Modeling and Characterization of Near-Crack-Tip Plasticity from Micro- to Nano-Scales

Edward H. Glaessgen, Erik Saether, Jacob Hochhalter, Stephen W. Smith, Jonathan B. Ransom
NASA Langley Research Center, Hampton, Virginia, 23681
Corresponding author: Edward.H.Glaessgen@nasa.gov

Vesselin Yamakov, Vipul Gupta
National Institute of Aerospace, Hampton, Virginia, 23681

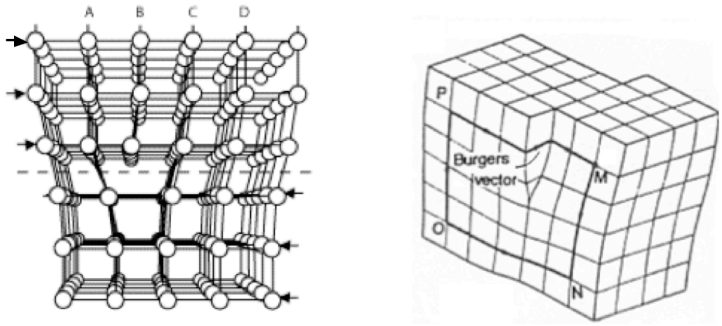
Abstract. Methodologies for understanding the plastic deformation mechanisms related to crack propagation at the nano-, meso- and micro-length scales are being developed. These efforts include the development and application of several computational methods including atomistic simulation, discrete dislocation plasticity, strain gradient plasticity and crystal plasticity; and experimental methods including electron backscattered diffraction and video image correlation. Additionally, methodologies for multi-scale modeling and characterization that can be used to bridge the relevant length scales from nanometers to millimeters are being developed. The paper focuses on the discussion of newly developed methodologies in these areas and their application to understanding damage processes in aluminum and its alloys.

1.0 INTRODUCTION

Fracture mechanics predictions of crack growth are based on the comparison between computed fracture parameters (i.e. K_I, G_I) to their empirically determined critical values (i.e. K_{Ic}, G_{Ic}). Thus, all fracture mechanics-based predictions of crack growth rely on the implicitly assumed similitude between the conditions under which the fracture parameters were determined and the operating conditions of the subject structure. This requires calibration based on extensive physical testing and does not currently represent a truly physics-based discipline.

A physics-based understanding of fracture requires modeling and characterization across length scales from nanometers to millimeters. For example, crack growth at length scales in which atomistic and microstructural details dominate the fracture processes can consume up to 80% of the total life of a structure. These details are not considered in a rigorous manner in static and fatigue crack growth analyses. As a result, high factors of safety are often introduced to account for the myriad of unknowns and potential differences between the test articles used to generate fracture parameters and operational structures. They result in overly conservative structural designs (i.e., increased material thickness resulting in increased weight) and reductions in prescribed service life. The improvement of our understanding of the fundamental processes that govern fracture is enabling to the development of more reliable, lighter, and safer materials and structures. Therefore, it is important to understand the plastic deformation mechanisms related to crack propagation at the nano-, meso-, and micro-length scales. This understanding becomes the basis for a ‘best-physics’ approach to fracture that reduces dependence on empiricism at each length scale and bridges lengths scales with a robust multiscale simulation methodology.

Various methods such as molecular dynamics (MD) or molecular statics (MS) can be used to simulate nanoscale damage and fracture processes using first principles in physics and provide an understanding of deformation and fracture processes at the atomistic level. Shown in Figure 1, dislocations are the characteristic deformation mechanism in all crystalline materials. They can be divided into two



a) Edge dislocation b) Screw dislocation

Figure 1. Configuration of edge and screw dislocations.

types: edge dislocations and screw dislocations as shown in Figure 1a and 1b, respectively.

Through their dynamic evolution and interaction, dislocations constitute the basis for plastic deformation and strain hardening in metallic polycrystals (see Weertman and Weertman, 1992). Because of the importance of understanding dislocation plasticity, dislocation dynamics methods (DD) have been developed that model mesoscale deformation and can provide an analytical bridge between atomistic and continuum material models.

