STATISTICAL MECHANICS MODELING OF MESOSCALE DEFORMATION IN METALS

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Program Manager: Dr. John S. Vetrano

Principal Investigator
Anter El-Azab, Professor

Current Affiliation and Contact Information:
School of Nuclear Engineering and School of Materials Engineering
Purdue University
400 Central Drive, West Lafayette, IN 47907-2017
E-mail address: aelazab@purdue.edu
Phone: 765-496-6864; Fax: 765-494-9570

This work was performed while the Principal Investigator was with the Florida State University.

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TABLE OF CONTENTS

FINAL TECHNICAL REPORT.....	1
Introduction	1
Research Highlights	2
1. Dislocation Statistics.....	2
2. Coupled Dislocation-Kinetics and Crystal-Mechanics Formalism and Computational Solution.....	12
3. Comparison with Experiments.....	15
Summary and Conclusions	18
References	19
Students and Post-Doctoral Support.....	21
Student Degrees Obtained under this Contract	22
Publications, Presentations and Activities Inspired by this Project	22
Journal publications.....	22
Journal manuscripts, to be submitted	22
Journal manuscripts under preparation.....	22
Conference publications	22
Edited Volumes by the PI (and others) Inspired by this Project	23
Invited and Keynote Presentations	23
Contributed Presentations.....	24
BIOGRAPHICAL SKETCH	26

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FINAL TECHNICAL REPORT

INTRODUCTION

The research under this project focused on a theoretical and computational modeling of dislocation dynamics of mesoscale deformation of metal single crystals. Specifically, the work aimed to implement a continuum statistical theory of dislocations to understand strain hardening and cell structure formation under monotonic loading. These aspects of crystal deformation are manifestations of the evolution of the underlying dislocation system under mechanical loading.

The project had three research tasks:

- 1) Investigating the statistical characteristics of dislocation systems in deformed crystals.
- 2) Formulating kinetic equations of dislocations and coupling these kinetics equations and crystal mechanics.
- 3) Computational solution of coupled crystal mechanics and dislocation kinetics.

Comparison of dislocation dynamics predictions with experimental results in the area of statistical properties of dislocations and their field was also a part of the proposed effort.

In the first research task, the dislocation dynamics simulation method was used to investigate the spatial, orientation, velocity, and temporal statistics of dynamical dislocation systems, and on the use of the results from this investigation to complete the kinetic description of dislocations.

The second task focused on completing the formulation of a kinetic theory of dislocations that respects the discrete nature of crystallographic slip and the physics of dislocation motion and dislocation interaction in the crystal. Part of this effort also targeted the theoretical basis for establishing the connection between discrete and continuum representation of dislocations and the analysis of discrete dislocation simulation results within the continuum framework. This part of the research enables the enrichment of the kinetic description with information representing the discrete dislocation systems behavior.

The third task focused on the development of physics-inspired numerical methods of solution of the coupled dislocation kinetics and crystal mechanics framework. To a large extent, this task has also been successfully started. We have developed a custom finite-element approach with mesh points being a subset of the underlying crystal structure. When used to predict the evolution of the dislocation system, the planar motion of dislocations is naturally captured for all slip systems, thus minimizing numerical errors and providing simple ways to investigate cross slip and dislocation reactions. Preliminary results in this direction show that we are closer than ever in building a predictive framework for dislocation dynamics and mesoscale plasticity based on the first principles of dislocation dynamics.

The rest of the report gives an overview of the research performed under this project and highlights the key results and open questions left for future investigations.

RESEARCH HIGHLIGHTS

1. Dislocation Statistics

1.1 Dislocation Correlations

For the purpose of understanding the dislocation statistics and to close the dislocation kinetic equations in the statistical framework, dislocation dynamics simulation models was used to simulate the spatial statistics of dislocations density, the temporal statistics of cross slip and dislocation reaction events, and the statistics of internal stress and elastic fields.

Analysis of the spatial and orientation statistics of dislocations focused on understanding various aspects of the dislocation correlation. We have simulated the radial, 3D, and orientation correlation of dislocations in both FCC and BCC crystals. The method of simulation and results are summarized in a publication [1]. This work revealed a number of important characteristics of dislocation correlations:

- The radial dislocation correlation is oscillatory and the associated oscillations die out at several micrometer separation distances and become weaker at higher strain and higher strain rates.
- The self-correlation (of dislocations of same Burgers vector) is stronger than the cross-correlation. The latter is about an order of magnitude weaker at short separation distances. The self-correlation is much stronger at short separation due to continuity of the dislocation lines.
- The correlations are anisotropic in the crystal and line-orientation space.

Figure 1 illustrates the radial self correlation. The oscillatory behavior of dislocation correlations has been attributed to the formation of dislocation patterns at early stage of deformation. These patterns arise due to the sparse initial sources used in dislocation dynamics simulations, which are also typical of real crystals having low initial dislocation density. The formation of dislocation patterns has been confirmed by computing the Fourier transform of the density.

The observed anisotropy of the 3D correlation, see figure 2, is partly due to dislocation patterning and partly due to geometrical relationships between crystallographic slip systems. This anisotropy, which is observed in both FCC and BCC crystals, represents a computational challenge for incorporating the dislocation correlations into the kinetic equations of the dislocation density in the crystal.

1.2 Temporal Statistics of Dislocations

Time series analysis has been used to model the temporal statistics of cross slip and junction reactions in dislocation dynamics. The objective of this analysis is to model the coarse graining time scale of dislocation dynamics, and to demonstrate how this time can be used to determine the source terms associated with cross slip and junction reactions in the kinetic theory of dislocations. The hypothesis underlying this investigation is as follows: the spatial and temporal coarse-graining of dislocations must go hand in hand, in the sense that a spatial coarse-graining allowing to model dislocations using a density parameter and hence permit the simulation of larger crystal volumes must also allow for longer simulation times. The analysis thus aims to

define the coarse graining time scale for dislocation dynamics, a scale that permits continuum representation of dislocation events in time.

Figure 1. Radiation self correlation functions in Mo at different strains for two different Burgers vectors. The ParaDiS dislocation dynamics code [2] was used to collect dislocation data during deformation simulation.

Figure 2. A slice of the 3D dislocation correlation graph in copper at a lower (a) and a higher strain (b) values. The microMegas dislocation dynamics code [3] was used to collect dislocation data during deformation simulation.

