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Micromechanics model for nanovoid growth and coalescence by dislocation emission: Loading and lattice orientation effects

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ABSTRACT

Dislocation loops emitting from the surface of void is a viable mechanism at the nanoscale for void growth and coalescence, which has been confirmed by experimental observations and molecular dynamics simulations. Based on this mechanism, a micromechanics model was developed to investigate the crystal orientation on nanovoid growth and coalescence in fcc single crystals. In this paper, uniaxial tensile loading along four representative lattice orientations were considered. The surface effect of nanovoid on the critical stress and direction of nanovoid growth was also analyzed. The results showed a strong dependence of nanovoid evolution on loading and lattice orientation: in the case of uniaxial loading along the [1 1 0] direction void grew most easily, and the largest applied stress was required for the void growth under the unixial loading along the [1 1 2] direction. The void evolution showed a strong dependence on the size of nanovoid, especially for the void radius less than 10 nm.

1. Introduction

It is well known that the micro-defects, such as voids and cracks, play a fundamental role in ductile fracture of crystalline materials as well as their composites [1–4]. The increasing trend toward the miniaturization of devices in micro/nano-technology necessitates the studying of deformation and failure in small scale. The mechanical properties and responses of such small devices are mainly determined by the deformation and fracture of single grains. Therefore, it is necessary to investigate the fracture and failure of single grains which constitute the crystallite.

Voids nucleated by matrix cavitation, cracking of the second phase and debonding at the interface between the matrix and the second phase are generally in micro- or nano-scale [5,6]. Early work on the growth and coalescence of voids has been done based on the plastic flow mechanism, and the materials are assumed to possess perfectly isotropic constitutive properties [7–10]. However, the actual materials are all anisotropic, which has a significant influence on the growth and coalescence of voids, especially in the initial stage of void growth where the scale of the voids are in nanometers. As noted in Hutchinson [11], the application of void growth prediction based on the conventional plasticity to micron-sized voids is probably unjustified. Therefore, investigating the void growth and coalescence in anisotropic materials provides the theoretical basis for the research on ductile fracture of actual materials.

Based on crystal plasticity model, a great number of studies had been performed including both the finite element method and theoretical model [12–15]. Potirniche et al. [16] studied the effects of crystallographic orientation and loading condition on void growth and coalescence using a 2D plane strain unit cell with one and two cylindrical voids. They concluded that the void evolution was strongly dependent on the crystallographic orientation with respect to the tensile axis for uniaxial tension conditions, and the lattice orientation had only a minor role in void growth rate under biaxial/triaxial loading. Recently, Liu et al. [17–19] used a 3D unit cell to study the effects of crystallographic orientation and misorientation on void growth and coalescence in fcc single crystal and bicrystal, respectively. Their results showed that void growth shape was significantly dependent on the crystallographic orientation, and large difference of orientation factor accelerates void coalescence at grain boundary.

However, these continuum models cannot reveal the fundamental physical mechanisms of void evolution. An recently employed tool to the study of void growth and coalescence is molecular dynamics (MD), which has the advantage over continuum models that no assumption need to be made about the mechanisms of void growth and coalescence. Using MD simulation, Belak et al. [20–22] investigated the void growth and coalescence in the fracture process of ductile materials, and the results showed that dislocations were nucleated in the neighboring of void when the void was subjected

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to tensile or compressive loading. Once the dislocation was trigged and emits toward the interior of the crystal, the void grew one Burgers vector. To investigate the effects of lattice orientations and loading conditions on void growth and coalescence based on the dislocation mechanism, MD simulations were performed by Zhu et al. [23]. Their study revealed that a nanovoid in copper grew to be a ellipsoidal shape and different loading directions ([1 0 0] and [1 $\bar{1}$ 1]) changed the orientation of its major axis. Later, Deng et al. [24] investigated the effect of configuration on coalescence in single-crystal copper using a MD simulation. The results showed that the 60° configuration coalescence most easily. In spite of the large number of MD studies on void growth and coalescence, only a few theoretical models of the growth and coalescence based on dislocation mechanism have been made.

The aim of this study is to develop a theoretical model to investigate the effects of loading and lattice orientations on nanovoid growth and coalescence by emission of dislocation in fcc single crystals. Since the void size is in the range of nanometers, the surface effect of nanovoid cannot be neglected. The slip direction and the critical stress for a dislocation emitting from the surface of void in elastic plane are calculated. Then, four representative orientations of uniaxial tensile axis are considered to investigate the loading and lattice orientations effects. The void size effects on the growth and coalescence are also discussed in details.

2. Theoretical model

2.1. Stress field of a cylindrical nanovoid by considering surface effect

To study the stress field around a void, we consider an infinite elastic plane containing a nanosized cylindrical void with radius a, as shown in Fig. 1. The bulk material is assumed to be linearly elastic, homogeneous, and isotropic. To simplify the problem, we use two polar coordinates (r,θ) and(ρ,φ), and the polar coordinates (r,θ) can be expressed in terms of the polar coordinates (ρ,φ), emanating from the surface of the void by using the following relationship:

$$r^2=a^2+\rho^2+2a\rho\cos\varphi,\quad \tan\theta=\frac{\rho\sin\varphi}{a+\rho\cos\varphi}. \tag{1}$$

