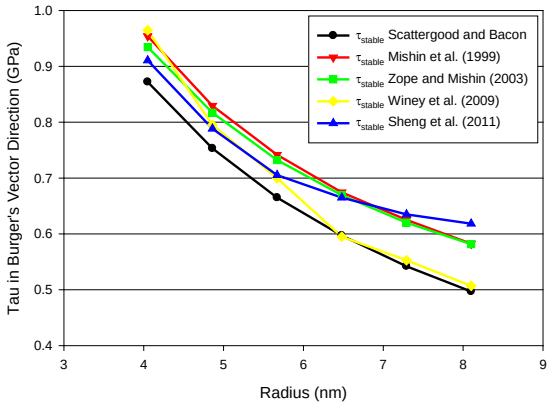


Figure 4. Influence of Al EAM potential on the resolved shear stress necessary to stabilize the dislocation loop.

2.3 Effect of Temperature

The dislocation loop construction algorithm is extended to consider finite temperature effects on the critical resolved shear stress for dislocation loop equilibrium. To determine this value for dislocation loops with different radii and at different temperatures, the algorithm presented in Fig. 5 is developed. This algorithm iterates over different values of resolved shear stress (applied via a three-dimensional state of stress acting on the simulation cell using the anisotropic elastic constants of the lattice) at a given temperature during a MD simulation and determines the resolved shear stress necessary for dislocation loop equilibrium. Again, the centrosymmetry parameter [16] is used to assess if the dislocation loop is expanding or collapsing during the MD simulation.

Figure 6 shows the effect of temperature on the critical resolved shear stress necessary for dislocation loop stabilization. Each data point in Fig. 6 is the average of five independent

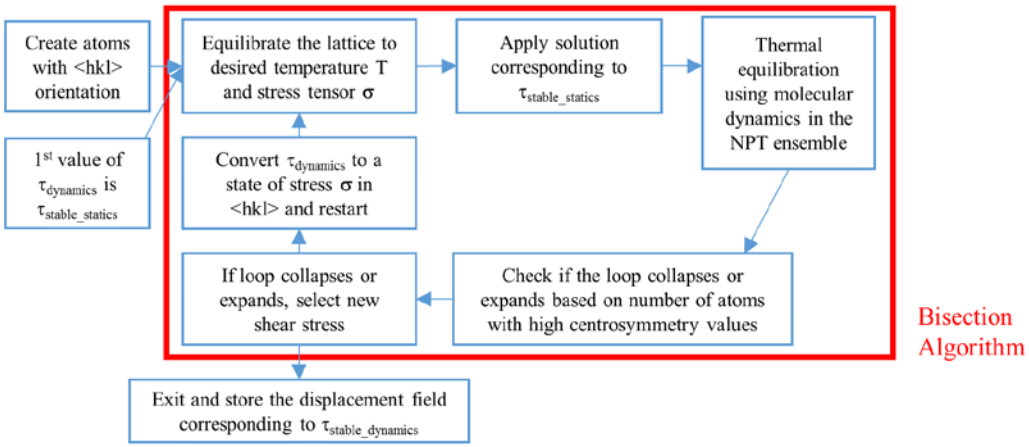


Figure 5. Bisection algorithm to resolve the stress necessary to stabilize a dislocation loop of given radius at finite temperature.