Despite advances in MD and DD, continuum methods will continue to play a dominant role in studying the deformation and fracture of structural materials because their computational efficiency enables interrogation of large domains. Examples of relevant methods that are being developed to address plastic deformation in metallic crystals include strain gradient plasticity and crystal plasticity. These plasticity paradigms are suitable for representing deformation at the micro scale and provide a mechanistic linkage to continuum material models for analysis at structural length scales.

This paper will outline several efforts that are aimed at understanding near-crack-tip plasticity at nano-, meso-, and micro-length scales and will discuss scale-dependent damage mechanisms at each of these length scales.

2.0 MULTISCALE ANALYSIS OF NEAR-CRACK-TIP PLASTICITY

Modeling and characterization approaches for understanding crack tip plastic mechanisms at atomistic, mesoscopic and continuum length scales are presented in the following subsections. Various simulation issues such as time and length scale affects in MD, dimensionality considerations in DD, and the predictive capability of continuum analysis will also be discussed.

2.1 Modeling Near-Crack-Tip Plasticity at the Nano Scale

As a crack grows within a metallic material, a plastic zone is formed as dislocations are generated, propagated and accumulated. Atomistic-based modeling methods such as molecular dynamics provide a means of explicitly examining fundamental deformation mechanisms and have been a topic of considerable study during the past two decades (see Allen and Tildesley, 1987).

Because of its ubiquitous usage in aerospace vehicles, aluminum is of particular interest. Recently, a number of atomistic simulation studies on intergranular and transgranular crack propagation in pure aluminum have been published (Farkas, 2001; Hai, 2001; Tadmor, 2003; Yamakov,

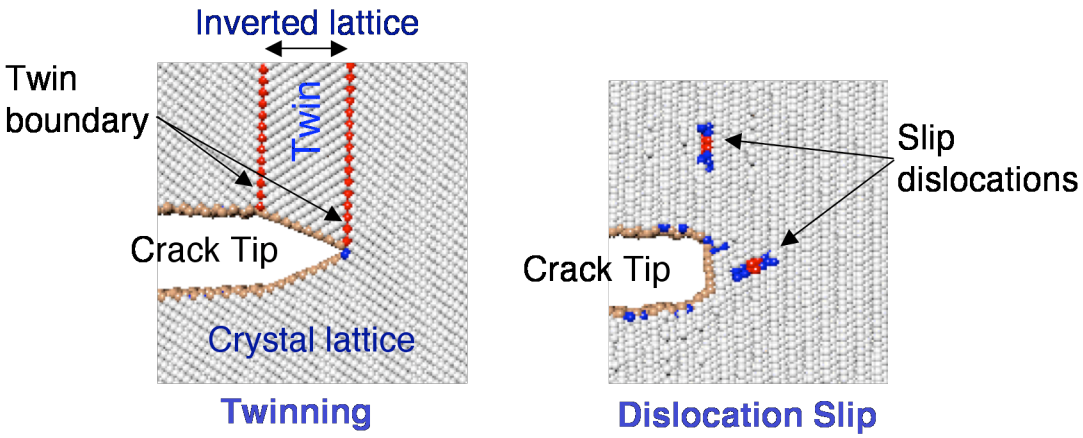


Figure 2. Twinning and slip near a crack tip in pure aluminum (Yamakov, 2009)

2006; Warner, 2007). The results of these investigations show that two main mechanisms of crack propagation and associated near-crack-tip plasticity operate at the nanoscale. These mechanisms include propagation through deformation twinning and propagation through the emission of full dislocations from the crack tip (see Figure 2). One major finding of these and other atomistic simulations of aluminum disagrees with experiment: most atomistic simulations predict deformation twinning as the dominant deformation mechanism whereas experimental observations show that dislocation slip is dominant (Tadmor, 2003).

The discrepancy between simulations and experiments has attracted considerable attention among researchers because it prevents the reliable and accurate modeling of nanoscale fracture, in particular, and puts doubt on the reliability of the atomistic simulations, in general (Tadmor, 2003; Warner and Curtin, 2007). Most likely, the source of this discrepancy is related to the very different length scales (nanometers vs. millimeters), time scales (nanoseconds vs. seconds) and stresses (GPa vs. MPa) at which simulations and experiments are usually performed. Nonetheless, the exact mechanism of how these length and time scales affect the propagation process remains unclear.

