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Crack growth versus blunting in nanocrystalline metals with extremely small grain size

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ABSTRACT

Fracture of nanocrystalline metals with extremely small grain size is simulated in this paper by structural evolution. Two-dimensional scheme is formulated to study the competition between crack growth and blunting in nanocrystalline samples with edge cracks. The scheme couples the creep deformation induced by grain boundary (GB) mechanisms and the intergranular crack growth. The effects of material properties, initial configurations and applied loads are explored. Either the enhancement in diffusion mobility, or the deterrence in the grain boundary damage, would blunt the crack and decelerate its growth, and vice versa. The simulations agree with the analytical predictions as modified from that of Yang and Yang [2008. Brittle versus ductile transition of nanocrystalline metal. Int. J. Solids Struct. 45, 3897–3907]. Upon the suppression of dislocation activities, it is validated that the brittle versus ductile transition of nanocrystals is controlled by the development of grain boundary-dominated creep versus grain boundary decohesion. Further simulations found that either decreasing the grain sizes or increasing the dispersion of grain sizes would blunt the growing cracks.

1. Introduction

In the search of unusual mechanical behavior, nanocrystalline metals have been widely studied (Gleiter, 1989; Meyers et al., 2006). Experiments such as nano-indentation, uniaxial tension and rolling were carried out. Some of the available data (Karch et al., 1987; Sanders et al., 1997; Koch et al., 1999) indicated that nanocrystalline metals appeared to have toughness and ductility lower than their coarse-grained counterparts. Different explanations were offered. Several authors (Koch et al., 1999; Hugo et al., 2003) attributed the lower ductility of nanocrystalline metals to the porosities and impurities introduced during the sample processing, since the high-purity nanocrystalline copper testing (Lu et al., 2000) demonstrated exceptional ductility; some (e.g. Zhang et al., 2002) regarded it as an inherent property of nanocrystalline materials; while others (e.g. Wang et al., 2002) emphasized the strain localization effect due to the lack of strain hardening of nanocrystals. To describe the brittle versus ductile transition via proper models, one has to understand the fracture behavior of nanocrystalline metals.

For metals with grain sizes below a critical level, theoretical analysis (Gryaznov, 1991) indicated that dislocations can hardly maintain stability in the grain interior, and the dislocation emissions cease to occur. Indeed dislocations were seldom observed in experiments when the grain size fell below, say, 10–15 nm (Meyers et al., 2006). Though traces of

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stacking faults indicating the passages of partial dislocations were observed (Liao et al., 2003), the contribution of dislocation activity to the deformation is rather minor (Kumar et al., 2003). Meanwhile, experiments (Ebrahimi et al., 1999; Conrad, 2004) indicated that the Hall–Petch relation of the size effect no longer held for the nanocrystalline metals. The reverse Hall–Petch relation was reported as the grain size shrunk to the range of 10 or 20 nm, and the maximum strength was believed to exist (Schiøtz et al., 1998; Schiøtz and Jacobsen, 2003). Several models (Zaichenko and Glezer, 1997; Conrad and Narayan, 2000) were proposed to explain the softening effects. The inapplicability of Hall–Petch relation could not be explained by the classical theory of dislocation-induced plasticity, but should rather be viewed as the manifestation of grain boundary (GB) mechanisms like GB sliding, GB diffusion and grain rotation. Lu et al. (2000) reported a stunning experiment result of rolling nanocrystalline Cu to 5100% elongation at room temperature. The grains kept equiaxed during the rolling, assembling the superplasticity simulation by Pan and Cocks (1993a). Yang and Wang (2004) and Wang and Yang (2004) incorporated the grain rotation to Ashby–Verrall mechanism (Ashby and Verrall, 1973) and proposed a grain-cooperated deformation model. The grain rotation mechanism was directly observed by experiments (Shan et al., 2004).