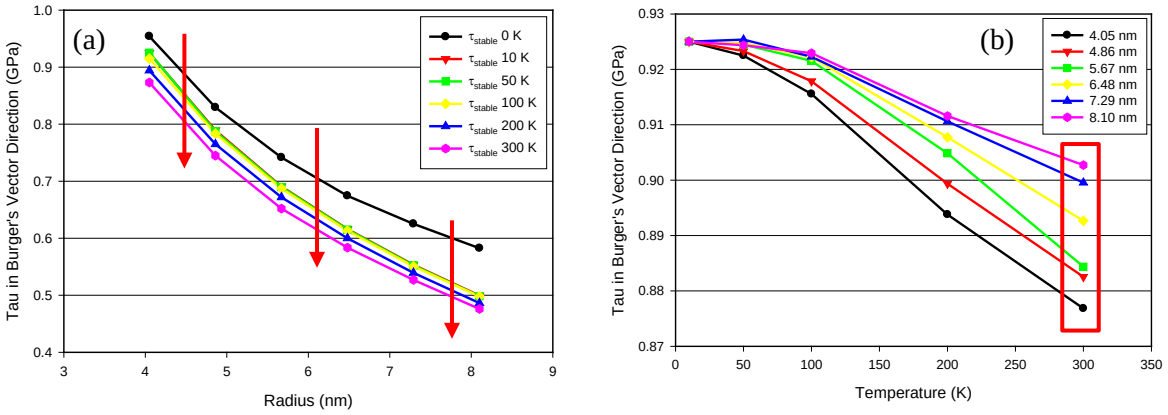


Figure 6. Influence of temperature on the resolved shear stress necessary to stabilize the dislocation loop. (a) Stabilizing shear stress as a function of dislocation loop radius showing the thermal source effect. (b) Stabilizing shear stress as a function of temperature normalized by the stabilizing stress value at 10 K to show the phonon drag effect.

simulations with different initial random velocities applied to the atoms in each model. The error between each of these runs is less than 10 MPa. In Fig. 6(a), it is clear that temperature lowers the resolved shear stress necessary for dislocation loop stabilization. Thermal vibrations act as an energy source for the dislocation loop cores to escape their local energy minima. When plotted as a function of temperature and normalized by the critical resolved shear stress for stabilization at 10 K, Fig. 6(b) shows the interplay between dislocation loop size (self interaction effects) and the stabilizing shear stress. The smallest dislocation loops are more significantly impacted by increases in temperature. The ordering of the data, highlighted by the box in Fig. 6(b), shows that the thermal source effect dominates phonon drag effects for nanosized dislocation loops.

2.4 Calibrating Discrete Dislocation Dynamics Simulations

The purpose of the atomistic simulations summarized in the prior sections is to provide data for calibration of DDD simulations of dislocation loop structure and mobility. Discrete dislocation dynamics simulations provide a meso-scale approach to model dislocation motion and interactions

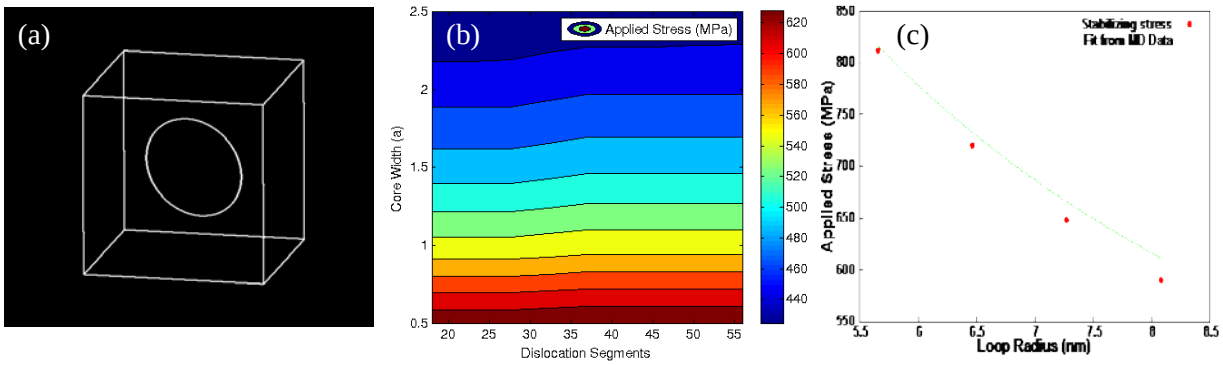


Figure 7. (a) Discrete dislocation dynamics model of a dislocation loop on the same slip system as in the atomistic simulations, (b) mesh contour plot showing the effect of dislocation loop discretization and core width parameter in the DDD code, (c) calibration of the DDD code to the atomistic simulation results.

without atomic-level detail, enabling larger simulation cell domains (and importantly the ability to model dislocation pile-ups at a grain boundary, which have length scale beyond MD simulations). However, the DDD simulation methodology is heavily dependent on the specification of rules that control the motion of dislocations and their reaction with other defects in the simulation cell (dislocations or interfaces). Further, numerical issues are also important, such as how a dislocation core is discretized.

Figure 7 shows the first step towards calibrating DDD simulations via the atomistic simulation data. Specifically, Fig. 7(a) shows a dislocation loop with 8.1 nm radius modeled using DDD simulations. Two parameters are adjusted to match the resolved shear stress data computed from atomistic simulations (shown in Fig. 3(b)): (1) the width of the dislocation "core" parameter in DDD formulation, and (2) the number of numerical segments used to discretize the dislocation loop. From Fig. 7(b), the number of segments used to discretize the dislocation loop has only a small effect on the value of the resolved shear stress necessary for loop stabilization. On the other hand, the core width parameter has a significant effect on the stabilizing stress. Using multiple dislocation loop radii, this parameter in the DDD code is tuned to match best the atomistic simulation data, as shown in Fig. 7(c). Note that most values typically used in the literature range from 0.5b to 1.5b. Yet such choice appears so far as relatively arbitrary. The present work allows for a rigorous choice of core radius.

