Physics Letters A 380 (2016) 917–922

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Discussion

Molecular dynamics simulations of void effect of the copper nanocubes under triaxial tensions ☆

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ARTICLE INFO

Article history:
Received 28 October 2015
Received in revised form 8 December 2015
Accepted 22 December 2015
Available online 31 December 2015
Communicated by R. Wu

Keywords:
Triaxial tension
Damage model
Molecular dynamics
Void

ABSTRACT

The isotropic copper nanocubes with different size cubic voids under triaxial tensions are investigated by the molecular dynamics method. For accuracy we present the hydrostatic stress, Mises stress, true stress, logarithmic strain and relationship between each other. In the simulation the number of model atoms is formulized and the hydrostatic stresses can replace triaxial stresses of model. We demonstrate that the yielding strengths will decrease with increase of void, particularly when the void percentage is reaching 0.2%. The models are breaking at 45 angle dislocation with tiny differences. Also, the Gurson model cannot well describe the trend of damage; instead the authors propose a modified model by relationship between Mises stress and hydrostatic stress.

1. Introduction

The conductive performance of copper is behind silver in the metal, but it is much cheaper than silver. And copper plays the part of 'leading role' in electrical industry. For its application performance, its mechanical properties need to meet a high standard. The crystal structures affect the material properties, and it is necessary to research crystal structures for making, using and developing materials. The materials around us cannot be perfect, where is the value of damage mechanics. Microcosmic voids, which will cause mesoscopic defects, are the sources of damage and failure. In 1995, the behavior of a void under a high direct current (DC) stress had been accomplished [1].

In recent years, researchers realized the importance of microcosmic models with voids. Void growth [2] and defects have always been the research hotspots in recent years. Void growth and coalescence in single crystal nickel [3,4], copper [5], magnesium [6] and λ-TiAl [7] have been investigated by molecular dynamics (MD). The deformation behavior of face-centered cubic single crystals containing microvoids by using finite element methods (FEM) was researched [8]. Three-dimensional FEM are completely different from molecular dynamics method. The different model styles including nanowires [9–11] and nanoimprint [12], different void styles including crack [13], point defect [14] and line defect [15], and the different analysis styles including plasticity deformation mechanism [16], collision cascades [17] and ductile failures [18], were all considered.

The previous studies were not considering stress triaxiality effects [19]. Fracturing and breaking are being popular in the mechanical field, and the single crystal structures cannot meet the demand. The fracture behaviors of twinned Cu nanowires are simulated under uniaxial tensile deformation [20,21].

This work will investigate the mechanics effect of void in isotropy nanocubes under triaxial tensions for approaching the macro mechanics and obtain microscopic damage models not in the mesoscopic damage mechanics by using molecular dynamics [22].

The rest of this paper is organized as follows. In Section 2, we introduce the model and method. The results will be discussed in Section 3. Finally, some conclusions are drawn from the present study in Section 4.

2. Method and model

2.1. Molecular dynamics simulation

The molecular dynamics simulations are performed with the modified software NanoMD [23], which is developed by Zhao's

☆ Supported by the Earthquake Industry Special Science Research Foundation Project Grant No. 201508026-02, the Natural Science Foundation of Heilongjiang Province Grant No. A201310, the Scientific Research Starting Foundation for Post Doctorate of Heilongjiang Province Grant No. LBHQ13040.

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http://dx.doi.org/10.1016/j.physleta.2015.12.030

Table 1
Parameters of EAM potentials for FCC metals of copper.

a	E_c	f_e	ϕ_e	α	β	γ
3.614 Å	3.54 eV	0.30	0.59	5.09	5.85	8.00

group (Nanjing University). In this work, MD simulations are carried out with the embedded-atom method (EAM) potential developed by Johnson [24], which could provide an effective description of the transition metals with a face-centered cubic (FCC) structure.

The total energy [25] is given by

$$E_{tot} = \sum_i E_i, \tag{1}$$

$$E_i = F_i(\rho_i) + \frac{1}{2}\sum_{j\neq i} \phi_{ij}(r_{ij}), \tag{2}$$

$$\rho_i = \sum_{j\neq i} f_j(r_{ij}), \tag{3}$$

where E_{tot} is the total internal energy of an assembly of atoms, E_i is the internal energy of atom i, ρ_i is the electron density contribution of all other atoms at atom i, $F_i(\rho_i)$ is the energy to embed atom i into the electron density ρ_i, r_{ij} is the distance between atoms i and j, $\phi_{ij}(r_{ij})$ is the pair potential with the distance between atoms i and j being r_{ij}, and $f_j(r_{ij})$ is the contribution of the atom j at r_{ij} to the electron density at atom i. The potential with nearest neighbor atom model is used. The pair potential and the embedded energy are given [26] by

$$\phi(r) = \phi_e \exp\left[-\gamma\left(\frac{r}{r_e} - 1\right)\right], \tag{4}$$

$$\rho(r) = \sum f(r) = \sum f_e \exp\left[-\beta\left(\frac{r}{r_e} - 1\right)\right], \tag{5}$$

$$F(\rho) = -E_c\left[1 - \frac{\alpha}{\beta}\ln\left(\frac{\rho}{\rho_e}\right)\right]\left[\frac{\rho}{\rho_e}\right]^{\alpha/\beta} - 6\phi_e\left[\frac{\rho}{\rho_e}\right]^{\gamma/\beta}, \tag{6}$$

where E_c, f_e, ϕ_e, α, β and γ are the parameters (see Table 1) of EAM potentials for FCC metal. The variables with subscript e refer to the equilibrium values of the variables.