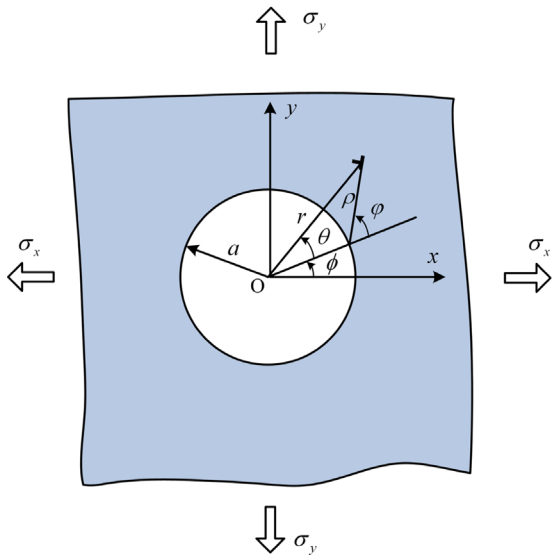

Fig. 1. Nanoscale void in an infinite elastic plane subjected to remote tensile stress. The two sets of polar coordinates (ρ,φ) and (r,θ) define the slip plane and the intersection of the slip plane with the surface of the void.

In isotropic elasticity plane in the absence of body forces, the equilibrium and constitutive equations can be expressed based on the theory proposed by Gurtin and Murdoch [25] and Gurtin et al. [26] as follows:

$$\sigma^b_{ij,j}=0, \tag{2}$$

$$\sigma^b_{ij}=\lambda\varepsilon_{kk}\delta_{ij}+2\mu\varepsilon_{ij}, \tag{3}$$

where λ and μ are the Lamé constants of the bulk, σ_{ij} and ε_{ij} are the stress and strain components, $\delta_{\alpha\beta}$ is Kronecker delta.

When the size of the void is in nanoscale, due to the high surface-to-volume ratio, the surface of the void is quite different from those in macroelasticity [27–29], where the traction-free condition is always assumed along the surface. In the Gurtin–Murdoch model, surface stress resulting from a surface free energy and a constant residual stress was suggested. So the equilibrium equation and the constitutive relation on the surface can be expressed as

$$\sigma^b_{ij}n_in_j=\sigma^s_{\alpha\beta}k_{\alpha\beta} \tag{4}$$

and

$$\sigma^s_{\alpha\beta}=\tau_0\delta_{\alpha\beta}+2(\mu^s-\tau_0)\,\varepsilon_{\alpha\beta}+(\lambda^s+\tau_0)\varepsilon_{\gamma\gamma}\delta_{\alpha\beta}, \tag{5}$$

where superscripts b and s denote the quantities corresponding to bulk and surface of void, n_i is the normal vector on the surface, τ_0 is the residual surface stress under unstrained condition, $k_{\alpha\beta}$ is the curvature tensor of the surface, and μ^s and λ^s are the surface Lamé constants, which depend on the material type and the surface crystal orientation.

The elastic stress field around the nanovoid for the plane strain condition is (see details in our previous work [30]):

$$\begin{aligned}
\sigma_{rr}&=\frac{1}{a}\left[2\mathrm{A}+\frac{2AB_1a^2}{r^2}-\left(\mathrm{B}+\frac{4BA_1a^2}{r^2}-\frac{3BB_2a^4}{r^4}\right)\cos\,2(\theta+\phi)\right],\\
\sigma_{\theta\theta}&=\frac{1}{a}\left[2\mathrm{A}-\frac{2AB_1a^2}{r^2}+\left(\mathrm{B}-\frac{3BB_2a^4}{r^4}\right)\cos\,2(\theta+\phi)\right],\\
\sigma_{r\theta}&=\frac{1}{a}\left(\mathrm{B}-\frac{2BA_1a^2}{r^2}+\frac{3BB_2a^4}{r^4}\right)\sin\,2(\theta+\phi),
\end{aligned} \tag{6}$$

where

$$A=\frac{(\sigma_x+\sigma_y)a}{4},\quad B=\frac{(\sigma_y-\sigma_x+2i\sigma_{xy})a}{2}, \tag{7}$$

$$\begin{aligned}
A_1&=\frac{-(1+2\Lambda_1)}{1+4\Lambda_1+\Lambda_1\Lambda_2},\\
B_1&=\frac{\tau_0/(2A)+\Lambda_1\Lambda_2-1}{1+2\Lambda_1},\\
B_2&=\frac{\Lambda_1\Lambda_2-1}{1+4\Lambda_1+\Lambda_1\Lambda_2},
\end{aligned} \tag{8}$$

and

$$\Lambda_1=\frac{2\mu^S+\lambda^S-\tau_0}{4\mu a},\quad \Lambda_2=\frac{2\mu}{\lambda+\mu}. \tag{9}$$

We analyze fcc single crystal Al as an illustrative example, and the elastic constants for aluminum are: Lamé constants $\lambda=$ 58.17 GPa, $\mu=G=26.13$ GPa, Poisson's ratio $\nu=0.345$, Burgers vector $b=0.255$ nm [31,32]. From previous experimental and atomistic simulations, the effective parameters of the aluminum surface are determined, and the results indicated that the surface elastic constants depend on the material type and the surface crystal orientation. For example, for Al [1 1 1] surface: $\lambda^s=6.8511$ N/m, $\mu^s=-0.3760$ N/m, $\tau_0=0.9108$ N/m [31]. In the case of the uniaxial loading $\sigma_x=0$ and $\sigma_y=\sigma$, the elastic stress field around the nanovoid with and without the surface effect are calculated. Fig. 2 shows the stress concentration factor as the function of void radius a/b with and without the surface effect. The horizontal line is the stress concentration factor without the surface effects. It can be