The temporal analysis of dislocation dynamics includes a collection of time series data for cross slip and junction reaction events using the method of dislocation dynamics simulation, stationarization of the time series and computing the correlation time. Figure 3(a) shows a typical time series (blue curve) for the junction density on slip system $[110](1\bar{1}1)$ in a copper single crystal deforming under $[100]$ loading at strain rate of $25s^{-1}$. The red plot in the same panel is the

stationarized time series. Using the latter series, the correlation time has been computed for both cross slip and dislocation reactions (junction formation and annihilation reactions) for all slip systems in deforming copper. The results are summarized in figure 3(b). It has been found that, the cross slip correlation time is larger than the junction reaction correlation time, and that the latter is approximately the same as the correlation time for dislocation annihilation reactions. The coarse graining time scale, which is a fundamental characteristic time of dislocation dynamics, is thus taken to be the cross slip correlation time. This correlation time has then been used to simulate the rates of cross slip and junction reaction rates in dislocation dynamics. The cross slip rate is set to be proportional to the density available for cross slip and the rate coefficient is found from a statistical averaging procedure explained in [4]. Similarly, the junction reaction rate is set to be proportional to product of the reacting species and the rate coefficient is found by time averaging of the junction events over the coarse graining time scale. Typical results are shown in figure 4; see [4] for more details. The left panel shows the rate coefficient for cross slip while the right panel shows a typical junction reaction rate coefficient. The cross slip coefficients rise from small value and approach a plateau value in an oscillatory fashion. The junction reaction coefficients exhibit large-scale oscillations superposed on a slowly growing background component. The oscillatory behavior of these quantities is closely related to the intermittent character of plastic flow in crystals [4].

Analysis of the oscillation of the junction formation rate showed that a fundamental scaling law can be derived for the reaction rate oscillations [4].

Figure 3. (a) Typical time series of the instantaneous junction density for a single slip system in a deforming copper single crystal. (b) Correlation time for cross slip and junction reactions for active slip system in a copper crystal deformed under [100] type loading. The dislocation data were collected using the microMegas code [3].

Figure 4. (a) Rate coefficient for cross slip for all active slip systems in a copper crystal loaded along $[100]$ direction. (b) Glissile junction reaction rate coefficients for the reaction: $[10\bar{1}](\bar{1}\bar{1}\bar{1}) + [\bar{1}10](11\bar{1}) \rightarrow [01\bar{1}](\bar{1}\bar{1}\bar{1})$.

1.3 Internal Elastic Field Statistics

A statistical analysis of the internal stress field of dislocations was conducted for the case of homogeneous deformation of FCC crystals. The analysis aimed to explain the difference between the internal stress in a crystal and its values at dislocation lines. The hypothesis underlying this investigation is as follows: since the dislocation lines (segments) represent a subset of the crystal points, the statistics of internal stress on segments must differ from the crystal counterpart. It is the former that must then be used to derive a law for internal stress versus velocity in the continuum dislocation dynamics models.

In the simplified implementation of a 2D continuum dislocations model by Yefimov et al [5], the internal stress field that drives the dislocation density was represented as the summation of two contributions. The first component includes the effect of all dislocations, assuming that they are uncorrelated, whilst the second accounts for the spatial correlation effect. Although it was possible to establish analytical expressions for the pair correlation functions by the aid of discrete dislocation dynamics simulations for 2D dislocation systems [6], the extension of such approach to three dimensional dislocation systems is complicated.

Two major journal papers on internal elastic field statistics are under preparation – the first summarizes the stress statistics and an approach for a stress-velocity connection in continuum dislocation dynamics and the second is on the characteristics of internal geometric field and comparison with X-ray measurements of the same.

In our construction of a continuum theory of dislocations, an eigenstrain approach is followed. This approach yields the stress field in the crystal space. In this case the internal stress field calculated at any point can be thought of as the average internal stress field sampled over a continuum element at that point. On the other hand, the average internal stress field that drives the dislocation density should be averaged over points located on the discrete dislocation segments included inside the same continuum element. Accordingly, statistical analysis is conducted to investigate the difference between the statistics of internal stress field when sampled over crystal points versus segments.

The statistical analysis is conducted for homogeneously deformed copper single crystal, with periodic boundary conditions applied during the simulations, using microMegas dislocation dynamics code [3]. A cubic crystal of edge size ~ 5 microns is subjected to constant tensile strain rate of 25 sec^{-1} up to strain level $\sim 1.3\%$. Based on dislocation configurations extracted from the simulations, the internal stress field is calculated as superposition of two contributions. The first contribution is the infinite medium field, which is the stress field generated by the dislocations contained inside the simulation volume itself, whereas the second contribution is the *image field* which accounts for the effect of dislocations outside this volume. The infinite medium stress field $\sigma^\infty(\mathbf{x})$ is calculated using the non-singular integral expression developed by Cai et al [7], where the integration is implemented numerically over the whole discrete dislocation network

$$\begin{aligned} \sigma_{\alpha\beta}^\infty(\mathbf{x}) = & \frac{\mu}{8\pi} \oint_C \partial_i \nabla^2 R_a (b_m \varepsilon_{im\alpha} dx'_\beta + b_m \varepsilon_{im\beta} dx'_\alpha) \\ & + \frac{\mu}{4\pi(1-\nu)} \oint_C b_m \varepsilon_{imk} (\partial_i \partial_\alpha \partial_\beta R_a - \delta_{\alpha\beta} \partial_i R_a) dx'_k \end{aligned} \quad (1)$$

The image stress field, $\sigma^I(\mathbf{x})$, on the other hand, is calculated by solving the boundary value problem (BVP) developed by Deng and El-Azab [8], which is stated as

$$\left. \begin{aligned} \nabla \cdot \sigma^I(\mathbf{x}) + \mathbf{f}(\mathbf{x}) &= \mathbf{0}, & \mathbf{x} \in \Omega \\ \mathbf{f}(\mathbf{x}) &= \nabla \cdot \sigma^\infty(\mathbf{x}), & \mathbf{x} \in \Omega \\ \sigma^I(\mathbf{x}) \mathbf{n}(\mathbf{x}) &= -\sigma^\infty(\mathbf{x}) \mathbf{n}(\mathbf{x}) & \mathbf{x} \in \partial\Omega \end{aligned} \right\}, \quad (2)$$

where $\mathbf{n}(\mathbf{x})$ is the outward unit vector normal to the domain boundary $\partial\Omega$ and $\mathbf{f}$ is a body force. In order to the boundary value problem (2), a Galerkin finite-element method program is developed. The total internal stress field is calculated on two sets of sampling points. The first is a set of uniformly distributed points in the crystal and the second set is a collection of points placed at the middle points of the discrete dislocation segments. The probability distribution function (PDF) is calculated for each set of sampling points to investigate the potential differences in their statistical characteristics.