2.2. Creating models

The crystal structure of copper is FCC. The homogeneity models, [100] isotropous models [27], are created with different size voids. Because of the atomic lattice symmetry, the number of atoms is reduced layer by layer from the inside to outside with the void sizes increasing.

The models are all [100] nanocubes, whose outside sizes are all $20a$ (a denotes the copper lattice constant 0.3614 nm) (Table 1) and whose tensile atoms' sizes are a (Fig. 1(a)), under triaxial tensile loadings. The model without voids has about 34 000 atoms. Fig. 1(b) shows the void styles clearly at z direction in the xy section.

During the simulations, conventional molecular dynamics calculation is used, which is corresponding to micro-canonical ensemble in statistical mechanics. At the beginning, velocities of atoms are initialized according to the Maxwell–Boltzmann [28]. Then systems achieve thermal equilibrium states at 30 K by at least 20 000 relaxation steps gradually. After enough relaxation, a combined Verlet leapfrog and cell-linked list algorithm is applied for Newtonian motion equations and the tensile atoms of the models are loaded by 0.01% ps^{-1} under triaxial tension. Some mechanical quantities are recorded and solved.

2.3. Mechanical quantities

The stress is computed by the virial scheme, which is on the average of all atomistic stresses. The nominal stress (engineering stress) is showed in terms of EAM potential functions as follows [29]:

$$\sigma_i^{\xi\eta} = \frac{1}{\Omega_i}\left\{-m_i v_i^{\xi} v_i^{\eta} + \frac{1}{2}\sum_{j\neq i}\left[\frac{\partial\phi}{\partial r_{ij}} + \left(\frac{\partial F}{\partial\rho_i} + \frac{\partial F}{\partial\rho_j}\right)\frac{\partial f}{\partial r_{ij}}\right]\frac{r_{ij}^{\xi} r_{ij}^{\eta}}{r_{ij}}\right\}, \tag{7}$$

where $\sigma_i^{\xi\eta}$ is the $\xi\eta$ component of the atomic stress tensor of atom i, Ω_i is average volume of atom i, m_i is the mass of atom i, v_i^{ξ} and v_i^{ξ} are the velocity components in the ξ and η direction of atom i respectively, r_{ij}^{ξ} and r_{ij}^{η} are the displacement components in the ξ and η directions of r_{ij} respectively.

The nominal strain is defined as

$$\varepsilon = (l - l_0)/l_0, \tag{8}$$

where l is the length of the current model, and l_0 is the length of the model after relaxation.

Due to the obvious necking of nanocubes, the true stress $\widetilde{\sigma}$ and the logarithmic strain $\widetilde{\varepsilon}$ are proposed by [30]

$$\widetilde{\sigma} = \sigma(1+\varepsilon), \tag{9}$$

$$\widetilde{\varepsilon} = \ln(1+\varepsilon), \tag{10}$$

where σ and ε are the nominal stress and the nominal strain respectively.

In order to considering comprehensive stress, hydrostatic stress σ_m and Mises stress σ_{eq} are defined respectively as follows:

$$\sigma_m = \frac{1}{3}(\sigma_x + \sigma_y + \sigma_z), \tag{11}$$

$$\sigma_{eq} = \sqrt{\frac{1}{2}\left[(\sigma_x - \sigma_y)^2 + (\sigma_y - \sigma_z)^2 + (\sigma_z - \sigma_x)^2\right]}, \tag{12}$$

where σ_x, σ_y, and σ_z are the stresses in the three directions.

The Gurson damage model has given four models containing voids, and the model of spherical voids will meet the yield surface equation [31]:

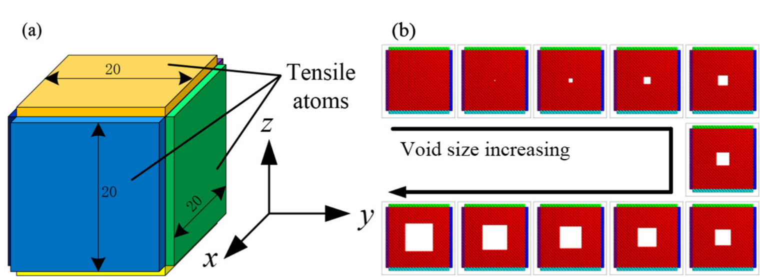

Fig. 1. (a) Schematic diagram of models under triaxial tensions (unit: a). (b) Atom figures of the models with void size increasing in the xy plane.