2.5 Dislocation – Grain Boundary Interaction Simulations

Using the displacement field computed from the energy minimization calculations (Section 2.2), molecular dynamics models are constructed with the dislocation loop placed in close proximity to a grain boundary. By applying a stress to the simulation cell boundaries, the dislocation loop is expanded to interact with the grain boundary at finite temperature. Driving the dislocation loop with sub GPa levels of stress (Fig. 3) avoids the prescription of a high strain rate boundary condition, as is used in most prior MD simulations. Figure 8 shows the reaction of a dislocation loop and a Σ5 {210}<100> symmetric tilt grain boundary in Al. To create the grain boundary structure, the model is constructed first without the dislocation loop (using a standard energy minimization procedure), and then the displacement field associated with the dislocation loop is applied at a selected position within the grain boundary model, as shown in Fig. 8(a). As shown

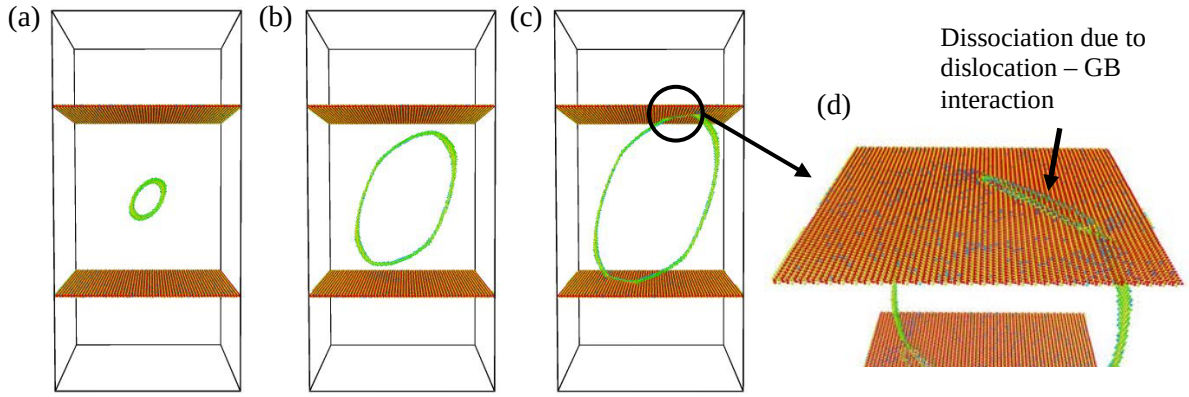


Figure 8. Interaction of a dislocation loop and a Σ5 {210}<100> symmetric tilt grain boundary. (a) 0 ps, (b) 35 ps, (c), 40 ps, (d) dissociation of the dislocation loop in the GB plane.

in Figs. 8(b) – 8(d), the dislocation loop interacts with the grain boundary at a specific location and with a specific inclination. At the intersection of the dislocation loop and the grain boundary, the dislocation is absorbed and dissociates within the grain boundary plane. One of the long-term objectives of this project is to characterize this reaction mechanism using virtual diffraction techniques and to calibrate DDD simulations to account properly for these type of reactions.

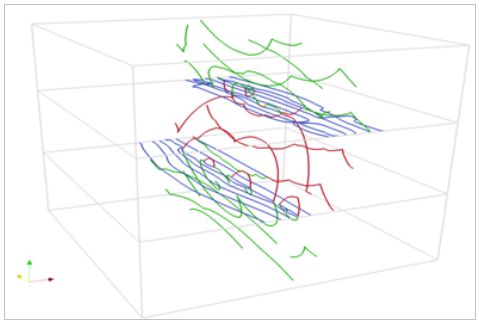


Figure 9. DDD simulations of dislocation-twin boundary interactions.

To match the atomistic simulation geometry, the DDD methodology is extended to consider a first case of dislocation – grain boundary interactions. Here, similar to the work of Jin et al. [18,19], a Frank-Read source was activated to send a dislocation segment onto a {111} coherent twin boundary and the dissociation process revealed by them and also by Dewald and Curtin [20–22] was reproduced by enforcing the Lee et al. [23] slip transmission criterion. Figure 9 shows the defect structure resulting from the continuous interaction of dislocations with the {111} twin boundary. Red and green segments correspond to glide dislocations in each lattice region, while blue segments represent interface dislocations generated from multiple dislocation – grain boundary reactions. This initial example shows the capability of the MD informed DDD framework towards studying the collective interactions of dislocations with grain boundaries.