Figure 5 shows the PDF for the internal stress field at crystal points and on segments at plastic strain level $\sim 1.3\%$. The key difference of interest between the two probability distributions is the symmetry. Looking closely at the PDF of stress on segments we see that some of the peaks are slightly shifted from the zero (mean value) point, which implies that the volume average of the internal stress field on segments has nonzero mean. This skewness was further confirmed by calculating the average value for the internal stress field on both sets. The skewness of the distribution becomes clear when the PDF of the internal stress field resolved on the 12 slip

systems FCC crystals is plotted. Figure 6 shows the distributions of the stress field resolved on 6 of the slip systems. The significant difference between both distributions, and so the corresponding average values, implies that the internal stress field calculated in the crystal has different statistical characteristics than the part that actually drives the dislocation motion. The results underscore the need to establish a mapping scheme between the stress in crystal and the stress on segments when establishing stress-velocity connection in continuum dislocation dynamics.

Figure 5. PDF for the components of stress field at strain level ~ 1.3% (a) Sampling points are crystal points and (b) sampling points are segments.

Figure 6. PDF for the resolved shear stress at 6 slip systems at strain level ~ 1.3%: (a) in the crystal, (b) on segments.

The aforementioned computation framework to calculate the internal stress field can also be used to calculate the elastic distortion fields of dislocation structure, namely the elastic strain and lattice rotation. The dislocation density tensor, which is a geometric measure of the incompatibility of the plastic distortion, can be determined from the elastic strain and rotation fields. Figure 7 shows a 3D map for the dislocation density tensor norm in a copper crystal at strain level $\sim 0.65\%$, which reveals the heterogeneity of the dislocation microstructure even at relatively small strain levels. The importance of computing those elastic distortion fields is attributed to the recent advances in X-ray microscopy that provides spatially resolved 3D X-ray microscopy measurements of the same fields [7], which makes it possible to conduct direct comparison between 3D computational data, as in figure (3), and the corresponding 3D experimentally measured maps.

Figure 7. 3D map for the density tensor norm (mrad/microns) in a copper crystal strained to $\sim 0.65\%$. The heterogeneity of the dislocation density tensor reflects the formation of cell structure in deformed copper.

The elastic lattice rotation field, ω , is important since it can be used to calculate two other geometrical measures, the misorientation angle and Nye dislocation density tensor. The misorientation angle between any two points is defined as the magnitude of the difference between their lattice rotation vectors, whereas Nye dislocation tensor, α_{ij} , is defined by [9]

$$\alpha_{ij} = \kappa_{ji} - \delta_{ij} \kappa_{kk}, \quad (3)$$

where $\kappa_{ij} = \partial_i \omega_j$. Figure 8 shows the PDF for the misorientation angle and dislocation density tensor norm at three strain levels. The figures reveal a great similarity of the PDF and its evolution with strain level for the two quantities. Such similarity implies that there can be direct correspondence between Nye dislocation density tensor norm and the misorientation angle in deformed crystals, although such relationship cannot be proved analytically. The claimed direct relationship can be verified by plotting the average misorientation angle versus the average Nye dislocation density tensor norm, as shown in figure 9; the plot reveals a linear relationship

between the averages of both geometric measures. The existence of such a relationship is of great importance as it paves the way to a potential link between the Transmission Electron Microscopy (TEM) and Orientation Imaging Microscopy (OIM) data, and between this data and the recent 3D X-ray measurements for the dislocation density tensor [10].

Figure 8. PDF for (a) Nye dislocation density tensor norm and (b) misorientation angle in a copper crystal undergoing homogeneous deformation.

Figure 9. The average misorientation angle versus the average Nye dislocation density tensor norm.

1.4 Dislocation Dynamics Simulation of Indentation

Indentation of FCC single crystal was simulated using a three-dimensional multiscale plasticity framework. This work aims to compare induced local elastic strain and lattice rotation fields with X-ray measurements of the same fields in 3D [10] for the case of heterogeneous deformation, in preparation for performing the same comparison at a later point using the continuum dislocation dynamics theory.

Previous simulations of indentation deformation using discrete dislocation dynamics considered mostly the macroscopic behavior, such as crystal hardness, rather than the evolution of the microscopic distortion fields. Fivel et al [11] implemented 3D simulation of indentation for copper single crystal where they qualitatively compared the evolved dislocation microstructure with experimental TEM micrographs.

Later on [12], the same framework was used to estimate some parameters to be used within crystal plasticity model. In addition, Widjaja et al [13,14] simulated single crystal indentation using a two dimensional model, where they investigated the effect of initial dislocation source density and indenter shape on the crystal hardness, in addition to potential size effects during indentation.

When simulating the plastic deformation of a finite domain using dislocation dynamics, the applied framework usually consists of coupling a dislocation dynamics library that explicitly simulates plasticity in the nanoscale with a finite element solver that applies the continuum mechanics laws in the continuum scale. In collaboration with the nano/micro mechanics laboratory at University of California, Los Angeles, the Mechanics of Defects Evolution Library (MODEL) was developed, where the contribution of our group was mainly to incorporate boundary value problem (BVP) solution into the library, which enables it to simulate finite domains with arbitrary boundary conditions. The dislocation dynamics core of MODEL is an extension of the parametric dislocation dynamics concept [15].