For conventional crystals, Rice and Thomson (1974) proposed that the brittle versus ductile transition is dictated by the competition between dislocation emission and cleavage. When the grain size is reduced to 10 or 20 nm, or the range of extremely small grains, the dislocation activity is suppressed. GB-induced mechanisms would dominate the fracture behavior due to the increasing volume percentage of grain boundaries and triple junctions. That leads to the following understandings:

1. In nanocrystalline metals, the grain interior is clean and devoid of dislocations, the grain boundary is sharp and straight. The grains are equiaxed and remain so during deformation. The deformation is dominated by the GB mechanisms such as GB sliding, GB diffusion and grain rotation.
2. Fracture of nanocrystalline metals proceeds intergranularly. The decohesion along the grain boundary is assisted by voiding at the triple junctions and nanocrack evolution along the grain boundaries.

Up to now, experimental data on the deformation and fracture behavior of nanocrystalline metals are still insufficient due to the lack of quality control in sample preparation, as well as to the difficulty in test control (Meyers et al., 2006). Due to the difficulty of preparing high-quality samples (Sanders et al., 1997; Agnew et al., 2000), reliable fracture data of nanocrystalline metals are inadequate to pinpoint the major mechanism of brittle versus ductile transition of nanocrystals. Since the fracture behavior involves different mechanisms, generally accepted theory has not yet been reached.

Computer simulations are widely used to investigate the deformation and fracture behavior of nanocrystalline metals. Molecular dynamics (MD) frequently serves for the purpose. As the grain size decreases, MD simulations (Schiøtz et al., 1998; Van Swygenhoven et al., 2001; Schiøtz and Jacobsen, 2003; Yamakov et al., 2004) suggest the transition from the dislocation-dominated mechanism to the GB-dominated one. The MD simulations of fracture in FCC and BCC nanocrystals (Farkas et al., 2002, 2005; Frederiksen et al., 2004) indicate that the crack growth proceeds along the grain boundaries, and the grain boundaries decohere by cavitations ahead of the crack, coinciding with the experiment of Kumar et al. (2003). Though furnishing information on the deformation and fracture of nanocrystals, the MD method has an intrinsic femto-second time step that makes the simulations of mass transport and grain rotation unfeasible.

Finite element method (FEM) is another way to simulate the deformation and fracture of nanocrystalline metals. One approach (Fu et al., 2004; Wei and Anand, 2004) treated the material as a composite of grain interior and grain boundary region, while another approach (Bower and Wininger, 2004; Wei and Gao, 2008; Wei et al., 2008) used sharp grain boundaries and considered effects of migration, diffusion and grain boundary slide. The latter approach couples the mechanisms in grain boundaries and grain interiors and possesses the capacity to model the deformation of metals with grain sizes from hundred nanometers to a few nanometers.

Yang and Yang (2008) proposed that the brittle versus ductile transition of nanocrystalline metals is dominated by two competing mechanisms: (1) GB-induced plastic deformation, which includes mass diffusion, GB sliding and grain rotation; and (2) grain boundary decohesion that includes grain boundary damage due to voids evolution. The first mechanism blunts the crack tip and relieves the stress concentration near the crack tip, while the second mechanism propagates the crack. The nanocrystals will show ductile properties if the first mechanism prevails or brittle properties if the second mechanism does.

The present paper intends to develop a computational scheme suitable for the study of the brittle versus ductile transition of nanocrystals to validate the above-mentioned proposal. Based on the formulations of structural evolution (Sun et al., 1994; Yang and Suo, 1996; Suo, 1997), Yang and Hong (2002) developed a computation scheme to simulate the deformation of nanocrystals. The method is capable of describing the structural evolution dominated by GB mechanisms. That approach is adopted here for the fracture of nanocrystals.

2. Model and computation scheme

To simulate the crack growth and blunting under GB-induced deformation and GB decohesion, one should devise a proper and efficient computation model that is capable of describing both mechanisms. Coupling between two mechanisms is assumed as weak based on the following considerations. (1) The grain boundary diffusion is driven by the