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AIAA 2002-1315

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**43rd AIAA/ASME/ASCE/AHS/ASC
Structures, Structural Dynamics,
and Materials Conference
April 22-25, 2002/Denver, CO**

MICROMECHANICS MODELING OF FRACTURE IN NANOCRYSTALLINE METALS

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Abstract

Nanocrystalline metals have very high theoretical strength, but suffer from a lack of ductility and toughness. Therefore, it is critical to understand the mechanisms of deformation and fracture of these materials before their full potential can be achieved. Because classical fracture mechanics is based on the comparison of computed fracture parameters, such as stress intensity factors, to their empirically determined critical values, it does not adequately describe the fundamental physics of fracture required to predict the behavior of nanocrystalline metals. Thus, micromechanics-based techniques must be considered to quantify the physical processes of deformation and fracture within nanocrystalline metals. This paper discusses fundamental physics-based modeling strategies that may be useful for the prediction of deformation, crack formation and crack growth within nanocrystalline metals.

Introduction

Fracture processes in materials such as nanocrystalline metals (see Figure 1¹), layered metals and powder metallurgy-formed materials cannot be modeled by traditional fracture mechanics-based concepts. While these materials often exhibit high strength, they also tend to have low ductility and low fracture toughness. Low ductility and toughness is a result of the nano-scale structure; here, Hall-Petch behavior is no longer valid when the structural size approaches the size of dislocations, thus disabling the mechanisms that produce ductility and toughness.² Therefore, it is critical to understand the mechanisms of deformation and fracture of these materials before their full potential can be achieved.³ This requires a new understanding at the micromechanics level. This paper discusses fundamental physics-based modeling strategies that may be useful for the prediction of deformation, crack formation and crack growth within nanocrystalline metals.

Classical Approaches

Fracture of standard engineering metals containing micro-sized structure is thought of in terms of brittle and ductile fracture. Brittle metals usually have either body-centered cubic (BCC) or hexagonal close packed (HCP) atomic structure whereas ductile metals have face-centered cubic (FCC) atomic structure. In BCC and HCP metals, there are few planes for dislocation movement allowing for little plastic deformation. In FCC metals, there are many planes for dislocation movement and hence they can undergo significant plastic deformation. Figure 2 shows these three types of atomistic structures.

In general, high strength materials often exhibit brittle fracture and low toughness whereas low strength materials exhibit ductile fracture and high toughness. Current fracture models employ classical fracture mechanics. Classical fracture mechanics is based on the premise that brittle fracture (in plane strain) will occur when $K_I > K_{IC}$, i.e. when the computed value of the stress intensity factor, K_I , is greater than or equal to the fracture toughness, K_{IC} . In classical fracture mechanics, fracture toughness is considered to be a property of the material, and the plane strain fracture toughness, K_{IC} , is the lowest value of material toughness.

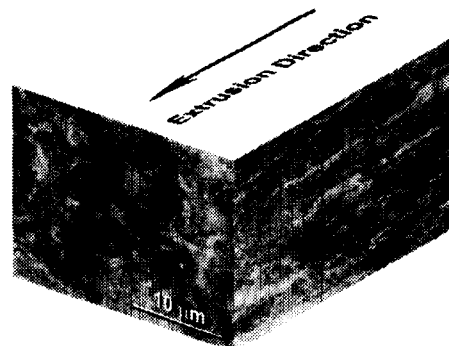


Figure 1. A 3D View of Microstructure of Extruded Al-Ti-Cu bulk Nanocrystalline Metal. (TEM Images)¹

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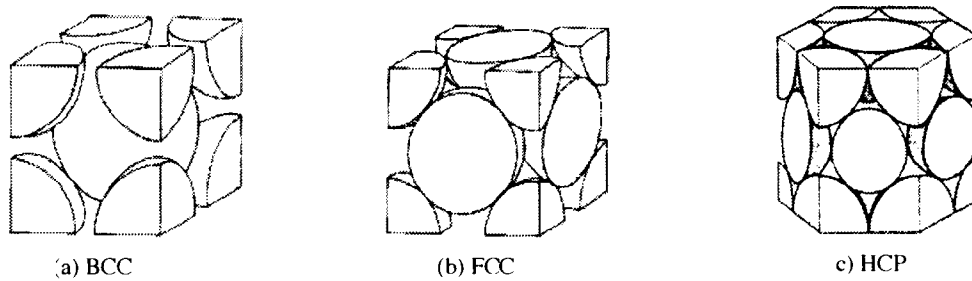


Figure 2. Three Atomic Structures Found in Typical Metals.