Finite domain dislocation dynamics simulations, with arbitrary boundary conditions, are usually enabled by applying the superposition principle proposed by van der Giessen and Needleman [16], which splits the internal fields generated by dislocations into an infinite medium contribution, that is calculated analytically, plus an image contribution that is calculated by solving the BVP,

$$\left. \begin{aligned} \nabla \cdot \boldsymbol{\sigma}^I(\mathbf{x}) &= \mathbf{0}, & \mathbf{x} \in \Omega \\ \mathbf{t}(\mathbf{x}) &= \mathbf{t}^a(\mathbf{x}) - \boldsymbol{\sigma}^\infty(\mathbf{x}) \mathbf{n}(\mathbf{x}) & \mathbf{x} \in \partial\Omega \\ \mathbf{u}(\mathbf{x}) &= \mathbf{u}^a(\mathbf{x}) - \mathbf{u}^\infty(\mathbf{x}) & \mathbf{x} \in \partial\Omega \end{aligned} \right\}, \quad (4)$$

where the superscript a refers to the externally imposed boundary conditions and ∞ refers to infinite medium fields generated by the entire dislocation structure. The BVP (4) is solved using a Galerkin finite element method and the resultant fields account for both the free surface effect and the imposed boundary conditions.

Two journal papers on the computational approach for simulating the indentation problem and on the characteristics of internal geometric field and comparison with X-ray measurements of the same are under preparation.

MODEL was developed using object oriented C++ language. The library is capable of simulating finite size domains with arbitrary shapes by enabling the users to provide their own domain triangulation (mesh) files to define the simulation domain. The domain mesh files are of great importance since they are used during the finite element solution of the BVP, and also to control the dislocations motion across the domain boundary. For example, when penetrable boundary is enabled, where dislocations are allowed to leave the simulation domain and generate a slip-step on the surface, the data provided by the domain mesh files is used to trim dislocations on the boundary. Moreover, the library is capable of conducting simulations with arbitrary/user-defined traction and/or displacement boundary conditions, where the user has also a complete control over the imposed boundary conditions though the whole course of simulation. Such high capabilities and flexibilities are unprecedented for a discrete dislocation dynamics library. Since the library is provided for public usage as an open source code, it can be considered as a boost for wider applications of dislocation dynamics simulations.

MODEL was used to conduct indentation simulations and compare the evolving distortion fields with experiments. Figure 10 shows a snapshot of the evolving dislocation structure underneath the indenter at indentation depth of ~ 13.0 nm, and a 3D map for the corresponding dislocation density tensor norm. Comparison between the preliminary results and experiments revealed similarities between the computed and the experimentally measured elastic distortion fields.

The development of the community library MODEL in collaboration with the UCLA Group is a major accomplishment of the current contract.

Figure 10. (a) Evolving dislocation structure underneath the indenter at indentation depth ~ 13.00 nm. (b) 3D map of the dislocation density tensor norm at the same depth.

2. Coupled Dislocation-Kinetics and Crystal-Mechanics Formalism and Computational Solution

This task includes the development of a continuum description of dislocation dynamics based on a dislocation density as a physical field, and the coupling of the resulting kinetic formulation with crystal mechanics to develop a mesoscale plasticity framework. This work is motivated by the need to simulate crystal response to realistic levels of strains and over experimentally relevant crystal volumes. Attempts to develop such a theory date back to the 1950s, when Nye [17] and Kroener [18], among others, started to develop continuum representation of dislocations based on density tensors. It was only recently, and after the introduction of dislocation dynamics simulation methods, that some authors started to employ the concepts of statistical mechanics to develop continuum theories of dislocations; see work by Groma [19,20] for 2D formalism and by El-Azab [1,21] for a 3D counterpart. These efforts motivated others to follow with additional work in the same direction [22,23].

In the current 3D formalism of continuum dislocation dynamics, the evolution of dislocations is governed by a coupled set of first-order hyperbolic equations and the mechanical response of crystal is described by stress equilibrium equations. The dislocation kinetics and stress field are coupled by calculating the plastic (eigen) strain from dislocation motion via a tensorial representation of Orowan's law in which the resolved shear stress drives the motion of dislocations. We thus follow an eigenstrain formalism for solving for the elastic fields when the crystal is deforming plastically. A staggered finite element scheme has been used to solve the dislocation kinetic equations and the elastic eigenstrain problems. The simulation is implemented for copper crystals undergoing multiple slip loading.

Acharya and co-workers [24] proposed Galerkin/Least-Square Finite Element Method (referred to as Galerkin/LSFEM) to discretize the evolution equation in space and the numerical result in such way conserves the solenoidality of dislocation distribution field. In this approach, they also simulated shear test [25,26], considering only one slip system and only pure edge dislocations. Sethna and coworkers [27,28] solved the evolution equation of plastic eigenstrain that gives the dislocation density field. By using their continuum model, some special and interesting dislocation morphology observed in experiment [29,30] (like fractal, cell pattern, self-organization) is also simulated [31,32,33].

In spite of a serious conceptual difference between our approach to continuum dislocation dynamics and the work by these authors, the latter work shows that a continuum approach to dislocation dynamics is a promising one to pursue. This difference is not a matter of approximation or assumption but rather an issue of correctness of the formalism itself.

The predictive power of the framework developed here is illustrated by presenting a few examples that show basic features of an evolving dislocation system using a continuum dislocation density. A simple example in this regard is the relaxation of an arbitrary dislocation system on more than one slip system. In figure 11, we show an initial dislocation structure consisting of four sets of loops on four slip systems (figure 11a). This system is left to relax without external loading until all dislocations stop

The details of the continuum modeling framework have not been published yet. We defer these details to a journal publication and report only some results illustrating the promise and potential of this approach.

moving (figure 11b). The cube dimensions are $5 \times 5 \times 5 \mu\text{m}$. A cell structure forms upon the relaxation process with minor change in the dislocation density. The cell structure is shown in figure 11b. The internal stress associated with these dislocation ensembles is shown in figure 12.

Figure 11. (a) A set of dislocation loops distributed over four slip systems in a copper crystal. (b) The dislocation density distribution after relaxation showing the formation of cell structure. Parts (c) and (d) show the density variation over section of the cube before and after relaxation, respectively.

Figure 12. Snapshots of the stress component σ_{33} (a) prior to and (b) after relaxation of the dislocation system shown in figure 11. The heterogeneity of the internal elastic fields is obvious.

