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Modeling Near-Crack-Tip Plasticity From Nano- to Micro-Scales

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Several efforts that are aimed at understanding the plastic deformation mechanisms related to crack propagation at the nano-, meso- and micro-length scales including atomistic simulation, discrete dislocation plasticity, strain gradient plasticity and crystal plasticity are discussed. The paper focuses on discussion of newly developed methodologies and their application to understanding damage processes in aluminum and its alloys. Examination of plastic mechanisms as a function of increasing length scale illustrates increasingly complex phenomena governing plasticity.

Introduction

Fracture mechanics predictions of crack growth are based on the comparison between computed fracture parameters (i.e., K_I, G_I) and 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. Examples of these conditions include loading mode mixity, material thickness and operating environment. Although this paradigm is usually successful for modeling crack growth at structural scales, it requires calibration based on extensive physical testing and does not currently represent a truly physics-based discipline. Therefore, to lessen the dependence on empirical input and advance the mechanistic basis of classical fracture

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mechanics, the fundamental processes that govern fracture across length scales must be thoroughly elucidated.

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. Typically, these details are not considered in a rigorous manner in static and fatigue crack growth analysis. 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. These factors of safety are manifested through overly conservative structural designs (i.e. increased material thickness resulting in increased weight) and reductions in prescribed service life. Hence, 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.

Further, the development and implementation of new materials for structural applications (i.e., nanocrystalline metals, layered metals, powder metallurgy-formed materials) is highly dependent on developing an understanding of their internal damage processes (Needleman, 2001). While many of these materials often exhibit high strength, some also tend to have low ductility and low fracture toughness. Low ductility and toughness can be a result of nanoscale structure; here, Hall-Petch* behavior is no longer valid when the grain dimension approaches the size of dislocations, thus disabling the mechanisms that produce ductility and toughness (Sanders, 1997). Since current engineering approaches are unable to explain these important phenomena, new modeling methods are being developed to predict material behavior at nano- to micro- length scales.

All material processes involved with damage and fracture are ultimately based on atomistic mechanisms occurring at nanometer length scales. Various methods such as molecular dynamics (MD) or molecular statics (MS) methods can be used to simulate these nanoscale processes using *first principles* in physics and provide an understanding of deformation and fracture processes at the atomistic level. These simulation methodologies promise the development of physics-based 'bottom-up' multiscale analyses

*Hall-Petch behavior refers to a general relationship where
material properties "improve" with decreasing grain size.

that can provide an understanding of the evolution of failure mechanisms across length scales. In this paper, nanoscale mechanisms will be examined through atomistic studies of crack tip behavior.

The characteristic deformation mechanism in all crystalline materials is the *dislocation*. Dislocations are a class of atomic lattice defects that consist of a central core containing a large distortion of the lattice that gradually diminishes with increasing distance, resulting in long-range straining of the atomic crystal (see Weertman and Weertman, 1992). Dislocations can be divided into three types: edge dislocations, screw dislocations and mixed dislocations. Dislocations are generally of mixed character, being a combination of the edge and screw dislocations shown in Figure 1a and 1b, respectively. The dynamic evolution of these dislocation fields constitutes the atomistic basis for plastic deformation and strain hardening in metallic polycrystals.

Dislocations of all types are often divided into two classes in continuum mechanics-based analyses. These are the *statistically stored dislocations* 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* that are required to enforce internal compatibility during non-uniform plastic deformation. Although statistically stored dislocations are dominant at large characteristic dimensions, geometrically necessary dislocations become increasingly important at smaller dimensions.
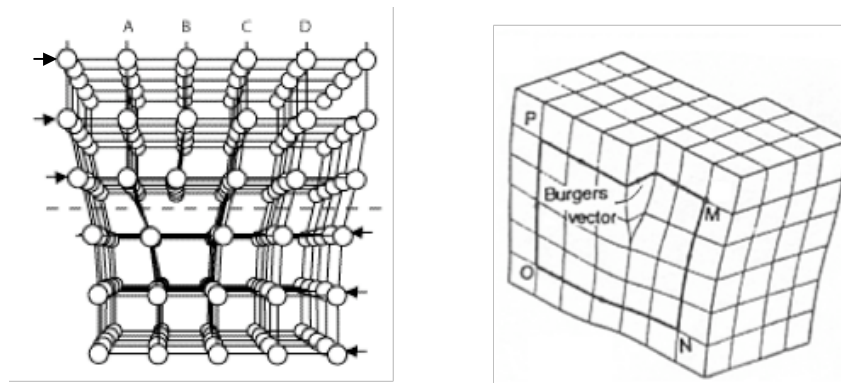
a) Edge dislocation   b) Screw dislocation

Figure 1. Configuration of edge and screw dislocations.