A second set of DDD simulations are performed employing the same atomistic configurations described in Fig. 8. The idea is to simulate the interaction of dislocations with a grain boundary by simply propagating a dislocation into a bicrystal interface as shown in Fig. 10. Here, the dislocation deposits Burger's vector content into the grain boundary plane. In future efforts, different transmission laws will be tested and refined to match the dislocation configurations obtained by atomistic simulations. Note that in DDD simulations, core energies and effects must be specified ad hoc. Therefore, it is proposed to quantify elastic strain energy distributions and their evolutions via the use of the virtual diffraction method. Elastic strain energy landscape will be used as a metric to evaluate the newly derived slip transmission laws. Ultimately, the idea to be pursued in future years is to not enforce hard-coded geometrical rules, but rather to allow the DDD code to choose a reaction according to both dislocation core dissociation criteria (to be obtained from atomistic simulations) and energy. The extended slip transfer criteria to be derived

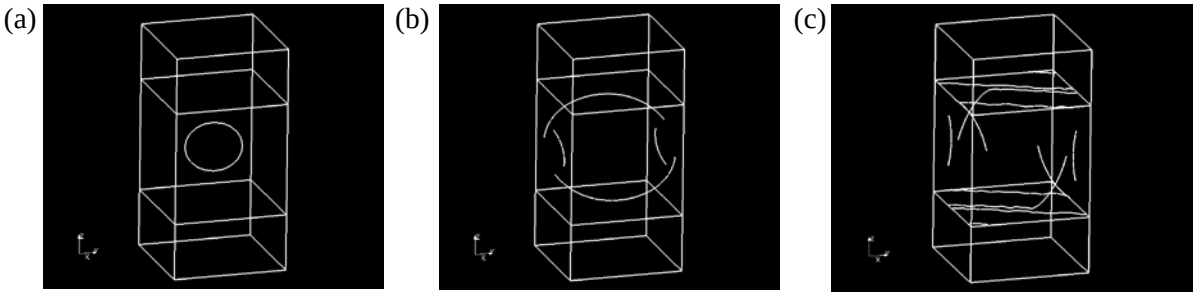


Figure 10. Discrete dislocation dynamics model of dislocation loop interactions with a Σ5 {210}<100> symmetric tilt grain boundary. The DDD code is calibrated via atomistic simulations and the stress state for driving the dislocation loop is identical to that in Fig. 8.

will thus simultaneously account for kinematics and kinetics of dislocation – grain boundary reactions.

3.0 Ongoing Research Activities

In addition to the activities described in this report, over the last two months additional atomistic simulations have been performed on models of periodic straight dislocations to determine the Peierls stress as a function of dislocation line character. The purpose of these simulations is to improve the ad hoc model for dislocation mobility used in DDD simulations to match the behavior observed using MD simulations. Traditionally, in DDD simulations, the mobility of edge and screw dislocations are specified, and the mobility of dislocations with line characters in between these bounds is computed using a linear interpolation between edge and screw values. Recent atomistic simulations [24], which are being validated and extended by Mr. Dang, have shown that the linear interpolation commonly used in DDD simulations is inaccurate. The Peierls stress (and hence the mobility) should be posed as a nonlinear function between edge and screw bounds, and this must be accounted for explicitly in DDD simulations of dislocation loop expansion to match the atomistic simulations. These activities will provide a second set of data to calibrate the DDD models using atomistic simulation input before dislocation loop – grain boundary interactions are studied extensively.

4.0 Bibliography

[1] S.P. Coleman, D.E. Spearot, L. Capolungo, Virtual diffraction analysis of Ni [010] symmetric tilt grain boundaries, Model. Simul. Mater. Sci. Eng. 21 (2013) 55020.

[2] M.V. Upadhyay, L. Capolungo, L. Balogh, On the computation of diffraction peaks from discrete defects in continuous media: Comparison of displacement and strain-based methods, J. Appl. Crystallogr. 47 (2014) 861–878.

[3] Y. Mishin, D. Farkas, M. Mehl, D. Papaconstantopoulos, Interatomic potentials for monoatomic metals from experimental data and ab initio calculations, Phys. Rev. B. 59 (1999) 3393–3407.