The relationship between the characteristic behavior of standard engineering materials and the types of fracture criteria that are applicable for these materials is shown in Figure 3.⁴ In this figure, LEFM denotes linear elastic fracture mechanics. The CTOD and CTOA are critical crack tip opening displacement and angle, respectively, and K - R and J - R curves are crack growth resistance curves based on K and the J -integral, respectively. The critical J -integral, J_{IC} , is yet another fracture criterion. In Figure 3, fracture behavior is captured in terms of empirical parameters (K_{IC} , J - R curves, CTOA, etc.) that are devoid of physics-based understanding. For example, plane strain fracture toughness (K_{IC}) is an empirical quantity that is only applicable to linear elastic fracture in thick materials.

Such empirical concepts used in classical fracture mechanics are not physics-based and do not capture the fundamental mechanisms associated with crack growth. For example, in many medium and low strength materials under plane stress, methods such as crack tip opening displacement (CTOD) or crack

tip opening angle (CTOA) are often used and tend to be associated with empirically determined length scales resulting in two-parameter criteria for crack growth. Additionally, energy-based methods such as the J -integral are unable to separate the relative contributions of the energy driving plastic deformation and the energy spent on the creation of new crack surfaces to the perceived crack growth resistance in ductile materials.

Computational Strategies

Because classical fracture mechanics is based on the comparison of computed fracture parameters (such as the stress intensity factor) to their empirically determined critical values, the concept does not adequately describe the fundamental physics of fracture required to predict the behavior of nanocrystalline metals. In a large part, classically formulated fracture mechanics (and classical continuum mechanics as a whole) is unsuitable for the prediction of deformation and fracture of nanocrystalline metals because it does not account for

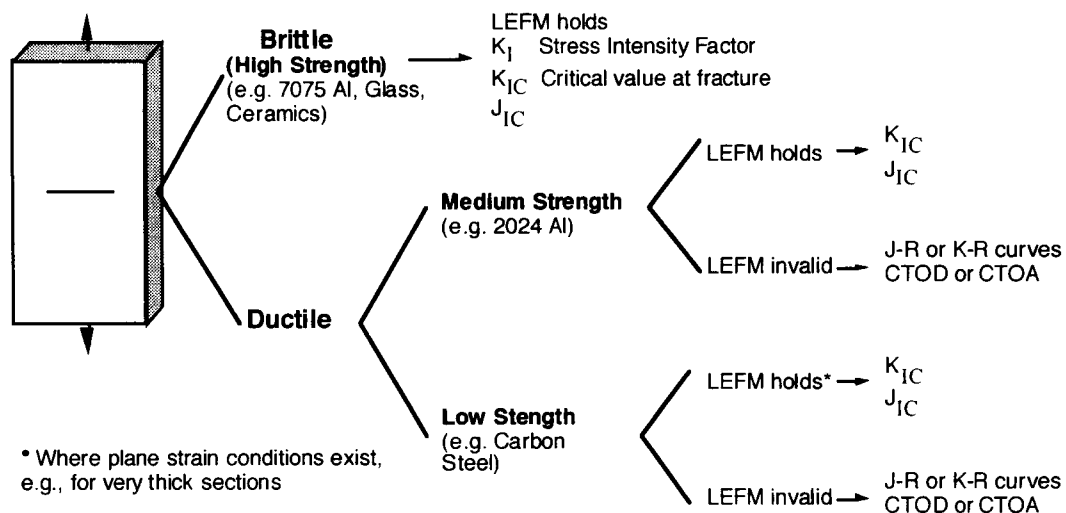


Figure 3. Relationship Between Material Behavior and Suitable Fracture Mechanics Analysis.

Table 1. Characteristic Scaling Lengths and Associated Simulation Method⁵

Length Scale, m	Upper Bound	Lower Bound	Simulation Method
10^0 - 10^{-3}	External load	Critical structural regions	Finite elements, finite difference
10^0 - 10^{-7}	External load	Grain size, dislocation cell size, crack size particle size	Microstructure mechanics Cohesive zone models
10^0 - 10^{-7}	External load	Grain shape	Variants of plasticity theory
10^0 - 10^{-9}	System size	Atomic clusters	Cellular automata
10^{-4} - 10^{-9}	Grain clusters	Burgers vector, annihilation spacing	Dislocation dynamics
10^{-6} - 10^{-10}	Cell size	Atom	Molecular dynamics
10^{-8} - 10^{-12}	Atom clusters	Ion, Electron	Ab initio molecular dynamics

the length-scale dependencies that tend to dominate the behavior of these materials. That is, the details of microstructural and nanostructural features are not considered. Table 1, adapted from reference 5, presents bounds on the domain of application for typical simulation methods over a broad range of length scales.