Dislocation interactions such as pile-ups and short-range entanglement (junction formation) are the primary mechanisms for increasing the resistance to subsequent dislocation motion, thereby enhancing material toughness. As additional dislocations are nucleated, their long-range interactions generate a many-body interaction problem involving the generation of Peach-Koehler forces† on neighboring dislocations that induce glide along slip planes. Dislocation jumps to adjacent slip planes can occur with the addition of thermal energy input typically above room temperature. Short-range interactions are described by local constitutive laws in which dislocations can annihilate, generate pile-ups, combine through complex junction formation, or become pinned to function as Frank-Read sources** for nucleating additional dislocations on associated slip planes. These interactions can result in the generation of internal dislocation structures such as shear bands, subcells and low-angle grain boundaries.

Examination of these nanoscale processes provides a remarkable amount of insight into the fundamental mechanisms of deformation and fracture. However, the largest domains that can be interrogated atomistically are much smaller than the grains found in all but a few nanocrystalline materials. Conversely, a grain of material in a typical aluminum alloy consists of billions of atoms with similar crystallographic orientation and millions of dislocations, each of which moves along a plane within the crystal lattice or between planes of the crystal lattice. The specific size of each of the grains and number of pre-existing dislocations is a function of material type and numerous processing parameters.

Although atomistic-based methods are enabling to the interrogation of the most fundamental mechanisms of deformation and fracture, the practical limitations stemming from the computational resources that are likely to be available for the foreseeable future dictate that other, more approximate, methods will continue to play a dominant role in studying the deformation of structural materials. Examples of relevant methods that are being developed to address plastic deformation in metallic crystals include discrete dislocation plasticity, strain gradient plasticity and crystal plasticity. These plasticity paradigms represent interrogation of deformation at the meso- to micro-scale and provide

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†Peach-Koehler forces are the forces on a dislocation.
**Frank-Read sources are one of the mechanisms that are responsible for the generation of dislocation loops within a slip plane.

a mechanistic connection to continuum material models for analysis at structural length scales.

There is an obvious and intimate linkage between each of these length scales. Less obvious are the details of the linkage between the mechanisms of deformation and between the various modeling paradigms that are suited to simulating deformation at each length scale. Despite inherent difficulties, the mechanics community has begun to realize the advantages of developing multiscale methodologies to link material models that span length scales encompassing atomistic to grain-scale micromechanical simulations.

In this paper, selected results from several efforts that are aimed at understanding the plastic deformation mechanisms related to crack propagation at the nano-, meso-, and micro-length scales will be presented. Issues related to the modeling of near-crack-tip plasticity across these length scales will be discussed. The paper will conclude with a summary of the work including a brief discussion of future directions for multiscale modeling of damage processes.

Modeling Near-Crack-Tip Plasticity at the Atomistic 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 (MD) provide a means of explicitly examining fundamental deformation mechanisms and have been a topic of considerable study during the past two decades. Early studies were focused on idealized perfect crystal structures (i.e., a single type of atom in a perfect lattice), but improved methodologies and increases in computing power are making the study of deformation and fracture in more complex atomic structures attainable (i.e., alloys with distributed lattice defects; for an overview of atomistic simulation, 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, 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).
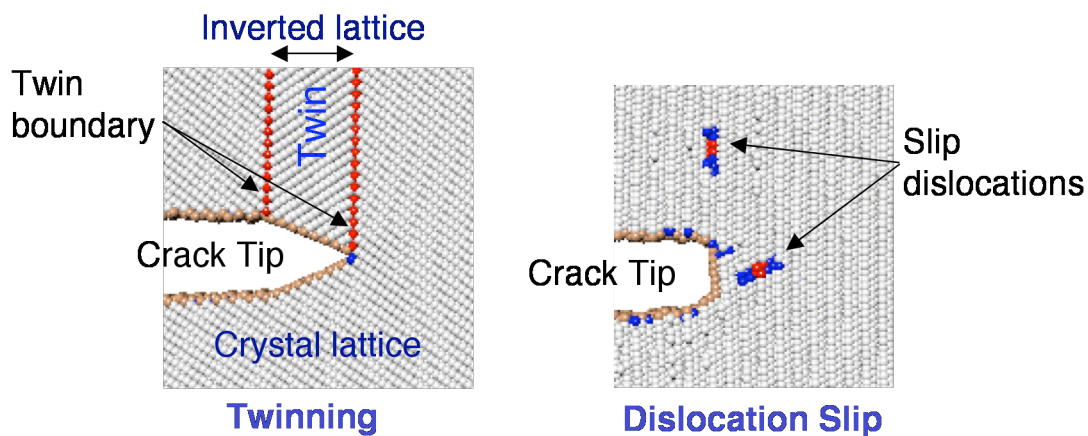

