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Plastic deformation of Cu single crystals containing an elliptic cylindrical void

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ABSTRACT

Molecular dynamics simulations are performed to study the plastic deformation of Cu single crystals containing an elliptic cylindrical void. The effects of initial void geometry including void ellipticity and void orientation angle on plastic deformation are examined by considering the stress–strain response, dislocation nucleation from the void surface, and porosity/void cross-sectional shape evolution. It is found that (i) the initial void geometry plays an important role and (ii) the growth of voids with an increasing initial ellipticity converges to that of a crack. Our results reveal the underlying mechanisms of initial void ellipticity- and orientation angle-dependent plastic deformation of metallic solids, and provide direct evidence that there is no dividing line between a void and a crack in terms of the mechanical responses of these solids.

1. Introduction

Nanovoid growth, important in ductile fracture and spallation of metals, has been the subject of extensive study for decades [1]. The following events are observed in ductile rupture of metals as plastic deformation advances: (i) voids are initiated at internal boundaries (e.g., grain boundaries) and/or due to vacancy aggregation; (ii) voids grow and change shape; (iii) large voids coalesce to form cracks which then propagate and grow; (iv) macroscopic cracks become observable and the material eventually fails [2]. The existence of voids also contributes to the hardening of metals by impeding dislocation migration [3]. As the continuum models of void growth and associated dislocation nucleation are very sensitive to the choice of various parameters and criteria (e.g., dislocation nucleation criteria and dissociation of dislocations) [4,5], atomistic methods such as molecular dynamics (MD) become the natural framework to understand the plastic response of voided metallic materials at the nano-scale [6–9].

Recently, a number of research efforts were devoted to studying the growth of elliptic cylindrical voids in Cu [10], Al [11,12], and Fe [13] by MD simulations. While these studies highlighted the significance of the initial void ellipticity in nanovoid growth, only a relatively small ellipticity ($\leqslant 0.8$) was considered. The void ellipticity is defined here as $e = \sqrt{(a^2 - c^2)/a^2}$, where a and c are length of the void major and void minor axes, respectively, as illustrated in Fig. 1 (b). Larger initial void ellipticity is worth investigating because the shape of the void would approach that of a crack as the void ellipticity approaches 1. While much MD work [14–17] has explored deformation of metals containing a crack, it remains unexplored to our best knowledge how a voided material grades into a cracked material as the initial void ellipticity increases. To address this, we conduct large scale MD simulations to quantify the effects of initial void ellipticity and orientation angle on tensile deformation of voided solids in face-centered cubic (FCC) Cu single crystals.

2. Materials and methods

The simulation cell for nanovoid growth study is presented in Fig. 1, with a model size of 15.1 nm (L_x) by 100.1 nm (L_y) by 100.1 nm (L_z) along the x, y, and z directions, respectively. Previous MD simulations [11,18] suggested that our simulation cells are large enough to ignore size effects on the onset of plasticity. The lattice orientations are $x[100]$, $y[010]$, and $z[001]$, with periodic boundary conditions applied along all directions. The lattice parameter is 3.615 Å, and each computational cell contains about 12.31 millions atoms. An elliptic cylindrical void is generated by removing all atoms throughout the specimen along the x axis and within the cross sectional shape on the y-z plane. The center of the void cross section, with an initial ellipticity of e, is at the center of the specimen. The void orientation angle θ is formed between the void major axis and the y axis. In this work, e varies from 0.8,