This paper discusses three of the physics-based analysis approaches shown in Table 1 to predict deformation, crack formation and crack growth in metallic materials. These approaches are molecular dynamics analysis⁶, cohesive zone models⁷ and variants of plasticity theory⁵. To varying degrees, these approaches have the ability to model aspects of the material architecture and their effects on fracture behavior while classically formulated fracture mechanics cannot model these aspects. These three computational methods will be discussed next followed by a brief discussion of their effects on the emerging field of computational materials.

Molecular Dynamics Analysis

Gaining accurate understanding of the mechanisms of fracture at a crack tip requires modeling at the atomistic level. Quantum mechanical solutions for the interaction among atoms rapidly become

intractable as the number of atoms considered increases, therefore, approximations to these interactions have been developed in the form of empirical and semi-empirical potentials describing the potential energy of the interactions among the atoms.⁶ Among the best known of the relationships for non-bonding potentials is the Lennard-Jones potential, Φ ,

$$\Phi = 4\varepsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^6 \right] \quad (1)$$

where ε is the depth of the energy well, σ is the van der Waals radius and r_{ij} is the separation distance between the i^{th} and j^{th} atoms in a pair. The r_{ij}^{-6} term represents the attractive contribution to the van der Waals forces between neutral molecules. The other component of the van der Waals interactions mimics the Coloumb interaction of the nuclei and the Pauli repulsion between overlapping electron clouds and is modeled by the short ranged r_{ij}^{-12} term.⁶

The Lennard-Jones potential was originally developed and is most accurate for interactions among atoms of noble gasses.⁸ However, it has been used for a broad variety of gasses, liquids and solids. Great care is needed in the selection of these potentials and further

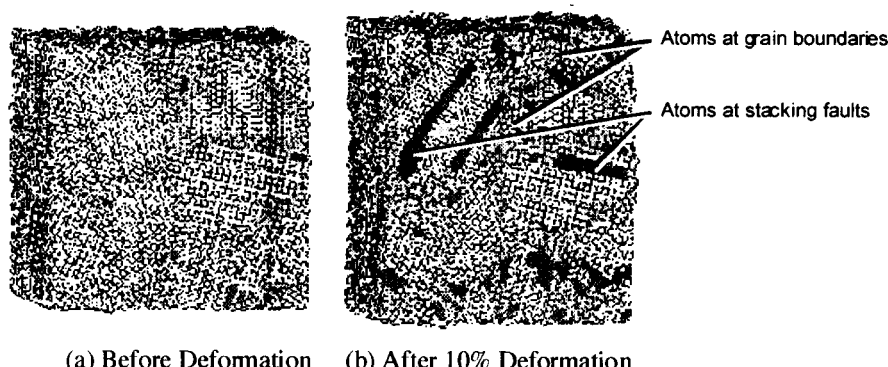


Figure 4. Nanocrystalline Copper Sample Containing 100,000 Atoms.⁹

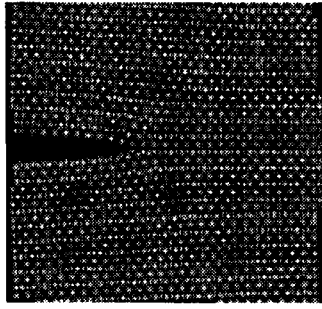


Figure 5. Fracture Along the Primary Cleavage {110} Planes of NiAl.¹⁰

work is needed in developing accurate potential energy functions for specific types of atomic interactions. Once developed, the interatomic potentials can be used in molecular dynamics (MD) simulations of deformation and fracture.

Molecular dynamics analysis mimics elementary atomistic path-dependent processes by solving the equations of motion for all atoms in the domain.⁶ MD simulations have yielded results such as the prediction of the deformation of nanocrystalline copper as shown in Figure 4. In this figure, stacking faults left behind by partial dislocations that have run through the grains during the deformation processes are clearly seen.⁹ As another example, fracture along the primary cleavage {110} planes of NiAl is shown in Figure 5.¹⁰

Atomistic simulations containing several hundred million atoms are possible, however this number of atoms corresponds to a cube of less than 1000 atoms on each side. One thousand atoms of titanium span approximately 400 nm. Thus, it is readily apparent that an atomistic approach is not practical for determining deformation and fracture in the vast

majority of materials. One exception involves certain classes of nanocrystalline materials wherein the characteristic length scales are very small. Typical grain diameters in nanocrystalline metals range from 5 to 50 nanometers.⁹ To resolve the issue of length scale in most other metals and larger domain problems in nanocrystalline materials, a multiscale modeling strategy has been proposed. The multiscale modeling strategy uses molecular dynamics models to provide constitutive input into cohesive zone relationships that can be embedded along regions of separation within finite element models of the grain structures.

