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Evolution of spherical nanovoids within copper polycrystals during plastic straining: Atomistic investigation

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ABSTRACT

The evolution, growth and coalescence, of nanovoids play a significant role in the plasticity of nanocrystalline metallic materials. Previous atomistic studies of void growth in face centered copper, and other metallic materials, have considered voids in single crystals, and those located at grain boundaries in polycrystals. The evolution of a spherical nanovoid in copper polycrystals under uniaxial tension is the focus of this atomistic investigation. In this paper, a critical stress based criterion is proposed for emission of dislocations from spherical void surfaces. The preference of dislocation source, GBs or spherical void surfaces, is determined by the relative magnitude of the critical stresses to emit dislocations from GBs or spherical void surfaces. The criterion reveals that there exists a grain size dependent critical void diameter at which the dislocation emission transits from GBs to spherical void surfaces as the spherical void grows. Simulation results show that, in intragranular voided models, the critical void diameter is 13 nm for simulation models with a 16.32 nm grain size and is 5.5 nm for simulation models with a 6.92 nm grain size. The critical void diameters revealed by simulations are in agreement with that obtained by the criterion. In addition, the simulation results indicate that the Gurson's model may be extended to predict the global yield conditions for simulation models with intragranular spherical voids. In the simulation models with intergranular voids, the spherical void continuously grows due to the initial dislocation emission from the intersections of GBs and spherical void surfaces.

1. Introduction

The ductile failure of metallic materials is generally considered to be controlled by the nucleation, growth and coalescence of nanovoids. Nanovoids extensively exist in experimental polycrystals. In experimental conditions, nanovoids can be generated in grain interior (intragranular nanovoids), deformation cells and at grain boundaries (GBs) (intergranular nanovoids) in nanocrystalline (nc) materials either during their synthesis process or in work conditions, such as inert-gas condensation, electrodeposition, radiation, quenching, serve plastic deformation (Van Petegem et al., 2003; Was, 2007;

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Zhou et al., 2009; Noell et al. 2017). The nucleation and evolution of nanovoids play an essential role in the plastic deformation behavior, mechanical properties and failure of these materials. For example, Meyers et al. (2006) report on the role of nano voids in the reduced tensile ductility of nanocrystalline materials. Molecular dynamics (MD) simulation results reported by Yang et al. (2007) demonstrate that the elastic moduli of spherical voided materials depend linearly on void volume fraction while the atomic stress concentration factor is dependent on void structural parameters. Nc materials with nanovoids exhibit a lot of different properties, such as lattice orientation sensitivity (Zhu et al., 2007; Zhao et al., 2009a, 2009b) and size-dependent yield stresses (Potirniche et al., 2006b; Traiviratana et al., 2008; Zhao et al., 2009b). In general, void growth rate is dependent on crystallographic orientation. The void growth rate is significantly higher in the [111] orientation than the other orientations at 1 and 3 stress triaxiality (Ling et al., 2016).