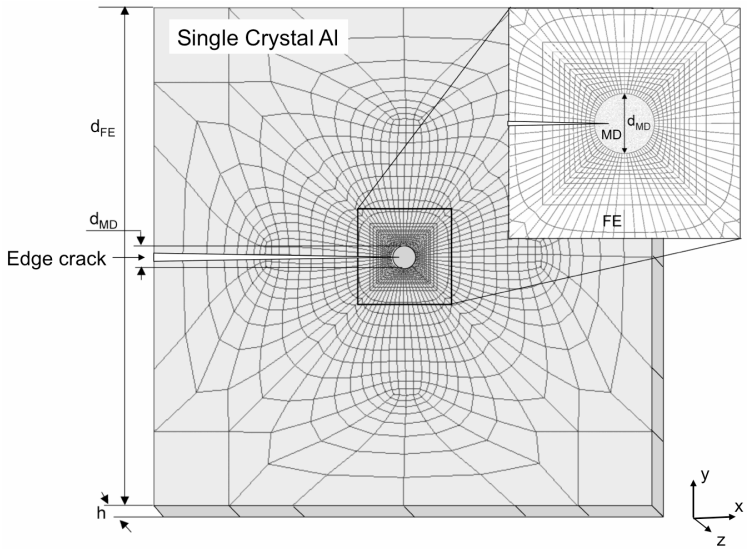


Figure 3. Model geometry of the MD-FEM coupled system with an embedded edge crack ending inside the MD domain.

To further improve the understanding of the sources of the discrepancy between simulation and experiment, a detailed study has been undertaken to determine the conditions under which twinning or dislocation emission occur at a crack tip under Mode I loading (Yamakov, 2009). The recently developed Embedded Statistical Coupling Method (ESCM; Saether, 2009) for concurrent multiscale modeling was used. ESCM was developed to enable much larger material domains to be simulated than can be considered using MD simulation alone by embedding the atomistic domain within a much larger continuum domain (see Figure 3) and thereby greatly reduce computational requirements. The atomistic region containing the crack tip is simulated using MD, while the surrounding continuum region is simulated using the finite element method (FEM). This approach was recently applied to study transgranular fracture in a single crystal of aluminum.

As shown in Figure 3, a circular MD domain was embedded in a square FEM mesh with a pre-existing edge crack propagating along the *x*-direction (Yamakov, 2009). The crack plane normal was along the *y*-direction, and the crack front was along the *z*-direction which was initially extended into the MD domain (see the enlarged central zone in the inset in Figure 3).

The crack front lies in the intersection of the $(11\bar{1})$ slip plane and the crack plane, thus the angle θ, as shown in Figure 4, is 90^o. The orientation of the crack front line is chosen as the *z*-direction in the model. Under these circumstances, the mechanism of crack tip dislocation nucleation is studied as a function of the twist angle, φ, formed between the crack plane normal (the *y*-direction in Figure 4) and the [112] twin axis, lying in the $(11\bar{1})$ slip plane.

Theoretical analysis by Tadmor and Hai (Tadmor, 2003) has shown that the tendency of the crack tip to nucleate a twin or a full dislocation under mode I loading is governed by the twist angle, φ, while the tilt angle, θ, affects only the critical load of nucleation. Studying the crack tip nucleation process at a fixed angle $\theta = 90^o$, while varying the angle φ and the applied stress intensity, K_I, reveals the existence of a transition stress intensity, K_{IT}, below which the crack emits full dislocations and above which deformation twinning becomes dominant. A minimum value of K_{IT} is reached at $\varphi = 0^o$ where twinning becomes the dominant crack propagation mode and a maximum value of K_{IT} at $\varphi = 30^o$ defines the region of full dislocation emission at typical MD loading rates. To be consistent with experimental observations, where deformation twinning at the crack tip in aluminum is rarely observed, this study suggests that crystallographic orientations close to $\varphi = 30^o$ should be used for

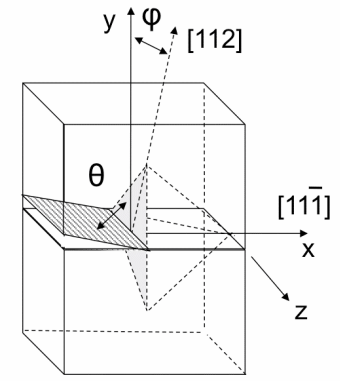


Figure 4. Crystallographic orientation of the crack with respect to the $(11\bar{1})$ slip plane in the fcc lattice.

atomistic characterization of crack tip plastic processes in aluminum. If orientations close to $\varphi = 0^o$ cannot be avoided, the results should be treated with caution as they may produce an artifact of deformation twinning.