Figure 2. Twinning and slip near a crack tip in pure aluminum (Yamakov, 2009)

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, 2007). Most likely, the source of this discrepancy is related to the very different length (nanometers vs. millimeters) and time (nanoseconds vs. seconds) scales at which simulations and experiments are usually performed. In an effort to determine whether or not it is possible for a MD-based method to predict the experimentally determined mechanisms, Warner and Curtin (Warner, 2007) used an extremely computationally-efficient multiscale analysis method to perform simulations. They developed a unique simulation in which they considered a time range spanning six orders of magnitude – from pico-seconds to micro-seconds. A transition in

the mechanism from twinning to dislocation slip was found when the crack propagation rate was decreased to about one millionth of the rate that is often used in atomistic simulations (Warner, 2007). Nonetheless, the exact mechanism of how these length and time scales affect the propagation process remains unclear and is a very active topic of research.

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. In ESCM, an atomistic domain is embedded within a larger continuum domain (see Figure 3). The atomistic region containing the crack tip is simulated using MD, while the surrounding continuum region is simulated using the finite element method (FEM). The authors have previously used the ESCM approach to study intergranular fracture along a grain boundary in aluminum (Saether, 2009). The same approach is applied here to study transgranular fracture in a single crystal of aluminum.

The model geometry used to study transgranular crack propagation in an aluminum single crystal is shown in Figure 3. A circular MD domain with a diameter $d_{MD} = 40$ nm was embedded in a square FEM mesh with side dimension $d_{FE} = 20d_{MD} = 0.8$ μm. In this model, the system represents a single crystal with a pre-existing edge crack propagating along the x-direction. The crack plane normal is along the y-direction, and the crack front is along the z-direction. The crack from the continuum region is initially extended into the MD domain equal to 1/4 d_{MD} (see the enlarged central zone in the inset in Figure 3). The atomically sharp crack tip in the MD domain is formed by screening the atomic forces between the atoms on both sides of the crack plane starting from the MD-FEM interface along a distance of 1/4 d_{MD} inside the MD domain.
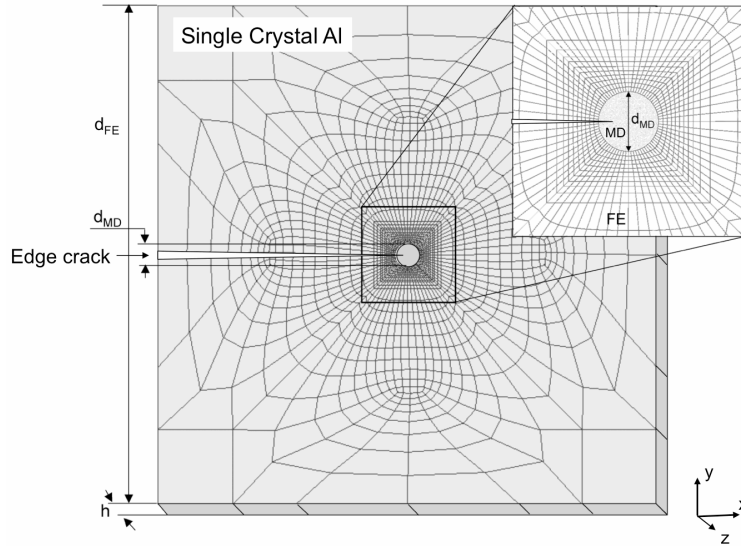
Figure 3. Model geometry of the MD-FEM coupled system with an embedded edge crack ending inside the MD domain.