The evolution of nanovoids intimately relates to dislocation activities in their vicinity. Previous research works (Rudd et al., 2007; Rudd, 2009) show that the evolution of spherical voids could be initiated by anisotropic dislocation nucleation and emission. The results, presented by Tucker et al. (2013) at room temperature using MD simulations, show that GBs in aluminum nanowires can be preferred nucleation sites for dislocations to free surfaces. Similarly, dislocation loops are emitted from GBs and expand into the grain interiors to carry plastic strain (Cao et al., 2015). Alternatively, void surfaces are another dislocation nucleation site. Void surface is a specific free surface. Plastic deformation can be initiated by the nucleation of dislocations at the atomic steps of the void surfaces. Lubarda et al. (2004) propose two mechanisms to account for the emission of geometrically necessary dislocations (GNDs) from void surfaces, i.e. prismatic and shear loops. They also show a decrease in the critical stress of dislocation emission with increasing void diameters, and an easy emission of dislocations with a wider core width than a narrower one. Dislocation loops associated with the cylindrical void evolution are nucleated and emitted at void surfaces (Lubarda et al., 2004; Meyers et al., 2009; Traiviratana et al., 2008). Traiviratana et al. (2008) perform atomistic calculations on bicrystalline copper models with a cylindrical or spherical void embedded right at the GBs. Their results reveal that shear loops are emitted from void surfaces and the shear loops dominate void evolution. The shear loops are similar to the well-known mechanisms of GNDs. In single crystal fcc (Potirniche et al., 2006a, 2006b; Segurado and LLoraca, 2010; Traiviratana et al., 2008), bcc (Xu et al., 2011) or hcp (Tang et al., 2010) metallic materials with a spherical void, dislocations are emitted from void surfaces during yield due to lack of alternative nucleation sites. Osetsky and Bacon (2010) find that dislocations in iron have a dipole-like configuration at void surface before breaking away due to the strong inhibition of voids. The dislocations leave the void surfaces when the dipole is unzipped at a critical stress. MD simulations are performed by Zheng and Zhang (2007) to study the role of preexisting ellipsoidal voids in the tensile deformation behavior of nc copper. Their results show that the dislocations emitted from void tips may assist the formation of shear planes. Dislocations are not absolutely emitted from GBs or void surfaces. Dislocation emission may transit from GBs to void surfaces. In a recent MD simulation study, Simar et al. (2011) investigate the interaction between gliding dissociated edge dislocations and voids in nickel. A transitive void diameter of 2 nm is found. For void diameter larger than 2 nm, the dominant attraction between the dissociated dislocations and the voids causes a detachment process. In contrast, for the void diameter below 2 nm, repulsive stress between the partials dominates the detachment of the leading partial dislocations from the voids while the trailing partial dislocations remain pinned at voids. These results demonstrate that the transition depends on the void separation distance along the dislocation line and the dissociation distance of partial dislocations, i.e. the stacking fault energy.

The works on nanovoid evolution in nc metallic materials are critical for understanding and improving the mechanical properties of these materials. The influential factors for void evolution include strain rate, loading method, initial porosity, initial void shape, specimen size, lattice orientation, etc. The void growth rate does not depend on initial void radius (Chang et al., 2013). Ductile failure micromechanisms in nc Cu at high strain rates are investigated by Dongare et al. (2009) using MD simulations. The results indicate that void growth is facilitated by the creation of a shell of disordered atoms around the voids, and not by the dislocation nucleation from void surfaces. Potirniche et al. (2006b) argue that stress triaxiality dominates void growth and coalescence in fcc single crystals. Potirniche et al. (2006b) demonstrate that specimen size changes the dislocation pattern, the evolving void aspect ratio and the corresponding stress strain response. Crystallographic orientation also plays an important role in void growth. It influences both the evolution direction and shape of nanovoids in fcc single crystals (Liu et al., 2007). Segurado and LLoraca (2010) use discrete dislocation dynamics to analyze void evolution in an isolated fcc single crystal deformed in-plane strain in the (-110) plane. The results indicate that void growth rate is dependent on lattice orientation in uniaxial tension due to anisotropic stress state. However, Borg et al. (2008) find that the lattice orientation does not significantly influence void growth rate under high stress triaxiality conditions. Dongare et al. (2009) find that void coalescence occurs by the shear of the disordered regions between the voids at high strain rates. The evolution of nanovoids by themselves and/or their interactions with neighbors often leads to void coalescence or collapse that may result in crack formation (Zhang and Cui, 2009). In addition, supersaturation of vacancies leads to void evolution (Fischera and Svoboda, 2008).

Though many experiments and simulations have been performed to reveal the nucleation and growth of nanovoids in monocrystals, bicrystals and polycrystals in which voids are located at GBs (intergranular voids) (Traiviratana et al., 2008; Segurado and LLoraca, 2010; Bachurin and Gumbsch, 2014), very few studies consider the evolution of an intragranular spherical nanovoid with different sizes in polycrystals. The aim of our study is the origin of plasticity as well as the void evolution in nc copper containing a spherical void. The intersection of void surfaces with surrounding GBs (intergranular voids, voids located at GBs) would make it hard to identify the origin of plasticity, i.e. the preference of dislocation emission from GBs or void surfaces. If the spherical void is embedded at GBs (intergranular voids), it is impossible to determine the role

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