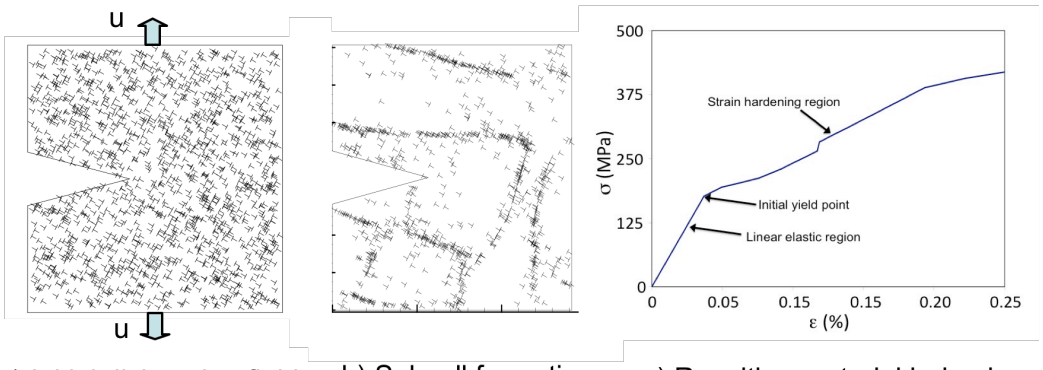
2.2 Modeling Near-Crack-Tip Plasticity at the Meso Scale

DD simulation methods have been developed to represent large numbers of dislocations, obstacles and sources discretely, but at relatively large length scales compared to atomic dimensions. In DD, the discreteness of individual atoms is homogenized with dislocations modeled as displacement discontinuities within an elastic medium and the strength of the discontinuity equal to the magnitude of the Burgers vector. Away from the core region, the displacement, stress and strain fields are suitably represented by analytic elasticity solutions. All the constitutive laws for DD are obtained directly from atomic theory, atomistic simulations, or from physical principles (Kubin et al. 1992). Simulations can involve infinite domains that are modeled using far-field boundaries or periodic boundary conditions, or as finite domains with various applied boundary conditions.

Dislocation dynamics is based on constitutive or field relations describing the short and long-range interactions between dislocations that are solved incrementally. During a simulation, the evolution of the dislocation field is obtained by forward integration of the governing equations and the plastic stress-strain relationship is directly obtained during the analysis. As discussed by van der Giessen and Needleman (1995), the computation of the deformation history is performed in an incremental manner as follows: (i) in the current state, the Peach–Koehler forces on each dislocation are determined based on the present stress fields; (ii) the change of the dislocation structure is obtained by integration of the equations of motion while governing relations are applied to test for dislocation nucleation, annihilation, short-range junction formation, and possible pinning at obstacles; (iii) updated stress state for the new dislocation configuration is repeated by returning to step (i).

Discrete dislocation plasticity simulations may be performed in either two or three dimensions. In two-dimensional simulations, dislocations are represented as point defects that are constrained to move on prescribed slip planes. This yields a simplified representation that provides qualitative results of dislocation interaction and the resulting plastic and hardening behavior of material domains. While the inelastic stress-strain and hardening behavior is an outcome of the analysis, much investigation has been made to determine the formation of dislocation structures such as subcells, shear bands, and low-angle grain boundaries.

Two-dimensional DD analysis has been enhanced by incorporating various three-dimensional processes such as junction formation resulting in dynamic sources and obstacle formation (Benzerga, 2004). An example is presented in Figure 5 in which a square aluminum domain having an edge notch is subjected to an applied external normal displacement in the *y*-direction (Figure 5a). The initial dislocation field shown in Figure 5a is randomly distributed while an evolved dislocation field showing subcell formation is shown in Figure 5b. The computed stress-strain relation is presented in Figure 5c and shows an initial linear elastic behavior followed by yielding and subsequent hardening due to dislocation interactions. Fully three-dimensional DD analyses are in the early stages of development and, although very promising, are very computationally intensive and currently have limited application (Arsenlis, 2007).



a) Initial dislocation field b) Subcell formation c) Resulting material behavior

Figure 5. Simulation using the two-dimensional DD-SIM code for a wedge configuration under normal tension loading in the *y*-direction.