The crack propagation direction, x, is fixed along the $[11\bar{1}]$ axis, so that the crack plane is perpendicular to the $(11\bar{1})$ slip plane. The crack front lies in the intersection of the $(11\bar{1})$ slip plane and the crack plane forming an angle θ, as shown in Figure 4, that equals 90°. 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 angle φ, while the angle θ affects only the critical load of nucleation.
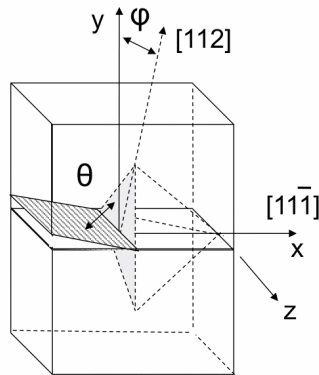

Figure 4. Crystallographic orientation of the crack with respect to the $(11\bar{1})$ slip plane in the f.c.c. lattice.

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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. The transition stress intensity depends on the crystallographic orientation, defined by the φ-angle. A minimum value of K_{IT} is reached at $\varphi = 0^o$ where twinning becomes the dominant crack propagation mode in MD simulations possibly due to their very large applied strain rates of 10^7 s^{-1} or higher. 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 atomistic characterization of crack tip plastic processes in aluminum. If orientations close to $\varphi = 0^o$ are to be examined using atomistic simulation at similar loading rates, the results should be treated with caution as they may produce an artifact of deformation twinning (Warner, 2007) that can substantially alter the predicted fracture parameters, such as the peak stress of debonding and energy of decohesion.

Modeling Near-Crack-Tip Plasticity at the Meso Scale

At the nanoscale, atomistic simulations predict the evolution of the atomic structure due to force interactions as described by an interatomic potential. At the microscale, continuum plasticity formulations are based on elastic-plastic constitutive behavior that must be assumed a-priori. However, at an intermediate scale, the mesoscale, discrete dislocation plasticity - based on dislocation dynamics (DD) - allows both the plastic stress-strain response and the corresponding evolution of the dislocation structure to be predicted as part of the solution of the boundary value problem (van der Giessen, 1995; Needleman, 2000; Cleveringa, 2000). DD simulation methods have been developed to represent large numbers of dislocations discretely, but at relatively large length scales compared to atomic dimensions. In these approaches, the discreteness of individual atoms is replaced through homogenization wherein all atoms are modeled as an elastic continuum and dislocations are represented as discrete entities centered along a

curvilinear core containing the displacement discontinuity where the strength of the discontinuity is 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 of material science. 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.

Discrete dislocation plasticity 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) the updated stress state for the new dislocation configuration is determined and the incrementation is repeated by returning to stage (i) (van der Giessen, 1995).

For finite geometries, a superposition approach is commonly used in which corrective displacement and stress fields are generated in a separate analysis and added to the infinite domain DD solution. This corrective solution is used to apply external loads and to generate dislocation image fields along boundaries to cancel internal normal tractions to recover free surface conditions. Although exact analytical expressions are available to yield correct boundary conditions for single or symmetric arrangements of dislocations, for complex distributions of dislocations, the corrective solution is typically obtained by solving a related boundary value problem using finite element analysis (van der Giessen,

1995; Needleman, 2000; Cleveringa, 2000). Although the body exhibits inelastic deformation at each increment in the solution, the material is assumed to be linear elastic with small strains, thus formally permitting the application of a superposition procedure.