While relaxation of dislocation ensembles is an important test case, the true predictive power of the modeling framework developed here can be shown by solving evolutionary problems. A test case of evolution of dislocation ensembles under uniaxial loading and double slip condition is discussed next. In this example, we show the evolution of the dislocation density and internal elastic fields, as well as the heterogeneous nature of the crystal distortion process. Figure 13 shows the evolution of the dislocation density with strain along with the internal dislocation density pattern evolution. After an initial plateau, the dislocation density increases with strain more like a square root function, exhibiting a behavior similar to that predicted by discrete dislocation dynamics (figure 14). The density increase is associated with the formation of high density of junctions as detected by inspecting the details of the dislocation pattern. The plastic slip pattern and the shape distortion of the crystal are illustrated in figure 15. The above results are only preliminary. More 3D testing of the modeling framework is underway.

Figure 13. Evolution of the dislocation density under uniaxial loading and double slip condition. Copper crystal properties are used but the double slip scenario is a hypothetical one.

Figure 14. Evolution of the dislocation density at different strain rates as predicted by discrete dislocation dynamics simulations (Zbib and co-workers).

Figure 15. Plastic slip pattern, internal axial stress and shape distortion associated with the simulation cases depicted in figure 13.

3. Comparison with Experiments

An analysis of the internal fields of mesoscale dislocation structures was conducted using the method of dislocation dynamics simulation for a copper crystal under compression and indentation loading. The purpose of this work was to make a direct comparison between dislocation dynamics and X-ray measurements of internal elastic strain, lattice rotation and dislocation density tensor. Due to the level of effort involved, one student was mutually supported by this contract and by another subcontract from Oak Ridge National Laboratory. The technical contact at Oak Ridge National Laboratory was Dr. Ben Larson.

In the case of uniform compression, the statistical properties of lattice rotation, elastic strain and dislocation density tensor were obtained and their probability distribution functions and two-point correlations were computed at pixel sizes appropriate for the comparison with X-ray data. It is found that the probability distribution of lattice rotation does not exhibit symmetry about the average lattice orientation, in agreement with the corresponding experimental observations (to be published by Larson and co-workers). Sample results for the statistical quantities of the internal elastic fields are displayed in figures 16 and 17. Analysis of the elastic fields also showed that the elastic strain and lattice rotation induced by the same dislocation ensemble exhibit different correlation length; basically, the correlation length of the lattice rotation field was found to be nearly double that for the elastic strain field, while the correlation length of the latter was comparable to that of the underlying dislocation system. These observations indicate that the spatial features of the dislocation microstructure cannot be inferred based only on experimental measurements of the induced lattice rotation field alone; *this is a significant theoretical result that will change the way X-ray data are currently analyzed.* It was further found that the elastic strain field has a significant contribution to the dislocation density tensor. This finding makes clear that Nye's tensor, which is based upon differential lattice rotation, differs from the full geometric measure of the dislocation density tensor as computed by the rotation of the elastic

distortion field. This discovery asserts the need to enhance the capabilities of current X-ray techniques to enable them to detect and measure the elastic strain in deformed materials with a higher level of resolution that currently possible in order to enhance our understanding of the role of the dislocation density tensor in low-scale size-effects in plasticity [34,35]. As a part of the analysis performed, which is fully documented in [36], we proposed a direct relationship between the average differential misorientation angle in deformed copper lattices and the average Nye's dislocation tensor. A final and important finding of the analysis of internal elastic fields in the case of uniform compression is that, the direct comparison between simulations and experiments of the lattice rotation field revealed similarities between simulations and experiments in the low-scale microstructural features manifested by rapid spatial fluctuations in the lattice rotation field. However, the experimentally observed large-scale features, with length scale in the order of 20 microns or higher, were not reproduced by simulations due to the simulation domain size limitations. Therefore, it was suggested that larger simulation domains should be considered when simulating the homogeneous deformation of metallic crystals through the dislocation dynamics method. This, however, remains a challenge to be addressed using the continuum dislocation dynamics framework.

Figure 16: Probability distribution function of the lattice rotation components at strain level of (a) 0.25% and (b) 0.85%.

In order to simulate micro-indentation, an accurate formulation of the boundary value problem of dislocation dynamics simulation has been carried out. In this formulation the formation of slip traces at the surface was accounted for by a special treatment of the intersection for dislocation with the sample boundary. The method of virtual dislocation segments was used in this formulation [37]. As previously mentioned, we collaborated with Ghoniem's group at to couple the elastic boundary value problem with a dislocation dynamics framework [38], which resulted in the Mechanics Of Defects Evolution Library (MODEL), an open-source dislocation dynamics library [39]. MODEL is capable of simulating finite domain deformation under mixed displacement/traction boundary conditions. MODEL's capabilities/flexibility, in addition to fact

that it is accessible for public users, represent a boost for broader applications of the dislocation dynamics method, which ultimately enhances the ongoing efforts dedicated to understand the plastic deformation physics. Simulation of indentation was carried out for a copper single crystal in the [111] direction. The crystal had a cubic shape with a 5 micron edge. An indentation depth of 35 nm was reached during the first phase of simulations. This indentation range is now being extended. The results compare with X-ray data nicely, where the experimentally observed pattern for the lattice rotation field was reproduced by simulations. Sample results of the internal elastic fields are shown in figures 18 and 19.

Figure 17. Radial self-correlation function of the lattice rotation components at strain level of (a) 0.25% and (b) 0.85%.

Figure 18. A display of the x-component of lattice rotation on two horizontal planes under the indenter. The split of the lattice rotation profile into positive and negative sides is a typical behavior as per X-ray data.

Figure 19. A display of the x-component of lattice rotation on a vertical plane under the indenter. The split of the lattice rotation profile into positive and negative sides and the reversal of the rotation sign at deeper spatial points is a typical behavior as per X-ray data.