2.3 Modeling Near-Crack-Tip Plasticity at the Micro Scale

Dislocations of all types are often divided into two classes in continuum mechanics-based analyses. These classes are the *statistically stored dislocations* (SSDs) that are generated by the manufacturing processes used to form the material (pre-existing dislocations) and by uniform deformation during loading, and the *geometrically necessary dislocations* (GNDs) that are required to enforce internal compatibility during non-uniform plastic deformation.

Both SSDs and GNDs are explicitly considered in molecular dynamics and dislocation dynamics models; however, neither is explicitly considered within conventional crystal plasticity (CCP) formulations. CCP formulations, like all constitutive models, must be calibrated for the specific material of interest. In CCP, the calibration usually consists of modeling a material microstructure with specific grain size, aspect ratio and crystallographic orientation, and matching a simulated response to an observed response by varying the material parameters.

Unlike CCP theories, the basic tenant of strain gradient plasticity (SGP) theories is that GNDs are produced by micron-scale gradients at a density comparable to, or greater than, that of SSDs, thus increasing the total dislocation density and the resistance to plastic flow. It is now generally accepted that any apparent increase in flow strength is due to the generation and storage of GNDs as required to maintain internal compatibility during non-uniform plastic deformation, e.g., localized gradients near crack tips or precipitates. Numerous SGP theories have been proposed recently with the purpose of extending the validity of continuum plasticity theories down to the micron scale. Inherent to SGP is the presence of a characteristic length scale over which the underlying mechanisms of plastic response are dependent on the magnitude of strain gradients. In addition to providing a more accurate model for work hardening, strain gradient plasticity models are closely related to and may be calibrated by the results of dislocation dynamics simulations, thereby providing a more natural tie to inelastic deformation processes at lower-length scales.

These microscale plasticity models can be integrated with detailed three-dimensional finite element models of microstructure to provide a new understanding of microstructural deformation. By incorporating models for slip accumulation, a relationship between plastic exhaustion and crack growth can be computed. Detailed three-dimensional finite element models of aluminum 7075-T651 employing

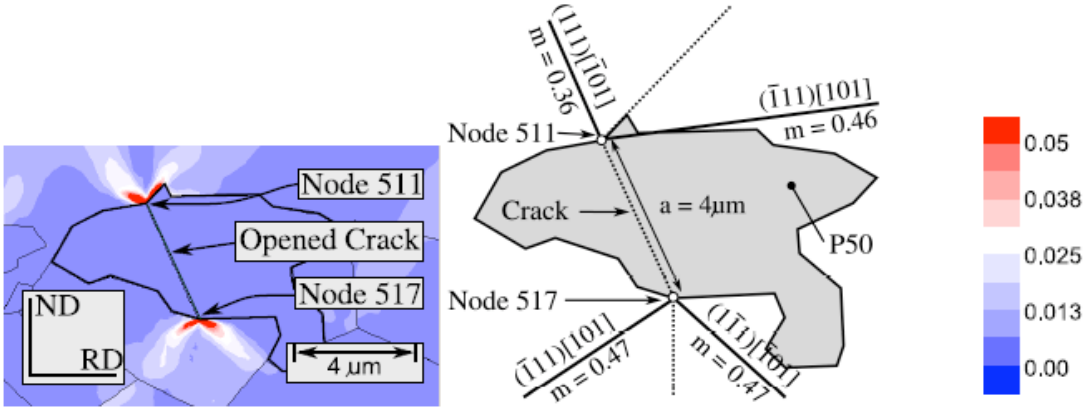


Figure 6. Computed slip fields near a cracked constituent particle that was observed to nucleate a crack into the surrounding grains.