As discussed in O'Day and Curtin (O'Day, 2004) and illustrated in Figure 5, the solution at any increment in a discrete dislocation plasticity simulation (the *Complete Problem* in Figure 5) is obtained as the superposition of: (i) the field of the current dislocations in an infinite space (the *DD Model* in Figure 5), and (ii) the field of a corrective problem which accounts for the particular geometry and any applied boundary conditions (the *FE Model* in Figure 5). The solution to (i) is known analytically by superposing the singular elasticity expressions for displacement and stress fields induced by each dislocation, while the solution to (ii) is smooth and can be found from a finite element calculation. Once the solution is found, the incremental procedure described previously is applied to advance the system by a specified time step.
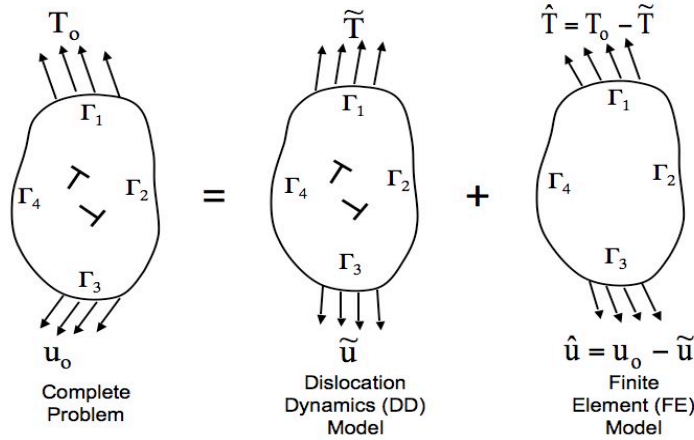

Figure 5. Superposition framework for performing finite geometry DD simulations.

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 idealization permits exact elasticity solutions to be derived for the displacement and stress fields and yields a simplified representation that provides qualitative results of dislocation interaction and 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.

The superposition procedure outlined in Figure 5 is the basis for a code (DD-SIM) that incorporates a DD analysis and a finite element procedure for correcting free edge boundary conditions using 4-node quadrilateral elements. The DD analysis has been enhanced by incorporating various two-dimensional representations of three-dimensional processes such as junction formation resulting in dynamic sources and obstacle formation (Benzerga, 2004). An example is presented in Figure 6 in which a square aluminum domain having side dimensions of 14.27 μm and an edge notch that is 5.71 μm long with an opening angle of 28.1^o is subjected to an applied external normal displacement in the y-direction of $u_y = 0.357$ μm (Figure 6a). The initial dislocations shown in Figure 6a are randomly applied and lie on $+60^o$ and -60° slip systems. After only 100 iterations, the simulation clearly shows the formation of subcell dislocation structures as depicted in Figure 6b. These internal structures are related to the material plastic response and, due to constraints on dislocation mobility, result in hardening or increased toughness of the material. The computed stress-strain relations is presented in Figure 6c and shows an initial linear elastic behavior followed by yielding and subsequent hardening due to dislocation interactions.

As illustrated by the results shown in Figure 6, two-dimensional DD simulation can provide qualitative information of dislocation behavior in idealized material domains. In contrast, three-dimensional modeling promises much more accurate predictions, but it requires a tremendous increase in computational resources. Three-dimensional DD modeling methods are still in relatively early stages of development with the most mature of the codes being the ParaDiS code (Arsenlis, 2007) that is being developed at Lawrence Livermore National Laboratory. Currently, the ParaDiS code accounts for three-dimensional dislocation loops, long-range and short-range interactions, but cannot simulate the affects of finite geometry on plasticity.