[4] V.Y. Bulatov, Current developments and trends in dislocation dynamics, J. Comput. Mater. Des. 9 (2002) 133–144.

[5] M.S. Daw, M.I. Baskes, Embedded-atom method: Derivation and application to impurities, surfaces, and other defects in metals, Phys. Rev. B. 29 (1984) 6443–6453.

[6] R.R. Zope, Y. Mishin, Interatomic potentials for atomistic simulations of the Ti-Al system, (2003) 46.

[7] J.M. Winey, A. Kubota, Y.M. Gupta, A thermodynamic approach to determine accurate potentials for molecular dynamics simulations, Model. Simul. Mater. Sci. Eng. 17 (2009) 55004.

[8] H.W. Sheng, M.J. Kramer, A. Cadien, T. Fujita, M.W. Chen, Highly optimized embedded-atom-method potentials for fourteen fcc metals, Phys. Rev. B. 83 (2011) 134118.

[9] R.D. Boyer, J. Li, S. Ogata, S. Yip, Analysis of shear deformations in Al and Cu: Empirical potentials versus density functional theory, Model. Simul. Mater. Sci. Eng. (2004) 1017–1029.

[10] M. Soleymani, M.H. Parsa, H. Mirzadeh, Molecular dynamics simulation of stress field around edge dislocations in Aluminum, Comput. Mater. Sci. 84 (2014) 83–96.

[11] S. Xu, L. Xiong, Y. Chen, D.L. McDowell, Sequential slip transfer of mixed-character

dislocations across Σ3 coherent twin boundary in FCC metals.pdf, NPJ Comput. Mater. 16 (2016) 15016.
[12] D.M. Barnett, The displacement field of a triangular dislocation loop, Philos. Mag. A. 51 (1985) 383–387.
[13] D.M. Barnett, R.W. Balluffi, The displacement field of a triangular dislocation loop – a correction with commentary, 87 (2007) 943–944.
[14] E. Bitzek, C. Brandl, D. Weygand, P.M. Derlet, H. Van Swygenhoven, Atomistic simulation of a dislocation shear loop interacting with grain boundaries in nanocrystalline aluminium, Model. Simul. Mater. Sci. Eng. 17 (2009) 55008.
[15] J.R. Shewchuk, An introduction to the conjugate gradient method without the agonizing pain, (1994).
[16] C. Kelchner, S. Plimpton, J. Hamilton, Dislocation nucleation and defect structure during surface indentation, Phys. Rev. B. 58 (1998) 11085–11088.
[17] R.O. Scattergood, D.J. Bacon, Dislocation shear loops in anisotropic crystals, Phys. Status Solidi. 25 (1974) 395–404.
[18] Z.-H. Jin, P. Gumbsch, E. Ma, K. Albe, K. Lu, H. Hahn, H. Gleiter, The interaction mechanism of screw dislocations with coherent twin boundaries in different face-centered cubic metals, Scr. Mater. 54 (2006) 1163–1168.
[19] Z.-H. Jin, P. Gumbsch, K. Albe, E. Ma, K. Lu, H. Gleiter, H. Hahn, Interactions between non-screw lattice dislocations and coherent twin boundaries in face-centered cubic metals, Acta Mater. 56 (2008) 1126–1135.
[20] M.P. Dewald, W.A. Curtin, Multiscale modelling of dislocation/grain-boundary interactions: I. Edge dislocations impinging on Σ11 (113) tilt boundary in Al, Model. Simul. Mater. Sci. Eng. 15 (2007) S193–S215.
[21] M.P. Dewald, W.A. Curtin, Multiscale modelling of dislocation/grain boundary interactions. II. Screw dislocations impinging on tilt boundaries in Al, Philos. Mag. 87 (2007) 4615–4641.
[22] M. Dewald, W.A. Curtin, Multiscale modeling of dislocation / grain-boundary interactions : III. 60º dislocations impinging on Σ3 , Σ9 and Σ11 tilt boundaries in Al, Model. Simul. Mater. Sci. Eng. 19 (2011) 55002.
[23] T.C. Lee, I.M. Robertson, H.K. Birnbaum, Anomalous slip in an FCC system, Ultramicroscopy. 29 (1989) 212–216.
[24] J. Cho, T. Junge, J. Molinari, G. Anciaux, Toward a 3D coupled atomistic and discrete dislocation dynamics simulation : dislocation core structures and Peierls stresses with several character angles in FCC aluminum, Adv. Model. Simul. Eng. Sci. 2 (2015) 1–17.