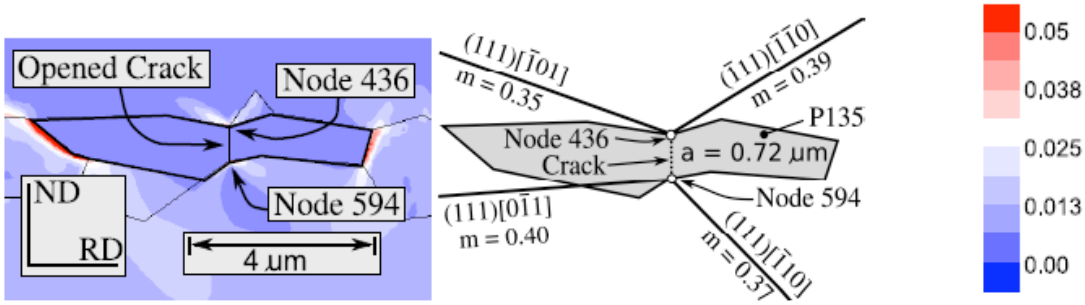


Figure 7. Computed slip fields near a cracked constituent particle that was observed not to nucleate a crack into the surrounding grains.

CCP have been generated to predict the initiation of cracking at the microstructural scale (Hochhalter, 2010). To better understand the slip accumulation during cyclic loading that precedes nucleation events, these finite element models were generated using observed microstructural data that included the configuration and location of constituent particles and grain microstructural details. Slip localization and accumulation was computed near cracked particles. Figures 6 and 7 illustrate the computed slip localization near two different cracked constituent particles in aluminum 7075-T651. The contoured fields in both figures are the maximum value of slip on any one of the twelve fcc slip systems; the corresponding values given by the contour bars are the magnitude of slip on the dominant system.

The particle shown in Figure 6 with high slip accumulation near the crack tip-grain interface was observed to nucleate a crack into the surrounding grains, while the particle in Figure 7 did not. Thus, it appears that slip localization and accumulation plays a governing role in crack nucleation at this scale; see Hochhalter (2010) for further discussion. Figures 6 and 7 also show the correspondence between computed slip localization and dominant slip system directions as measured using electron backscattered diffraction (EBSD). However, the directions of slip localization did not correspond with the nucleation direction given by the dotted line in Figure 6. This observation leads to two possible hypotheses, that crack trajectories are based on alternating shear or on local maximum tangential stress. More simulations and experimental characterizations are currently underway to investigate these hypotheses.

2.4 Characterization at the Meso and Micro Scales

Even though considerable progress in computational methodologies and algorithms has been made, an in-depth understanding of damage processes is still heavily dependent on experimental characterization. Small-scale experimental methods are being developed to understand damage processes and validate simulations at the meso and micro length scales. In one example, an experimental methodology that uses an environmental scanning electron microscope (ESEM) equipped with *in situ* loading frame and EBSD system has been employed to characterize damage processes in single crystals of pure aluminum and polycrystalline aluminum alloys. The EBSD orientation mapping tools can be used to measure the extent of high plastic deformation near the fatigue crack tip and crack tip wake. Plasticity near the crack tip is related to the plastic strain gradients and thus the geometrically necessary dislocation (GND) density.

These GNDs result in bending of the lattice and may be detected as an orientation gradient within a single grain. Additionally, a zone of "significant plastic strain" about a fatigue crack tip and crack tip wake can be determined by measuring the width of the highly defected region (e.g., green-to-red rainbow color scheme on misorientation maps). Experimentally determined locations of orientation discontinuities, e.g., at sector boundaries, slip bands, near the crack-tip and GND densities estimated from local lattice rotations can be compared with model predictions to enable the *physics-based* models to include correct input parameters, such as source and obstacle densities.

Recent studies (Sun, 2000; Kysar, 2002) of single crystals and bicrystals have shown that it is possible to extract some of the components of the Nye dislocation density tensor (Nye, 1953) using orientation data obtained by EBSD mapping, provided that the crystal orientation and deformation conditions are carefully controlled to constrain the number of independent components. The present work follows that of Sun (Sun, 2000) and Kysar (Kysar, 2002), and considers a connection between the GND content and the lattice curvature tensor through spatially resolved local-orientation measurements using EBSD.

For the purpose of illustration, these approaches have been applied to the EBSD orientation data obtained from the vicinity of a fatigue crack in precipitation-hardened aluminum alloy Al-Cu-Mg 2024-T351. The intra-grain misorientation map (Figure 8a) displays changes in the local orientation, along with large amounts of intra-granular misorientation associated with the large plastic deformation in the vicinity of a crack tip wake (Gupta, 2009). White regions in Figure 8a correspond to pixels that were not indexed. The misorientation map reveals distinctions in the morphology of plastic damage, e.g., the presence of slip-bands near the crack tip wake. These maps suggest the presence of a high dislocation content resulting in extensive misorientation.