SUMMARY AND CONCLUSIONS

Under this contract, the PI and his student and post-doctoral associates collaborators have accomplished the following:

- Developed and tested a continuum dislocation dynamics framework for predicting the collective behavior of dislocations in deforming metals. This framework couples the kinetic equations of dislocations with crystal mechanics and it tracks the dislocation density, plastic slip and all internal stresses during the course of loading. Although only initial results were obtained, the framework is likely to form the basis for a predictive mesoscale plasticity theory capable of capturing the hardening behavior and dislocation patterning.
- Developed a comprehensive methodology for the analysis of the statistics of dislocations and their internal fields, including dislocation correlations, elastic strain field, lattice rotation and dislocation density tensor distributions and correlations. We also performed the first temporal statistical analysis in dislocation dynamics to cast cross slip rates and dislocation reactions into information suitable for informing the kinetics of a continuum dislocation dynamics framework and for guaranteeing the equivalence between discrete and continuum representations of dislocation ensembles.
- We have performed the first direct comparison between 3D experimental data and dislocation dynamics models, through the collaboration with the X-ray spectroscopy group at Oak Ridge National Laboratory (Larson and co-workers).
- Contributed to the development of a community code MODEL for mesoscale simulation. This library of subroutines is becoming popular in the plasticity modeling community.

We envision that future work in this area will include:

- Incorporation of cross slip and dislocation reactions in the continuum dislocation dynamics framework. This requires the development of sophisticated search algorithms to decompose the dislocation density field in the crystal to its constituents and to implement statistical rules for cross slip rates and annihilation reactions based on discrete simulation results.
- The treatment of finite lattice rotation in the continuum dislocation dynamics framework. This part is non-trivial because the kinetic equations of dislocation dynamics are yet to be developed in conjunction with finite deformation kinematics.
- Dealing with the computational complexity of multiple slip under arbitrary loading in the continuum framework.
- Validation of the continuum theory using X-ray data.

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STUDENTS AND POST-DOCTORAL SUPPORT

Over the performance period of the project, 6/1/2008-5/31/2012, the following students and post-doctoral associates were supported.

- Jie Deng was supported for 7 months as a doctoral student and 7 months as a post-doctoral associate.
- Mamdouh Mohamed was supported for 35 month as a doctoral student. He was also partially supported via a subcontract from Oak Ridge National Laboratory.
- Shengxu Xia was supported for 24 month as a masters and doctoral student.
- Thomas Hochrainer was supported for 2.5 months as a post-doctoral associate.

- The PI was supported for a total of two summer months.

STUDENT DEGREES OBTAINED UNDER THIS CONTRACT

- Jie Deng obtained his PhD in the fall semester of 2008. He obtained post-doctoral positions at Sandia National Laboratory and at the University of Wisconsin-Madison.
- Mamdouh Mohamed obtained his Ph.D. degree in the fall semester of 2012. He obtained a post-doctoral position with the Computational Mechanics group at KAUST.
- Shengxu Xia obtained his M.S. degree in the fall semester of 2011. He is now working toward his doctorate degree at Purdue University.

PUBLICATIONS, PRESENTATIONS AND ACTIVITIES INSPIRED BY THIS PROJECT

Journal publications

1. Jie Deng and Anter El-Azab, Mathematical and Computational Modeling of Correlations in Dislocation Dynamics, *Modelling and Simulation in Materials Science and Engineering*, 17 (2009) 075010:1-31
2. Jie Deng and Anter El-Azab, Temporal statistics and coarse graining of dislocation ensembles, *Philosophical Magazine*, v 90, n 27-28, p 3651-3678 (2010).
3. Anter El-Azab, The Statistical Mechanics of Strain Hardened Metals, *Science*, 320 (2008) 1729-1730

Journal manuscripts, to be submitted

1. Mamdouh Mohamed, Jie Deng and Anter El-Azab, Statistical characterization of internal stress in dislocation dynamics: comparison between crystal stress and stress on dislocation lines, *J Statistical Mechanics: Theory and Experiments* (projected submission date: June 2013)
2. Mamdouh Mohamed, Ben Larson and Anter El-Azab, Statistics of internal elastic fields in deformed crystals, *J Statistical Mechanics: Theory and Experiments* (projected submission date: June 2013)

Journal manuscripts under preparation

1. Mamdouh Mohamed, Giacomo Po, Nasr Ghoniem, Ben Larson, and Anter El-Azab, Dislocation dynamics modeling of indentation experiments (projected submission June, December 2013)
2. Shengxu Xia and Anter El-Azab, Continuum dislocation dynamics: theoretical development and numerical implementation in fcc crystal (projected submission date, July 2013)

Conference publications

1. Mamdouh Mohamed, Anter El-Azab and B. C. Larson, Elastic distortion of dislocations in deforming FCC crystals, in *Fundamental Science of Defects and Microstructure* in

Advanced Materials for Energy, MRS Proceedings, 1363, mrss11-1363-rr03-04
doi:10.1557/opl.2011.1428

2. Mamdouh Mohamed, Jie Deng, Anter El-Azab and B. C. Larson, Statistical Modeling of Elastic Strain, Lattice Rotation and Dislocation Density Tensor in FCC Crystals, in: Proceedings of Fifth International Conference on Multiscale Materials Modeling, Edited by: Peter Gumbsch and Erik Van der Giessen, The Fifth International Conference on Multiscale Modeling of Materials, Freiburg, Germany, October 4-8, 2010, pp310-313.
3. Jie Deng and Anter El-Azab, Temporal coarse graining in dislocation dynamics, , in: Proceedings of Fifth International Conference on Multiscale Materials Modeling, Edited by: Peter Gumbsch and Erik Van der Giessen, The Fifth International Conference on Multiscale Modeling of Materials, Freiburg, Germany, October 4-8, 2010, pp 389-392.
4. Jie Deng, Anter El-Azab and Ben Larson, Statistics of Internal Elastic Fields and Dislocation Density Tensor in Deformed FCC Crystals, in: Computational Materials Design via Multiscale Modeling, symposium proceedings, Editors: Y. Qi, H.E. Fang, N. Reynolds, Z-K. Liu, Mater. Res. Soc. Symp. Proc. Volume 1130E, Warrendale, PA, 2009, paper # 1130-W12-11
5. Anter El-Azab, The Quest for a Physical Theory of Metal Plasticity: Can Statistical Mechanics Help? In: A. Dominguez-Rodriguez, D. Gomez-Garcia and A. Munoz Bernabe (Eds.), Proceedings of the II International Workshop: Relation Microstructure-Properties and Multiscale Modelling of Plasticity, Seville University, 2009, pp. 73-78
6. Jie Deng and Anter El-Azab, Theoretical and Computational Modeling of the Statistics of Internal Elastic Fields in 3D dislocation Systems, in: Proceedings of Fourth International Conference on Multiscale Materials Modeling, Editor: Anter El-Azab, October 27-31, 2008, pp. 119-122
7. Mamdouh Mohamed, Jie Deng, Anter El-Azab, Dislocation statistics in FCC crystals, in Proceedings of The Vasek Vitek Honorary Symposium on Crystal Defects, Computational Materials Science and Applications, Editor(s): Mo Li, David Srolovitz, Adrian Sutton, Vaclav Paidar, Jeff De Hosson, TMS, 2010 v2 pp 61-68.

