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Void growth in metals: Atomistic calculations

Sirirat Traiviratana [a], Eduardo M. Bringa [b], David J. Benson [a], Marc A. Meyers [a,c,*]

[a] Department of Mechanical and Aerospace Engineering, University of California, San Diego, La Jolla, CA 92093, USA
[b] Materials Science Department, Lawrence Livermore National Laboratory, Livermore, CA 94550, USA
[c] NanoEngineering, University of California, San Diego, La Jolla, CA 92093, USA

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Abstract

Molecular dynamics simulations in monocrystalline and bicrystalline copper were carried out with LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) to reveal void growth mechanisms. The specimens were subjected to tensile uniaxial strains; the results confirm that the emission of (shear) loops is the primary mechanism of void growth. It is observed that many of these shear loops develop along two slip planes (and not one, as previously thought), in a heretofore unidentified mechanism of cooperative growth. The emission of dislocations from voids is the first stage, and their reaction and interaction is the second stage. These loops, forming initially on different $\{1\,1\,1\}$ planes, join at the intersection, if the Burgers vector of the dislocations is parallel to the intersection of two $\{1\,1\,1\}$ planes: a $\langle 1\,1\,0\rangle$ direction. Thus, the two dislocations cancel at the intersection and a biplanar shear loop is formed. The expansion of the loops and their cross slip leads to the severely work-hardened region surrounding a growing void. Calculations were carried out on voids with different sizes, and a size dependence of the stress threshold to emit dislocations was obtained by MD, in disagreement with the Gurson model which is scale independent. This disagreement is most marked for the nanometer sized voids. The scale dependence of the stress required to grow voids is interpreted in terms of the decreasing availability of optimally oriented shear planes and increased stress required to nucleate shear loops as the void size is reduced. The growth of voids simulated by MD is compared with the Cocks–Ashby constitutive model and significant agreement is found. The density of geometrically necessary dislocations as a function of void size is calculated based on the emission of shear loops and their outward propagation. Calculations are also carried out for a void at the interface between two grains to simulate polycrystalline response. The dislocation emission pattern is qualitatively similar to microscope observations.

Keywords: Void growth; Dislocations; Nanocrystalline materials; Copper; Molecular dynamics simulations

1. Introduction

Fracture of ductile metals occurs by nucleation, growth and coalescence of voids [1]. There have been a number of continuum models proposed for the growth of voids in both two and three dimensions [2–5]. However, until recently there was no well established atomistic mechanism for void growth, and the model proposed by Cuitiño and Ortiz [6] is based on vacancy pipe diffusion. The only exception is Stevens et al. [7], who proposed a dislocation model for void growth in spalling.

Lubarda et al. [8] demonstrated that the vacancy diffusion mechanism is only applicable at low strain rates and/or high temperatures, and is therefore only relevant in creep deformation. Indeed, failure in creep is preceded by void nucleation and growth at the grain boundaries, and has been successfully modeled using the diffusion equation by Raj and Ashby [9]. Under these conditions vacancies definitely play a key role. The strain rates encountered in conventional deformation are on the order of $10^{-3}\ s^{-1}$; in laser shock the strain rates are on the order of $10^{6}\ s^{-1}$ and higher. Hence, one cannot envisage a vacancy diffusion mechanism under most operating conditions.

Analytical results by Lubarda et al. [8] and molecular dynamics simulations by Rudd and co-workers [10–13]

* Corresponding author. Tel.: +1 858 534 4719.
E-mail address: mameyers@ucsd.edu (M.A. Meyers).

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and Marian et al. [14,15] indicate that dislocation emission from the growing voids is the primary mechanism of radial material transfer required for void expansion. Void collapse calculations [16,17] lead to similar (but opposite in sign) dislocation configurations. Both prismatic and shear loops were postulated [8] and observed in molecular dynamics (MD) simulations [10–15,18]. Potirniche et al. [19] studied the expansion of voids with radii varying between 0.75 and 4.5 nm in monocrystalline nickel using a modified embedded atom method. Fig. 1 shows the two types of dislocation loops. It should be noted that Ashby [20–22] had also postulated prismatic and shear loops in the deformation of metals containing rigid particles to accommodate the strain gradients imposed; these are the "geometrically necessary dislocations". Seitz [23] and Brown [24] postulated prismatic loops forming at the interface between rigid article and the matrix. Thus, the suggestion that void growth takes place by shear and prismatic loop expansion is well rooted in inhomogeneous plastic deformation. It is the objective of this report to analyze the growth of voids in greater detail. The grain-boundary nature and void size were altered to examine their effect on growth mechanisms.