Cohesive Zone Models

Cohesive zone models assume cohesive interactions among the grains of a material and permit the appearance of fracture surfaces in the continuum.⁶ One of the popular cohesive zone models is attributed to Tvergaard and Hutchinson,¹¹ where the normal and shear components of the traction and displacement are combined into single measures, t and λ , respectively, so that the responses are coupled.¹² The coupled cohesive zone model (CCZM) given in reference 12 defines a traction potential, Φ

$$\Phi(\delta_n, \delta_t) = \delta_n^c \int_{\lambda} t(\lambda') d\lambda' \quad (2)$$

where λ is a nondimensional measure of the relative normal (δ_n) and tangential (δ_t) displacements as defined by

$$\lambda = \left[\left(\frac{\delta_n}{\delta_n^c} \right)^2 + \left(\frac{\delta_t}{\delta_t^c} \right)^2 \right]^{1/2} \quad (3)$$

where δ_n^c and δ_t^c are the critical values for the normal and tangential modes, respectively, and the initiation of a crack is assumed to occur when λ reaches a value

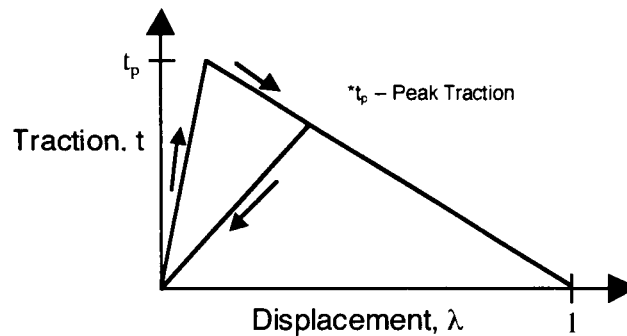


Figure 6. Traction-Displacement Relationship in CCZM.¹¹

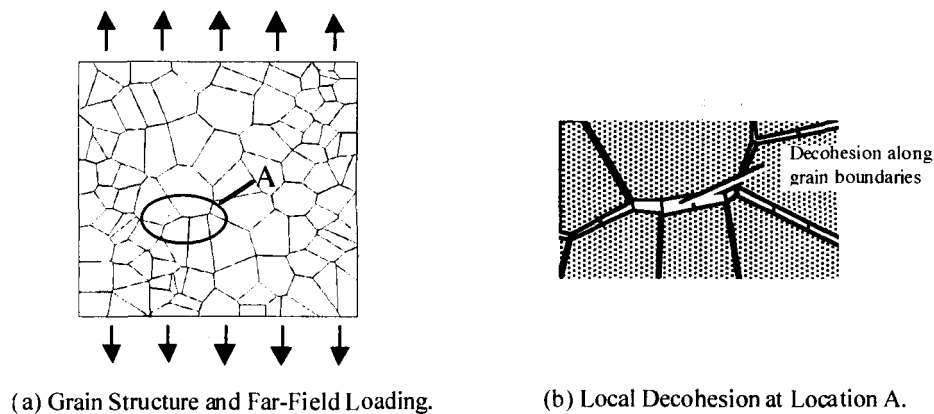


Figure 7. Decohesion Among Grain Boundaries of a Crystalline Metal.¹²

of unity. A graphical representation of the CCZM is shown in Figure 6.

Grain boundaries in metals exist because of incoherence in the atomic lattice. Decohesion may occur between the atoms within an individual grain (intragranular) or along the boundaries between the grains (intergranular). Currently, most analyses that implement cohesive zone models consider only the intergranular failure problem. Figure 7 shows results that are typical of a finite element calculation that uses cohesive zone models to predict separation between the grains.¹² Figure 7(a) is a representation of the grain structure, and Figure 7(b) is a detail of the decohesion among the grains at location A. While the results in reference 12 use heuristically derived relationships to define the coupled cohesive zone model, the CCZM can also be developed from results of molecular dynamics analyses allowing the physical insight of the MD analysis to be embedded in the more computationally efficient finite element models.