Edited Volumes by the PI (and others) Inspired by this Project

1. *Fundamentals Science of Defects and Microstructure in Advanced Materials for Energy*, Volume 1363 (MRS Proceedings, 2011), Eds. A. El-Azab, B. Uberuaga, G.M. Stokes, Cambridge University Press, ISBN-13: 9781605113401
2. *Collective behavior of complex dislocation structures*, Philosophical Magazine Special Issue number 27-28, Volume 90 (2010), pp. 3617-3786 (Eds. S. Sharafat, A. El-Azab, L. Kubin, S. Zinkle, H. Huang)
3. *Microstructure evolution in materials*, Modeling and Simulation in Materials Science and Engineering, Issue 6, Volume 17 (2009), papers # 064001-064010 (Eds. A. El-Azab, D. Weygand, J. Simmons)

Invited and Keynote Presentations

1. Anter El-Azab, Mamdouh Mohamed, Giacomo Po, Ben Larson, Nasr Ghoniem, Dislocation Dynamics Simulation of FCC single crystals during indentation; Symposium

G: Multiscale Modeling of Crystal Plasticity-From Discrete Modelnig to Generalized Continua, Multiscale Materials Modeling Conference, Biopolis, Singapore, October 15-19, 2012 (invited)

2. Anter El-Azab, A mesoscale theory of dislocation dynamics and crystal deformation, Symposium: Plasticity-Bridging the Scales from Micro to Macro, International Workshop on Computational Mechanics of Materials, IWCMM XXII, September 24-26, 2012, Baltimore, MD (invited)
3. Anter El-Azab, The Closure Problem in Density-Based Modeling of Dislocation Dynamics: Part I: Temporal Statistics. Symposium: Effects of small size scale in materials modeling; 23rd International Congress of Theoretical and Applied Mechanics (ICTAM2012), IUTAM, Beijing, August 19-24, 2012 (invited)
4. Anter El-Azab, The Closure Problem in Density-Based Modeling of Dislocation Dynamics: Part II: Spatial Statistics; Pre-Nominated Session: Plasticity, Viscoplasticity and Creep. 23rd International Congress of Theoretical and Applied Mechanics (ICTAM2012), IUTAM, Beijing, August 19-24, 2012 (invited)
5. Anter El-Azab, The Closure Problem in Density-Based Modeling of Dislocation Dynamics. Advances in Heterogeneous Material Mechanics; 3rd International Conference on Heterogeneous Material Mechanics (ICHMM-2011), Shanghai (ChongMing Island), China, May 22-26, 2011 (invited)
6. Anter El-Azab, On the Closure Problem in Density Based Modeling of Dislocation Dynamics; Symposium on Multiscale Modeling and Dislocation Density Based Models in Plasticity, IV European Conference on Computational Mechanics, Palais de Congrès, Paris, France, May 16-21, 2010 (keynote)
7. Anter El-Azab, Stochastic Modeling of Dislocation Dynamics and Mesoscale Deformation of Metals, International Conference of Numerical Analysis and Applied Mathematics, ICNAAM 2009, September 18-22, 2009, Crete, Greece (invited)
8. Anter El-Azab, The Quest for a Physical Theory of Metal Plasticity: Can Statistical Mechanics Help? II International Workshop: Relation Microstructure-Properties and Multiscale Modelling of Plasticity, Fuenteheridos, Huelva (SPAIN) June 17th-21st, 2009 (invited)

Contributed Presentations

1. Shengxu Xia and Anter El-Azab, Continuum Dislocation Dynamics Modeling of Mesoscale Deformation of Single Crystals, Symposium: Modeling and Experimental Validation of Multiscale Mechanical Behavior from Atomic Scale to Macro Scale, 2013 TMS Annual Meeting & Exhibition, March 3-7, 2013, San Antonio, TX
2. Mamdouh Mohamed, Giacomo Po, Ben Larson, Nasr Ghoniem and Anter El-Azab, Indentation of FCC Single Crystals: Comparison between Dislocation Dynamics Simulations and Experiments, Symposium: Modeling and Experimental Validation of Multiscale Mechanical Behavior from Atomic Scale to Macro Scale, 2013 TMS Annual Meeting & Exhibition, March 3-7, 2013, San Antonio, TX
3. Mamdouh Mohamed, Giacomo Po, Ben Larson, Nasr Ghoniem, Anter El-Azab, Investigation of dislocation-induced elastic fields during indentation of fcc single crystal

by dislocation dynamics simulations, Symposium TT: Defects and Microstructure Complexity in Materials, Materials Research Society Fall 2012 Meeting, Boston, MA, November 25-30, 2012.