a) Initial dislocation field   b) Subcell formation after 100 iterations
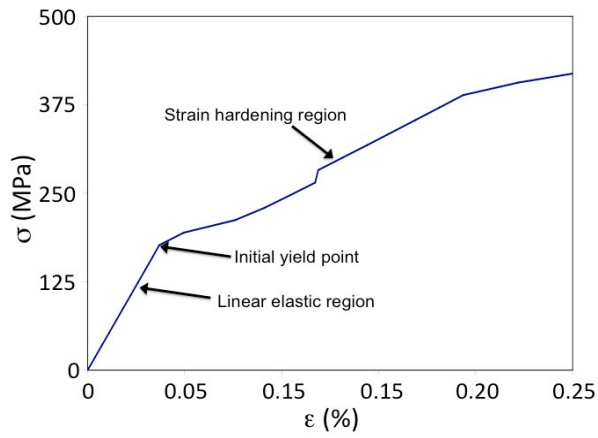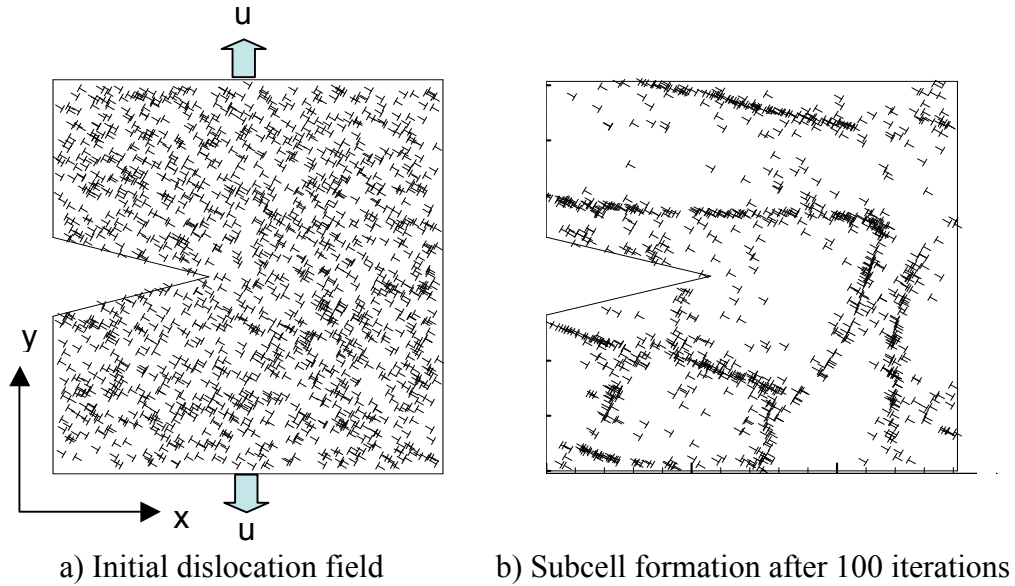
c) Resulting material behavior

Figure 6. Simulation using the two-dimensional DD-SIM code for a wedge
configuration under normal tension loading in the *y*-direction.

The results of a ParaDiS simulation of the evolution of dislocations in a cubic domain
with side dimension of 9.174 μm that is loaded at a uniaxial strain rate of 100 sec^{-1} are
shown in Figure 7. An arbitrary initial configuration of straight dislocations was assumed
to have been generated during the initial processing of the material and is depicted in
Figure 7a. Figure 7b presents the configuration of the system after approximately 3.8 x
10^{-8} sec of simulation wherein dislocation generation together with bending and folding
of the dislocation segments have occurred. These processes continue to evolve the
system of defects at the micron scale that, when averaged over the entire material

domain, are the basis for the overall stress-strain behavior and plastic yielding characteristics of the microstructure.
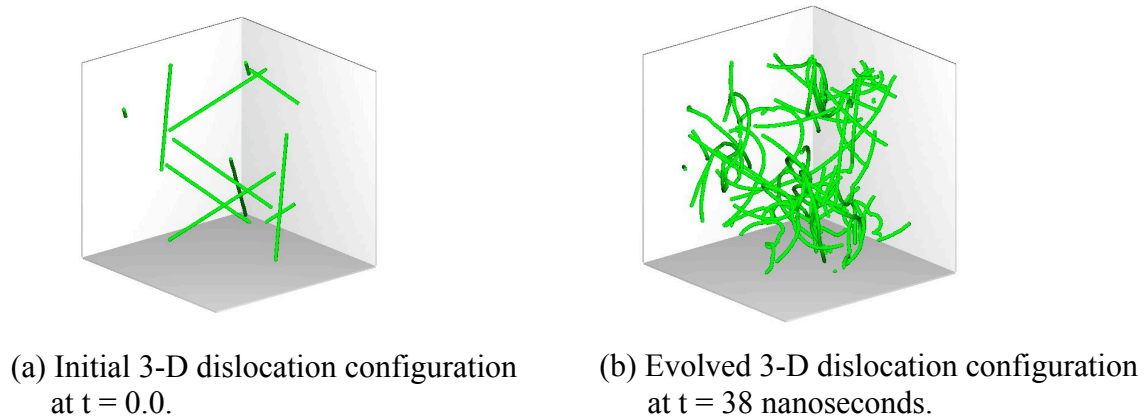

(a) Initial 3-D dislocation configuration at t = 0.0.

(b) Evolved 3-D dislocation configuration at t = 38 nanoseconds.

Figure 7. Dislocation evolution during dislocation dynamics simulation.