Variants of Plasticity Theory

Because of the complexities involved in developing meaningful representations of atomistic or grain configurations and the computational power required to solve the resulting systems of equations, approaches allowing for homogenization of the domains of interest may facilitate study of the deformation and fracture problems. One such top-down approach is to use models based on variants of plasticity theory. Among these approaches are polycrystalline plasticity, strain gradient plasticity and discrete dislocation plasticity.

Polycrystalline plasticity replaces the microstructure of the material by an appropriate constitutive description and can, to some extent, account for the

heterogeneous character of crystalline microstructure.⁵ For example, polycrystalline plasticity models have been used to examine strain localization at triple points and grain boundaries.¹³ Compared with standard continuum plasticity models, the predictions of the polycrystalline plasticity-based analyses show a more heterogeneous and physically realistic strain field. Recently, crystalline plasticity has been extended to a more general theory based on classical crystalline kinematics; classical macroforces; microforces for each slip system consistent with a microforce balance; a mechanical version of the Second Law of Thermodynamics that includes, via the microforces, work performed during slip; and a rate-independent constitutive theory that includes dependencies on plastic strain gradients.¹⁴

Based on the general framework of Cosserat couple stress theory, strain gradient plasticity allows for the inclusion of a single material length scale, l , and reduces to the conventional J_2 plasticity theory when geometric length scales are large compared with l .^{15, 16} The technique has been used to show strain, curvature and strength dependencies of materials containing rigid particles on the prescribed radius of the particles. For materials with a strain hardening index between 1 and 10, strength was shown to increase by values of between approximately 6 and 8 when the ratio of material length scale to particle size increased from 0 to 1.

Another variant on plasticity theory is discrete dislocation plasticity.¹⁷ In discrete dislocation plasticity, dislocations are treated as line singularities in an elastic solid. The formulation consists of two parts: a many body interaction problem involving the discrete dislocations and a fairly conventional solid mechanics boundary value problem. The long-range interactions between dislocations are accounted for using the continuum elasticity fields, while the short-

range interactions are incorporated through a set of constitutive rules. The technique has been used to predict the local deformations including localization of plastic flow within small ($48\mu\text{m}^2$) blocks of material under tension and bending and may be a useful intermediary between atomistic and continuum formulations.¹⁷

Computational Materials

Over the centuries, the materials processing community has taken an Edisonian approach to materials processing. This Edisonian paradigm is archaic and needs to be replaced. Simultaneously, the mechanics of materials community has developed analytical approaches based on empirically determined parameters such as modulus of elasticity, strength and toughness. These empirical parameters offer limited insight into the internal mechanisms from which they arise. Approaches such as the ones outlined in this paper have the potential to revolutionize mechanics of materials and couple it to materials processing allowing material microstructures to be designed and processing parameters to be determined before physical processing.

The work being undertaken to address the closely interwoven goals of developing techniques to predict the effects of processing parameters on microstructure evolution and to determine the effects of material microstructure on properties will lead to true computationally-designed materials. Materials that can be computationally designed at the microstructural level, can sense microstructural damage and repair themselves to retard development of macroscopic cracks and have redundant internal load-paths that can circumvent damage once it does form appear to be possible.

Concluding Remarks

Several analyses that may contribute to the understanding of deformation and fracture in materials such as nanocrystalline metals, layered metals and powder metallurgy-formed materials have been briefly described. These methods include molecular dynamics analysis, cohesive zone models and several variants on plasticity theory including polycrystalline plasticity and discrete dislocation plasticity.

Each of these methods has unique strengths and weaknesses. For example, the molecular dynamics analysis provides considerable insight into the mechanisms of dislocation formation and the details of fracture at a crack tip but because of limitations in computing power, it is not suited for solutions of

systems exceeding a few hundred million atoms. In contrast, the cohesive zone models are suited for larger domains including modeling decohesion along individual grain boundaries, but do so with a loss of detail near the crack tip. Plasticity-based models tend to be even more homogenized, but lend themselves to modeling larger domains.

The real power of these techniques is not seen when the methods are implemented individually, but rather, when the methods are combined. For example, molecular dynamics solutions can be used as the basis for discrete dislocation plasticity models of deformation and as the foundation for cohesive zone relationships used in polycrystalline models of crack initiation.

Through these efforts, the mechanics of materials and materials processing communities have embarked on a bold paradigm shift that will lead a transition from the traditional separate, empirical and heuristic qualitative methods that have existed for centuries to integrated physics-based quantitative methods that will allow numerical experiments to drive materials processing. Many early steps have been taken to develop useful techniques for modeling materials over a broad range of length scales. Some of them have been outlined in this paper.

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