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A computational study of the mechanical behavior of nanocrystalline fcc metals

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Abstract

We have conducted a finite-element-based study of the deformation and failure behavior of nanocrystalline face-centered cubic metals. A rate-dependent amorphous plasticity model which accounts for cavitation and related failure phenomena is used to model the grain boundaries, while a crystal plasticity model is used for the grain-interiors. Our numerical simulations using material parameters estimated to represent the macroscopic rate-dependent stress–strain response of nanocrystalline nickel (nc-Ni), show that there is a transition in deformation mechanism from grain-interior shearing to grain-boundary shearing, as the average grain-size decreases from 50 nm to 10 nm, and that the low ductility of nc-Ni is the result of intergranular failure due to grain-boundary shearing and resulting cavitation at triple-junctions and other high stress points in the microstructure. Our numerical simulations also show that the strength of nc-Ni is expected to be slightly higher in compression than in tension, primarily due to the easier operation of cavitation failure of the grain boundaries in tension.
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1. Introduction

Nanocrystalline metals are polycrystalline metallic materials with grain sizes typically less than 100 nm. These materials have been the subject of intense, worldwide research over the past two decades, and due to this research activity the micromechanisms governing their macroscopic mechanical behavior are now beginning to be better understood (e.g. [1,2]). Recent reviews on the topic, and references to the vast amount of literature, may be found in Kumar et al. [3] and Wolf et al. [4]. Nanocrystalline metals contain a high volume fraction of ''grain-boundary''-intercrystalline regions. For example, idealizing a unit cell containing a crystalline grain interior and an intercrystalline grain-boundary region as a sphere of diameter d, with an intercrystalline shell of thickness δ and a crystalline core of diameter $d - 2\delta$, the volume fractions of grain-boundary regions for a fixed value of $\delta \sim 0.5$ nm, and grain sizes d of 10 nm and 40 nm are 27.1% and 7.3%, respectively. Thus, a substantial fraction of the atoms in nanocrystalline materials lie in the intercrystalline grain-boundary regions, and these regions play an increasingly significant role as the grain size decreases below the 100 nm level. The nature of the intercrystalline grain-boundary regions depends on how the material has been processed. High-resolution transmission electron microscopy (TEM) studies on nanocrystalline materials show that while many grain boundaries appear sharp and well-defined, others show considerable disorder, with the maximum disordered region (measured perpendicular to grain boundaries) being approximately 2–3 lattice spacings; i.e., less than 1 nm [5].

In this paper we focus our attention on continuum-level modeling of the low temperature mechanical response of nanocrystalline fcc metals. A broad picture of the operative

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micromechanisms of inelastic deformation in this class of materials in this temperature range is beginning to emerge. The following features of the operative micromechanisms are now reasonably widely-accepted [1–4,6–8]:

- There is a strong interplay between dislocation-based deformation in the crystalline grain interiors and the inelastic deformation mechanisms operative in the grain-boundary regions.
- Grain boundaries act as both sources and sinks for dislocations.
- Let Γ denote the stacking fault energy of the face-centered cubic (fcc) material, G its nominal shear modulus, and b the magnitude of the Burgers vector of a perfect dislocation, then there exists a critical grain size d_c, given by $d_c \approx (2/3)(Gb^2/\Gamma)$, above which plastic deformation in nanocrystalline grain interiors occurs by the emission of complete dislocations from grain boundaries, and below which the plastic deformation occurs by emission of partial dislocations. The partial dislocations produce stacking faults as they glide through the grains [9,10].
- The number of dislocations or stacking faults that need to traverse a typical grain in the nanocrystalline range to produce an overall strain of the order of 5% is quite small, typically less than 10–15. Thus, dislocation based plasticity in the grain interiors is quite discrete in nature.
- When the grain size d becomes smaller than d_c, dislocation-based slip processes become less effective in producing overall inelastic deformation, and grain-boundary-region-based inelastic deformation mechanisms start to dominate [11–13].
- The grain-boundary inelastic deformation mechanisms are loosely called "grain-boundary sliding", but at low temperatures atomistic simulations show this to be stress-activated shear-shuffling of atoms located in the intercrystalline regions, and the cooperative result of numerous such shear-shuffles leads to substantial overall shearing of the intercrystalline regions; this process is not dominated by thermal diffusion of atoms in the grain-boundary regions. Such a deformation mechanism is reminiscent of that in metallic glasses, where inelastic deformation occurs by local shearing of clusters of atoms – "shear transformation zones" [14].
- Nanocrystalline fcc materials show a room-temperature strain-rate sensitivity which is almost an order of magnitude higher than their microcrystalline counterparts. The mechanism underlying this enhanced strain-rate sensitivity is not fully understood at present, but is probably due to the enhanced strain rate sensitivity of the intercrystalline grain-boundary regions, relative to the rate sensitivity of the crystalline grain-interiors.
- The ductility of these materials, as measured by elongation in tensile experiments, is significantly reduced from the values observed for their microcrystalline counterparts, and seldom exceeds 5%. Since this occurs even for materials at the high end of grain sizes in the nanocrystalline range (~100 nm), one can infer that even though there is some accommodation of the overall imposed deformation by dislocation-mediated plasticity in the grain interiors, this accommodation is insufficient. Additional, intergranular accommodation mechanisms, such as cavitation and microcracking, must be operative. It must be noted that while widespread distributed grain-boundary damage prior to final macroscopic fracture has not been experimentally observed, atomistic simulations do show void formation and decohesion leading to intergranular fracture in nanocrystalline materials [6–8].

As reviewed in [3,4], much of the understanding of the micromechanisms operative during the inelastic deformation of nanocrystalline materials has been obtained from large-scale molecular dynamics (MD) studies published in the past few years. Although MD methods of studying atomic-level mechanical response of materials are useful for gaining valuable insight, these methods are at present not suitable for carrying out simulations of deformation and failure under conditions similar to those under which physical experiments on nanocrystalline materials are carried out, i.e., macroscopic-sized specimens with complicated boundary conditions, involving realistic strain rates. MD simulations are inherently limited to small, idealized microstructures and extremely high strain rates, typically $>10^7$/s, which corresponds to a strain of 1% in 1 ns.

In contrast to MD methods, finite-element methods (FEM) for simulation of micromechanical interactions and prediction of local as well as overall response of materials have been effectively used to study the mechanical response of variety of composite material systems in recent years, and such methods do not possess the major limitations of the MD methods listed above. However, use of continuum-mechanical-based FEM methods is contingent upon the assumptions of continuum mechanics – suitable smoothness of displacement fields, the notion of stress, and balance laws of linear and angular momentum – continuing to hold at the nanoscale. Further, just as the results from MD simulations depend crucially on the reliability of the interatomic potentials used in such studies, the results of FEM simulations depend crucially on the reliability of the continuum-level constitutive equations used in such analyses. While the concepts of continuum elasticity are expected to be approximately applicable at small scales approaching the nano-level, the concepts of classical continuum plasticity being applicable at this scale are highly questionable. Nevertheless, based on a pragmatic engineering approach, and bolstered by the success of (length-scale-independent) crystal-plasticity theories and attendant FEM simulation methodologies to represent grain-scale shear localization phenomena and texture evolution (cf., e.g. [15]), a few investigators have recently carried out continuum-level FEM simulations of the inelastic deformation and failure response of nanocrystalline materials (cf., e.g. [17,18]). Although

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