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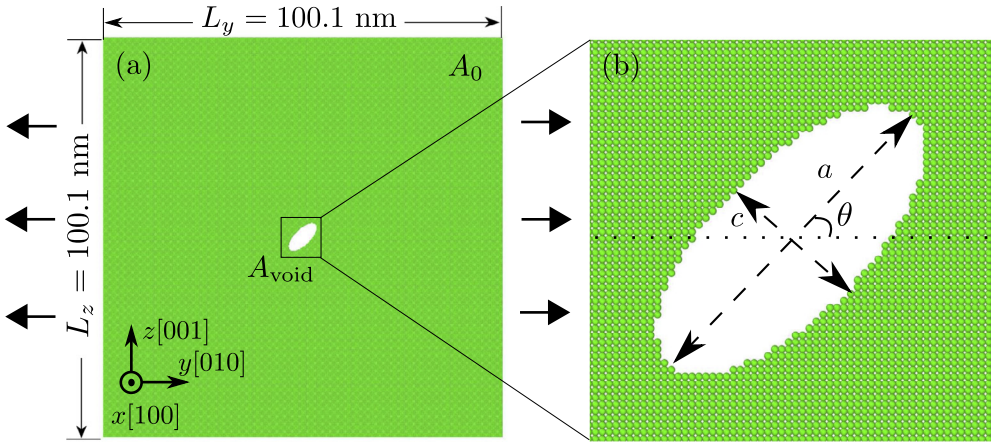
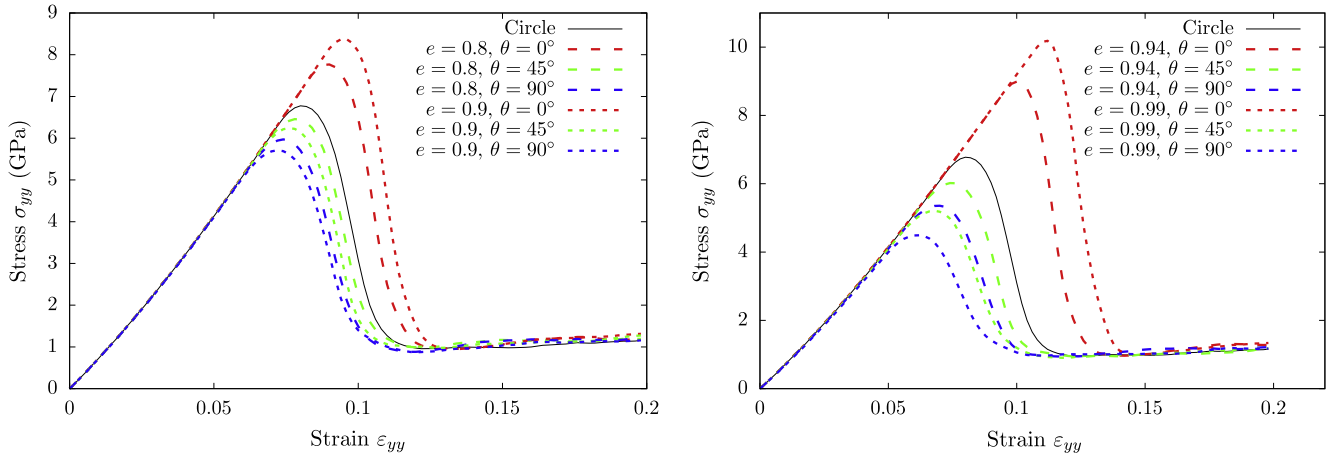


Fig. 1. Simulation cell of a Cu single crystal containing an elliptic cylindrical void formed by removing all atoms throughout the x axis and within the cross sectional shape on the y-z plane. The depth of the model in one supercell $L_x = 15.1$ nm. a and c are the length of the void major and void minor axes, respectively. The orientation angle θ, formed between the void major axis and the y axis, is either $0^\circ, 45^\circ$, or 90°. $A_0 = L_y L_z$ is the initial simulation cell area, and A_{void} is the cross-sectional area of the void; both are on the y-z plane.



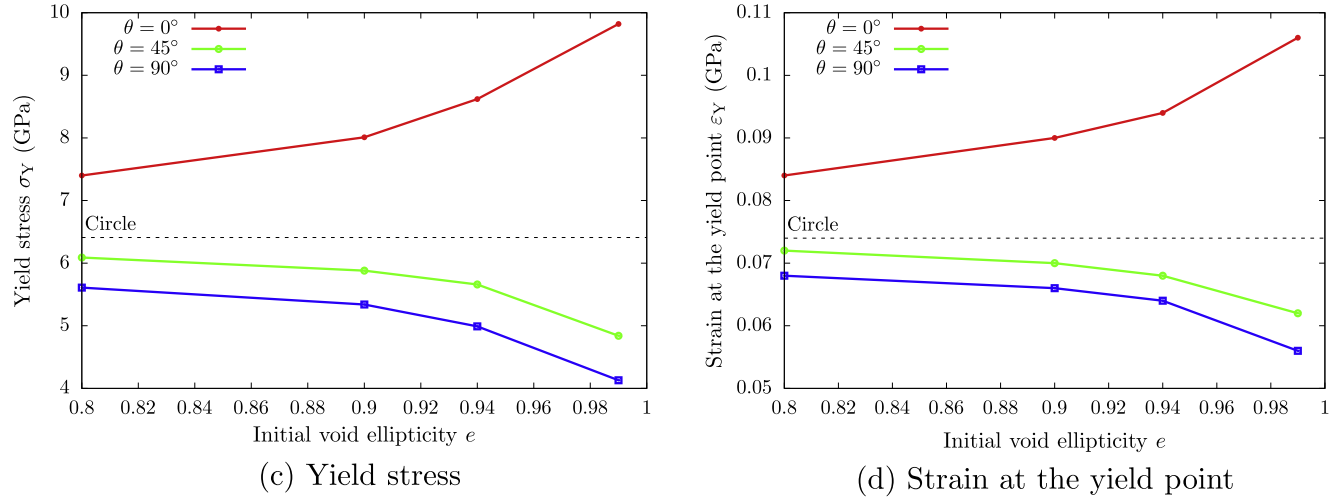


Fig. 2. Stress–strain curves in the cases of initial void ellipticity (a) $e = 0.8$ and 0.9, (b) $e = 0.94$ and 0.99, with initial void orientation angle $\theta = 0^\circ, 45^\circ$, or 90°. (c) Yield stress σ_Y and (d) strain at the yield point ε_Y as a function of both e and θ are also presented. The cases with an initially circular cylindrical void are given as solid curves in (a) and (b) and horizontal dash lines in (c) and (d) for references.