Figure 8b shows the estimated distribution of GND density within the scanned area. The regions of lower dislocation density (i.e., base material, ~0.5-1x10^{14} /m^2) are separated by regions of higher dislocation density (i.e., *plastically-deformed* crack-wake, ≥10^{15} /m^2 and higher), and can be identified by marked orientation change (Figure 8a) or by the enhanced dislocation density (Figure 8b; Gupta, 2009). The boundaries of these banded structures (dislocation patterning) contain a high GND density, and regions within the bands are relatively free of dislocations that contribute to lattice curvature. An inhomogeneous distribution of the dislocation density becomes obvious for such cases.

The measurements of local orientation changes and estimates of GND content near the crack tips and deformed wakes of

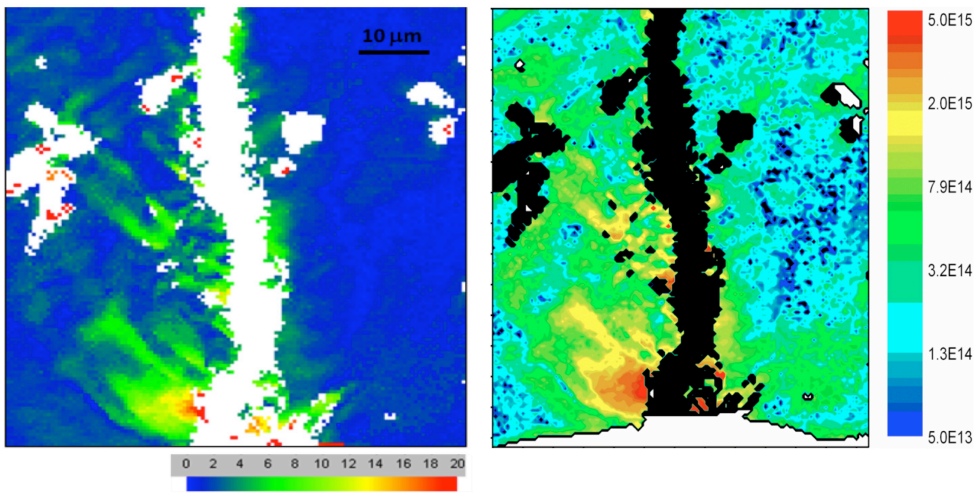
fatigue cracks can be qualitatively compared with those predicted by computational models developed with the aid of molecular dynamics and finite element simulations. This experimental effort will contribute a significant quantitative and physical understanding of damage mechanisms that will enable next-generation damage models to progress beyond the current empirical models.

3.0 SUMMARY

An examination of plastic mechanisms as a function of length scale reveals that the phenomena governing plasticity become increasingly complex as the length scales increase. At the nanoscale, plasticity is characterized by the formation and movement of individual dislocations. Assumptions at the nanoscale are related to very fundamental quantities such as the interatomic potential, structure of the crystal lattice, and the presence of alloying elements. At the mesoscale, the discrete dislocations interact with each other, with sources and with obstacles. DD simulations can model the behavior of micron-sized domains, but must use aggregated values of source and obstacle strength and spacing in addition to approximate solutions for dislocation interaction. At the microscale, the complex physical interactions within a grain interact with those occurring in neighboring grains and form an even more complex deformation field. Crystal plasticity and strain gradient plasticity formulations can account for plastic slip in a homogenized sense, but must be calibrated against experimental data or smaller-scale simulations.

Thus, a consequence of the limitations of existing modeling tools and finite computer resources is that the simulation of increasingly complex domains necessitates a corresponding decrease in the fidelity of the analyses.

The promise of these various computational methods for modeling near-crack-tip plasticity is not seen when the methods are implemented individually, but rather, when the methods are integrated with each other and with the understanding gained from small-scale experiment. For example, molecular dynamics simulations can be used as the basis for discrete dislocation plasticity models, which, in turn, can be used to inform the parameters needed in gradient and crystal plasticity models. The results from small-scale experiment can then be used to validate and augment these simulations.



(a) EBSD misorientation map (b) Enhanced dislocation density map

Figure 8. Maps of misorientation and geometrically necessary dislocation density

4.0 REFERENCES

Allen, M.P. and Tildesley D.J., *Computer Simulation of Liquids*, Oxford Science Publications, Oxford, 1987.