Modeling Near-Crack-Tip Plasticity at the Micro Scale

Both statistically stored dislocations and geometrically necessary dislocations are explicitly considered in molecular dynamics and dislocation dynamics models; however, neither is explicitly considered within conventional crystal plasticity (CCP) formulations. Rather, the effect of these dislocations is implicitly considered in the form of various rules that describe plastic slip. CCP formulations, like all constitutive models in continuum mechanics, 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. To make the calibration process tractable, a simple uniaxial tensile configuration is typically assumed. However, since no gradients of strain are imposed on the polycrystal scale, the resulting calibration is largely a result of plastic deformation caused by SSDs and not GNDs. Because the GNDs are not considered, the resulting formulation cannot account for large deformation gradients. The length-scale dependent effect of GND exclusion within conventional crystal plasticity formulations is overviewed by Hutchinson wherein the issue of underestimated work-hardening during plastic deformation within a strain gradient

dominated field is discussed (Hutchinson, 2000).

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 at small length scales 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 a given material, there may be several mechanisms and physical features that determine a characteristic length scale. During plastic deformation, length scales that are related to dislocation structures, such as typical distances between dislocations and sizes of dislocation cells, are believed to be of greatest importance. However, irrespective of the physical feature to be considered, the number of dislocations within a typical representative volume element must be sufficiently large such that meaningful averages over the dislocations can be taken, thus establishing an absolute lower bound on an effective length scale. In addition to providing a more accurate model for work hardening, strain gradient plasticity models are closely related to and calibrated by the results of dislocation dynamics simulations, thereby providing a more natural tie to inelastic deformation processes at lower-length scales.

While numerous SGP theories of continuum plasticity have been developed, work to incorporate length scale effects within crystal plasticity formulations is limited. Similarly, although CCP formulations do not accurately capture some aspects of plastic deformation at and below the micron scale, they are commonly employed to study material state fields near a crack within a microstructure. The common justification is

that meaningful results can still be gained provided that the limitations of CCP models are considered.

CCP constitutive 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. Some recent notable studies include Flouriot, 2003; Manonukul, 2004; Dunne, 2007; Arakere, 2009. Among these references, Flouriot, et al. generated three-dimensional finite element models of single crystal Compact Tension specimens of a nickel-based superalloy and validated simulated fields with experimentally observed deformation modes. They concluded that the computed deformation compared well with the experiment outside of a core region directly surrounding the crack front where intense discrete slip lines were not captured in the finite element modeling. Manonukul, et al. generated a two-dimensional finite element model of a nickel-based polycrystalline alloy and computed accumulated slip. A simple critical accumulated slip rule was found to correspond with the Coffin-Manson relationship in low cycle fatigue and the Basquin relationship for high cycle fatigue. Dunne, et al. replicated the microstructure of a nickel-based alloy with prismatic grains using finite element models. The locations where nucleation was observed to occur corresponded to locations where highly localized slip was predicted from the finite element model. It was also shown that, even in a two-dimensional analysis, the slip localization direction was accurately simulated. Arakere, et al. generated three-dimensional models of a single crystal nickel-based alloy modeled as an elastic anisotropic material and showed that, even with this simplified model for crystal response, the dominant slip systems within zones near the crack front could be predicted.

Similar to the studies of nickel-based alloys, detailed three-dimensional finite element models of aluminum 7075-T651 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 8 and 9 illustrate the computed slip localization near two different cracked constituent particles in aluminum 7075-T651 denoted P50 and P135.

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 8, P50, was observed to nucleate a crack into the surrounding grains, while the particle in Figure 9, P135, did not. It appears that slip localization and accumulation plays a governing role in crack nucleation at this scale; see Hochhalter, 2010 for further discussion. Figures 8 and 9 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 8. This observation leads to two possible hypotheses, that crack trajectories are based on alternating shear or on local maximum tangential stress. More simulations are currently underway to investigate these hypotheses.
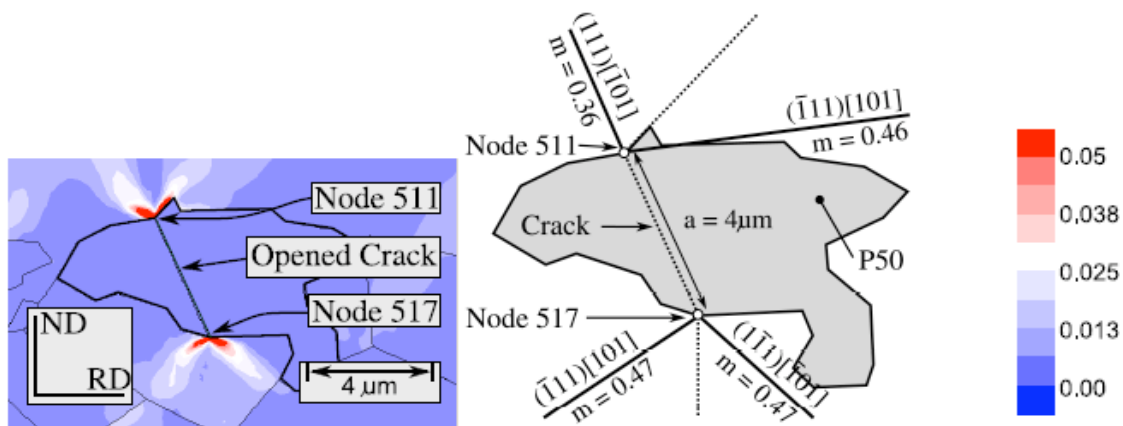

