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Plastic deformation of a porous bcc metal containing nanometer sized voids

C.J. Ruestes [a,e,f,*], E.M. Bringa [a,b], A. Stukowski [c], J.F. Rodríguez Nieva [d], Y. Tang [f], M.A. Meyers [f]

[a] Instituto de Ciencias Básicas, Univ. Nac. de Cuyo, Mendoza 5500, Argentina
[b] CONICET, Mendoza 5500, Argentina
[c] Darmstadt University of Technology, Darmstadt, Germany
[d] Massachusetts Institute of Technology, MA 02139, USA
[e] Instituto Balseiro, Univ. Nac. de Cuyo, Bariloche 8400, Argentina
[f] University of California, San Diego, La Jolla, CA 92093, USA

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ABSTRACT

Nanoporous materials, can present an outstanding range of mechanical properties. Both molecular dynamics and dislocation analysis were used to evaluate and quantify the evolution of plasticity in a porous Ta single crystal containing randomly placed voids with 3.3 nm radii and average initial porosity of 4.1%, when subjected to uniaxial compressive strain. Nanovoids act as effective sources for dislocation emission. Dislocation shear loops nucleate at the surface of the voids and expand by the advance of the edge component. The evolution of dislocation configuration and densities were predicted by the molecular dynamics calculations and successfully compared to an analysis based on Ashby's concept of geometrically-necessary dislocations. Resolved shear stress calculations were performed for all bcc slip systems and used to identify the operating Burgers vectors in the dislocation loops. The temperature excursion during plastic deformation was used to estimate the mobile dislocation density which is found to be less than 10% of the total dislocation density.

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1. Introduction

Metallic foams exhibit an outstanding range of properties obtained through the tailoring of void configuration and size [1–4]. The reduction in size of the voids in metals leads to high strength levels that are enabled by nanoscale effects. Biener et al. [1] demonstrated that nanoporous gold can reach a flow stress of 4.5 GPa. This is akin to the results of nanopillar strength by Greer et al. [5] and Nix et al. [6]. Kim et al. [7] also showed strong size effects in nanopillars (both in compression and tension) for various bcc metals, including Ta. In addition to the high strength achieved in nanofoams, their effectiveness in radiation resistance has been proposed. This is due to the size of the ligaments which, if properly chosen, produces a "self-healing" foam [3]. The nanoscale foams inhibit the formation of the collision cascade by providing sinks for the radiation induced defects. In addition to high porosity metallic foams as the ones described above, there are samples with low porosity at the nanoscale, like radiation damaged samples [8], or pre-spalled samples [9,10], where mechanical properties of samples are also of interest.

In the last few decades there has been a tremendous advance in the understanding of plasticity under extreme conditions such as the high pressures and strain rates achievable by shock compression. The extremely high strain rates obtained with laser compression (10^7–10^9 s^{-1}) and the ultrashort durations (1–10 ns) of the pressure pulse render this technique a unique tool to explore extreme regimes of plastic deformation, pressure, strain rate and temperature. Although plastic deformation is being studied intensively experimentally through the characterization of recovered specimens, direct simulations provide important insights into the dynamic processes of plastic deformation. Experiments that probe pressure-induced nanovoid collapse at the relevant nanoscopic length and ultrashort time scales are extremely difficult or impossible with current set-ups, while continuum models might not work at the nanoscale. Reisman et al. [8] measured VISAR profiles of a sample with a collection of radiation-induced voids, and were able to reasonably fit their data using a dislocation-based model with a size-dependent plastic threshold for the voids. Several authors [11–13] showed how molecular dynamics simulations can be coupled with laser-driven shock experiments to provide

* Corresponding author at: University of California, San Diego, La Jolla, CA 92093, USA. Tel.: +1 858 900 8425.
E-mail address: cjruestes@hotmail.com (C.J. Ruestes).

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insight into the plastic deformation mechanisms in such extreme regimes.

Despite these advances, nano-scale plasticity under extreme conditions remains poorly understood for bulk materials, and even more so for materials including porosity, where there are relatively few studies. Nanoscale porosity appears in many different scenarios: radiation damage [8], laser ablation [14], incipient spall [9], metallic and non-metallic nanofoams [15], etc. The understanding of the role of porosity on mechanical behavior is important for the assessment and development of materials such as metallic foams [1], and materials for new fission and fusion reactors [3], with improved mechanical properties.

Although there are a number of studies focusing on single voids in fcc [16–20] and bcc metals [21–25], void assemblies and the more general problem of a porous metal have not yet been thoroughly investigated in simulations, except for relatively few studies [10,18,26,27].

We aim to develop a mechanistic understanding of the microstructural changes induced by high strain rate compression of a material with nanoscale porosity. For that purpose, and given the typical size limitations of molecular dynamics, we chose to conduct this study by adding a few nanovoids to a bulk bcc Ta sample reaching a relatively low porosity (~4%) [26]. We found that dislocation production leads to an anomalous Taylor type relationship between dislocation density and stress, and that porosity collapse was directly related to plastic activity. In this study we focus on a detailed analysis of dislocation activity including activated dislocation systems and dislocation velocity, and present models to account for the lower plastic threshold, as compared to the case of a single void, and for the resulting density of geometrically necessary dislocations (GNDs). We also analyze plastic heating during void collapse and several other aspects of the evolution of the sample under compression. Although we are focusing here on a material with a low void fraction, the size of the voids and the acquired ligaments can be compared to those found in novel yet-laboratory scale nanofoams and therefore get that the conclusions reached herein can be extrapolated to higher porosities, in the regime of importance for both mechanical performance and radiation resistance.