Arsenlis, A., Cai, W., Tang, M., Rhee, M., Oppelstrup, T., Hommes, G., Pierce, T.G. and Buylatov, V.V., "Enabling Strain Hardening Simulations with Dislocation Dynamics," *Modeling and Simulation in Materials Science and Engineering*, vol. 15, 2007, pp. 553-595.

Benzerga, A., Brechet, Y., Needleman, A. and Van der Giessen, E., "Incorporating Three-Dimensional Mechanisms into Two-Dimensional Dislocation Dynamics," *Modeling and Simulation in Materials Science and Engineering,* vol. 12, 2004, pp. 159-196.

Farkas, D., Duranduru, M., Curtin, W. A., Ribbens, C., "Multiple-Dislocation Emission from the Crack Tip in the Ductile Fracture of Al," *Philosophical Magazine A*, vol. 81, 2001, pp. 1241-1255.

Gupta, V.K., Ph.D. Dissertation, University of Virginia, Charlottesville, 2009.

Hai, S. and Tadmor, E. B., "Deformation Twinning at Aluminum Crack Tips," *Acta Materialia*., vol. 51, 2003, pp. 117-131.

Hochhalter, J.D., Littlewood, D.J., Christ Jr., R.J., Veilleux, M.G., Bozek, J.E., Ingraffea, A.R., Maniatty, A.M., "A Geometric Approach to Modeling Microstructurally Small Fatigue Crack Formation: II. Physically based modeling of microstructure-dependent slip localization and actuation of the crack nucleation mechanism in AA 7075-T651," *Modeling and Simulation in Materials Science and Engineering*, vol. 18, 2010, pp. 1-32.

Kubin, L.P., Canova, G., Condat, M., Devincre, B., Pontikis, V. and Brechet, Y., "Dislocation Microstructures and Plastic Flow: A 3D Simulation," *Solid State Phenom*., vol. 23/24, 1992, pp. 455-472.

Kysar, J.W. and Briant, C.L., "Crack Tip Deformation Fields in Ductile Single Crystals," *Acta Materialia*, Vol. 50, 2002, pp. 2367-2380.

Nye, J.F., "Some Geometrical Relations in Dislocated Crystals," *Acta Metallurgica*, Vol. 1, 1953, pp. 153-162.

Saether, E., Yamakov, V. and Glaessgen, E.H., "An Embedded Statistical Method for Coupling Molecular Dynamics and Finite Element Analyses," *International Journal for Numerical Methods in Engineering*, vol. 78, 2009, pp. 1292-1319.

Sun, S., Adams, B.L. and King, W.E., "Observations of Lattice Curvature Near the Interface of a Deformed Aluminum Crystal," *Philosophical Magazine A*, Vol. 80, No. 1, 2000, pp. 9-25.

Tadmor, E.B. and Hai, S., "A Peierls Criterion for the Onset of Deformation Twinning at a Crack Tip," *Journal of the Mechanics and Physics of Solids*, vol. 51, 2003, pp. 765-793.

Van der Giessen, E. and Needleman, A., "Discrete Dislocation Plasticity: A Simple Planar Model," *Modeling and Simulation in Materials Science and Engineering,* vol. 3, 1995, pp. 689-735.

Warner, D.H., Curtin, W.A. and Qu, S., "Rate dependence of Crack-Tip Processes Predicts Twinning Trends in f.c.c. Metals," *Nature Materials*, vol. 6, 2007, pp. 876-880.

Weertman, J, Weertman, J.R., *Elementary Dislocation Theory,* Oxford University Press, Inc., New York, New York, 1992.

Yamakov, V., Saether, E., Phillips, D.R. and Glaessgen, E.H., "Molecular-Dynamics Simulation-Based Cohesive Zone Representation of Intergranular Fracture Processes in Aluminum," *Journal of the Mechanics and Physics of Solids*, vol. 54, 2006, pp. 1899-1928.

Yamakov, V., Saether, E., and Glaessgen, E.H., "A Continuum-Atomistic Analysis of Transgranular Crack Propagation in Aluminum," 50th AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics and Materials Conference and Exhibit, Palm Springs, CA, May 4-7, 2009.