Figure 8. Computed slip fields near a cracked constituent particle that was observed to nucleate a crack into the surrounding grains.
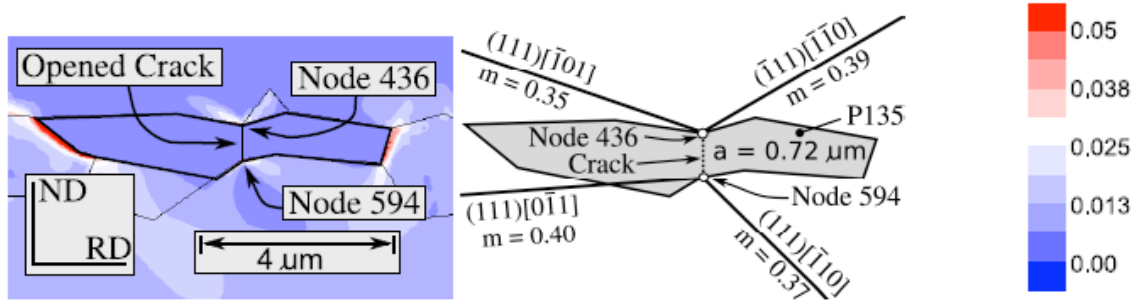
Figure 9. Computed slip fields near a cracked constituent particle that was observed notto nucleate a crack into the surrounding grains.

Modeling Near-Crack-Tip Plasticity Across Length Scales

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 small numbers of 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 methods for modeling plasticity is not seen when the methods are implemented individually, but rather, when the methods are integrated. 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. While the view elucidated by this paradigm is somewhat futuristic, the initial stages of the work are currently being undertaken.

Summary

The results of efforts that are aimed at understanding the plastic deformation mechanisms related to crack propagation at the nano-, meso- and micro-length scales has been discussed including atomistic simulation, discrete dislocation plasticity, strain gradient plasticity and crystal plasticity. Recent advances in nanoscale atomistic simulation include determination of the influence of crystallographic orientation on the crack tip plastic deformation modes during transgranular fracture. This work also revealed the existence of a transition stress intensity, K_{IT}, below which the crack emits full dislocations and above which deformation twinning becomes dominant. However, as discussed in the paper, there are issues relating to strain rate that could potentially influence the simulation of dislocation nucleation. Recent advances in mesoscale discrete dislocation plasticity simulation showed the formation of subcell dislocation structures near a notch in an aluminum plate. These internal structures are related to the material plastic response and, due to constraints on dislocation mobility, result in hardening or increased toughness of the material. Finally, recent advances in microscale crystal plasticity showed the role of slip localization and accumulation on crack nucleation.

Through these and many similar efforts, the mechanics of materials community has embarked on a bold paradigm shift that will lead a to transition from the traditional empirical and heuristic qualitative methods that have been used to predict plastic deformation and fracture to integrated physics-based quantitative methods that will allow numerical experiments to drive the development of continuum fracture parameters and guide materials processing. Many early steps have been taken to develop useful techniques for modeling materials over a broad range of length scales. This paper has illustrated aspects of a multiscale hierarchy of material models spanning nanoscale MD,

mesoscale DD, and microscale CCP and SGP approaches that may ultimately constitute components of an enhanced mechanistic approach to predict material behavior.

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