2. Computational modeling

The compression simulations were performed with LAMMPS [28] and bcc Ta was modeled with an extended Finnis–Sinclair potential [29]. Based on static equilibrium simulations, this potential predicts pressure–volume relations comparable to experimental data [29]. It gives generalized stacking-fault energies comparable with ab initio results [24], and it has been used in previous work on void collapse [24–26], as well as rapid compression of bcc metals [30,31]. Non-equilibrium shock simulations are a challenge for empirical potentials because solid–solid phase transitions [32,33] or soft-phonon modes [34] may appear artificially. No artificial behavior that may affect our simulations is known for pressures under 60 GPa, being 50 GPa the maximum pressure reached in our studies.

The simulation domain was initially set up as a cubic sample containing 100^3 unit cells. Ten spherical voids with radii of ~3.3 nm where created inside the sample, with an average distance (between void surfaces) of 10.5 nm, resulting in a 4.1% volume fraction of voids and 1.9 million remaining atoms. Periodic boundary conditions were imposed in all directions. The sample was equilibrated to zero pressure at an initial temperature of 300 K.

A uniaxial compressive strain rate of 10^9 s^{-1} was applied in the [0 0 1] direction for 200 ps, resulting in a total of 20% volume strain. Lateral strains were impeded. This strain state simulates early stages of laser shock compression experiments [11,12,35–37]. A 1 fs time step was chosen and the simulation was run with a constant NVE integration consistent with the micro-canonical ensemble. In this manner, no temperature control was imposed and we were able to measure temperature effects produced by plastic activity.

Defect tracking was done by means of the Common Neighbor Analysis (CNA) [38], a structural filter known to be suitable for bcc metals. During the computational run, non-bcc atoms were filtered by the built-in CNA available in LAMMPS. An improved version [39] of the recently developed dislocation extraction algorithm technique (DXA) [40], was also used to identify line and surface defects. Visualization of dislocations and void surfaces was performed using VMD [41] and ParaView [42].

3. Results

The computational procedures for the global stress–strain response and resolved shear stresses are explained in Sections 3.1 and 3.2 respectively. The dislocation activity is discussed in Section 3.3 and dislocation densities were computed independently in Section 3.4 (CNA), Section 3.5 (DXA), Section 3.6 (Mobile dislocation density) and Section 3.7 (geometrically-necessary dislocations).

3.1. Global uniaxial stress–strain response

The stress in the loading direction, σ_{zz}, was monitored during the simulation and is plotted in Fig. 1, next to the calculations of Tang et al. [24] for a sample of the same dimensions containing a single void of 3.3 nm radius. The stresses at the point where plastic flow starts are marked by arrows. As one might expect, the stress is about 20% lower in the sample with ten voids than for a single void. Wu and Markenscoff [43] calculated the singular stress amplification between two holes of equal radius r, showed in Fig. 2. The simplest form of this calculation is given, for uniaxial loading and at a point midway between the two holes, where this amplification, σ_{max}, is highest:

$$\sigma_{max} \sim \left[\frac{1.94}{\left(\frac{d}{2r}\right)^{\frac{1}{2}}} \pm \frac{\sqrt{2}}{2\left(\frac{d}{2r}\right)^{\frac{1}{2}}}\right]\sigma_{\infty} \tag{1}$$

where σ_{∞} is the stress at an infinite distance from the holes, r is the hole radius, and d is the distance between the edges of the holes. The minus sign corresponds to the hole centers aligned with the

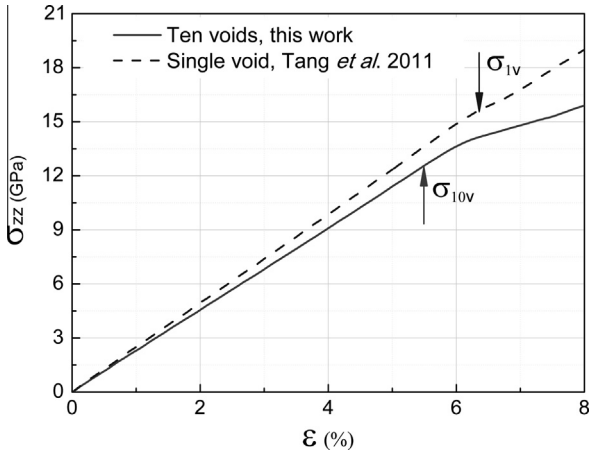

Fig. 1. Stress–strain curve for void collapse under uniaxial strain. Void radius is 3.3 nm. Yield strains at which defects start to nucleate are indicated by arrows. The elastic modulus reduction in our simulation is a direct consequence of the porosity.

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