4. Shengxu Xia, Anter El-Azab Continuum theory of dislocation dynamics, Symposium TT: Defects and Microstructure Complexity in Materials, Materials Research Society Fall 2012 Meeting, Boston, MA, November 25-30, 2012.
5. Mamdouh Mohamed, Ben Larson, Giacomo Po, Nasr Ghoniem, Anter El-Azab, Dislocation Dynamics Simulation of FCC single crystals during indentation; Symposium: From Macro to Nano, Understanding Mechanical Behavior across Length Scales: A Structural Materials Division Symposium in Honor of Robert Ritchie, 2012 TMS Annual Meeting & Exhibition, Orlando, FL, March 11-15, 2012
6. Anter El-Azab, Mamdouh Salem and Jie Deng, The Closure Problem in Density-Based Modeling of Dislocation Dynamics: Time Coarse Graining; Fifth International Symposium on Defect and Material Mechanics, ISDMM11, Sevilla, Spain, June 27-July 1, 2011
7. Mamdouh Mohamed, Ben Larson, Anter El-Azab, Statistical Modeling of Elastic Strain, Lattice Rotation and Dislocation Density Tensor in FCC Crystals; Symposium RR: Fundamentals Science of Defects and Microstructure in Advanced Materials for Energy, 2011 MRS Spring meeting, San Francisco, April 25-29, 2011
8. Mamdouh Mohamed, Jie Deng, Anter El-Azab, Ben Larson, Statistical Modeling of Elastic Strain, Lattice Rotation and Dislocation Density Tensor in FCC Crystals; The Fifth International Conference on Multiscale Modeling of Materials, Freiburg, Germany, October 4-8, 2010
9. Jie Deng and Anter El-Azab, Statistics of Internal Stress of Dynamical Dislocation Ensembles, The Fifth International Conference on Multiscale Modeling of Materials, Freiburg, Germany, October 4-8, 2010
10. Jie Deng and Anter El-Azab, Temporal Coarse Graining in Dislocation Dynamics, The Fifth International Conference on Multiscale Modeling of Materials, Freiburg, Germany, October 4-8, 2010
11. Anter El-Azab, A Perspective on the Development of Density-Based Models of Dislocation Dynamics; Symposium on Defects in Materials, The Fourth International Conference of Multiscale Materials Modeling, October 27-31, 2008, Florida State University, Tallahassee, FL
12. Anter El-Azab (2008) A New Frontier of Kinetic Theory Applications in Solid Mechanics: the Discrete-Continuum Connection in Dislocation Dynamics; Symposium on Mathematical Issues in Multiscale Modeling of Materials, The Fourth International Conference of Multiscale Materials Modeling, October 27-31, 2008, Florida State University, Tallahassee, FL

BIOGRAPHICAL SKETCH

Anter El-Azab, Professor
School of Nuclear Engineering and School of Materials Engineering
Purdue University
400 Central Drive
West Lafayette, IN 47907-2017
Phone: 765-494-5741; Fax: 765-494-9570
E-mail: aelazab@purdue.edu

Research interests

Computational Microstructure Science; Radiation Effects in Nuclear Alloys and Fuels; Defect Disorder in Oxides; Surface and Interfacial Science; Methods of Multiscale Modeling in Materials

Education and Training

Ph.D. (1994), Nuclear Engineering/Materials and Mechanics, University of California, Los Angeles

M.S. (1989) and B.S. (1986), Nuclear Engineering, University of Alexandria, Egypt

Professional Experience

2012-	Professor of Nuclear Engineering and Materials Engineering, Purdue University
2010- 2011	Professor of Computational Materials Science, Department of Scientific Computing, Florida State University
2008-2010	Associate Professor of Computational Materials Science, Department of Scientific Computing, Florida State University
2008-2011	Faculty Member, Materials Science and Engineering Program, Florida State University
2006-2008	Associate Professor (joint), School of Computational Science & Mechanical Engineering Department, Florida State University
2004-2006	Associate Professor, Mechanical Engineering Department, Florida State University
2003-2004	Senior Research Scientist, Fundamental Science Directorate, Pacific Northwest National Laboratory, Richland, WA
1998-2003	Senior Research Engineer, Energy & Fundamental Science Directorates, Pacific Northwest National Laboratory, Richland, WA
1995-1998	Senior Development Engineer and Lecturer, Mechanical and Aerospace Engineering Department, University of California, Los Angeles

Some Synergistic Activities

Chairman, 4th International Conference on *Multiscale Modeling of Materials*, October 27-31, 2008, Florida State University – the World’s Largest Forum on Computational Materials Science

Lead Organizer, MRS Symposium on *Defects and Microstructure Complexity in Materials*, Fall 2012, Boston

Guest Editor: Several special journal issues on defects and microstructure modeling in materials (Phil. Mag.; J. Appl Phys.; Modell. Simul. Mater. Sci. & Engng.; SIAM J. Multiscale Modeling)

Member of Executive Committee, Energy Frontier Research Center for Materials Science of Nuclear Fuel, DOE/BES

Reviewer, DOE, NSF, DoD

Co-Director, CMCSN Project on Computational Microstructure Science, DOE/BES Program

Five Related Publications

1. Jie Deng and Anter El-Azab, Mathematical and Computational Modeling of Correlations in Dislocation Dynamics, *Modelling and Simulation in Materials Science and Engineering*, 17 (2009) 075010:1-31
2. Jie Deng, Anter El-Azab and Ben Larson, On the Elastic Boundary Value Problem of Dislocations in Bounded Crystals, *Philosophical Magazine*, 88 (2008) 3527-3548
3. Anter El-Azab, The Statistical Mechanics of Strain Hardened Metals, *Science*, 320 (2008) 1729-1730
4. Anter El-Azab, Jie Deng and Meijie Tang, Statistical Characterization of Dislocation Ensembles, *Philosophical Magazine*, 87 (2007) 1201-1223
5. A. El-Azab, Statistical Mechanics Treatment of the Evolution of Dislocation Distributions in Single Crystals. *Physical Review B*, 61 (2000) 11956-11966

Five Other Significant Publications

6. Anter El-Azab (Editor), *Tackling Materials Complexity via Computational Science: Proceedings of the 4th International Conference on Multiscale Materials Modeling*, Florida State University, 2008, ISBN: 978-0-615-24781-6 (989 pages)
7. S.K. Rokkam, P.C. Millett, D. Wolf and A. El-Azab, Phase field simulation of void growth in irradiated materials, in: *Proceedings of Fourth International Conference on Multiscale Materials Modeling*, October 27-31, 2008, pp. 405-408
8. Srujan Rokkam, Anter El-Azab, Paul Millett, Dieter Wolf, Phase Field Modeling of Void Nucleation and Growth in Irradiated Metals, *Modelling and Simulation in Materials Science and Engineering*, vol. 17 (2009) pp 064002: 1-18
9. Paul Millett, Srujan Rokkam, Anter El-Azab, Michael Tonks, Dieter Wolf, Void Nucleation and Growth in Irradiated Polycrystalline Metals: A Phase Field Formulation, *Modelling and Simulation in Materials Science and Engineering*, vol. 17 (2009), pp 064003: 1-12
10. Paul C. Millett, Dieter Wolf, Tapan Desai, Srujan Rokkam, and Anter El-Azab, Phase-field simulation of thermal conductivity in porous polycrystalline microstructures, *J. Appl. Phys.* 104 (2008) 033512:1-6