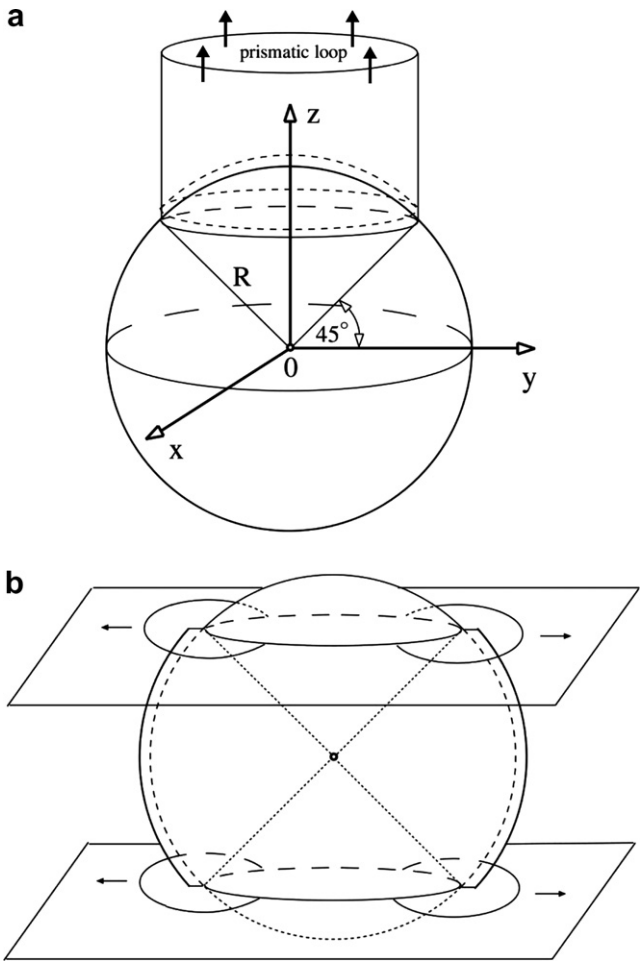

Fig. 1. Dislocation loops postulated by Lubarda et al. [8]; direction of dislocation motion marked by arrows. (a) Prismatic loops and (b) shear loops.

Atomistic simulation performed by Horstemeyer et al. [25] in simple shear using between 10^2 and 10^8 atoms revealed significant differences in the flow stress when expressed as a function of a scale parameter (volume/surface of sample). The resolved shear stress for plastic flow increases significantly with the decrease in size-scale, confirming experimental measurements related to gradient plasticity effects (e.g., Fleck et al. [33,34]). Interestingly, the MD results indicate that dislocation nucleation effects and not strain gradient effects (calculations in simple shear do not produce strain gradients) are responsible for the significant differences in shear flow stress obtained with the change in dimensional scale. These results have a significant bearing in what is perceived to be gradient plasticity.

2. Experimental observation

Dislocation activity around a void growing in the spall regime of shock compressed copper was reported by Meyers and Aimone [26] and Christy et al. [27]. There are also reports in the literature of a work-hardened layer surrounding a growing void (e.g. Ahn et al. [18]). Fig. 2 shows slip bands emanating from voids that nucleated at grain boundaries in copper. It is clear that void expansion did not occur by vacancy migration or prismatic loop emission, since slip bands, emanating from the void surface, are clearly seen. However, the exact nature of dislocation generation and evolution cannot be obtained from these observations. This requires detailed analysis methods such as MD.

3. Computational approach

The molecular dynamics LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) [28] code was used in this investigation. For the face-centered cubic copper structure, an EAM [29] Mishin et al. [30] potential was used. The number of atoms was varied from 10^5 to 10^7, and calculations were performed on parallel PCs and on the supercomputer at San Diego super computer center.

The single crystal copper domain was $10 \times 10 \times 10$ nm with 1 nm radius spherical void at center. This gives a void volume fraction of 0.42%. A periodic boundary was used with uniaxial expansion strain. The domain size was reduced for 0.5 nm radius void and enlarged for 2.0 nm radius void while fixing void volume fraction at 0.42%. The different sized domains were subjected to uniaxial strain along [0 0 1]. All simulations were done at a strain rate of 10^8 s^{-1} (2000 ps, 20% volume strain). Visualization of stacking faults representing dislocations was done with a filter using a centrosymmetry parameter [31].

A bicrystal copper domain was constructed with two single crystal cubes sharing a tilt boundary making an angle, $\theta = 43.6°$. The random angle of 43.6° between two grains (1, left and 2, right) was chosen because it rotates the atoms into positions that produce simple indices in LAMMPS. A counterclockwise rotation around [1 0 0] of