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Discussion

Mechanical properties of gold twinned nanocubes under different triaxial tensile rates

Zailin Yang [a,*], Guowei Zhang [a], Gang Luo [a], Xiaoqing Sun [a], Jianwei Zhao [b,*]

[a] College of Aerospace and Civil Engineering, Harbin Engineering University, Harbin 150001, PR China
[b] College of Materials and Textile Engineering, Jiaxing University, Jiaxing 314000, PR China

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ABSTRACT

The gold twinned nanocubes under different triaxial tensile rates are explored by molecular dynamics simulation. Hydrostatic stress and Mises stress are defined in order to understand triaxial stresses. Twin boundaries prevent dislocations between twin boundaries from developing and dislocation angles are inconspicuous, which causes little difference between triaxial stresses. The mechanical properties of the nanocubes under low and high tensile rates are different. The curves of nanocubes under high tensile rates are more abrupt than those under low tensile rates. When the tensile rate is extremely big, the loadings are out of the nanocubes and there are not deformation and fracture in the internal nanocubes.

1. Introduction

Nowadays, nanomaterials are popular with researchers because their properties are different from macromechanics. Face centered cubic structure materials, such as copper, gold and silver, are widely used in micronanomechanics, optical measurement and biological monitoring fields. Their mechanics properties must be researched accurately and micro mechanics are concerned to calculate the material properties. Molecular dynamics method is the effective means when the models scale is nanometer.

The properties of twin crystal nanomaterial are superior to general nanomaterials. Ref. [1] shows that the defect emission and propagation in fivefold twinned silver nanowire is prevented by the preexisting twin boundaries. Creep mechanisms in nanotwinned metals [2], dynamics of grain boundary atoms in the bulk nanocrystalline aluminum [3], plastic deformation of nanocrystalline copper [4], deformation behavior of nanopillars with and without twin boundary [5], the fracture behavior of a nanotwinned Cu specimen [6,7], secondary twinning contribution to the ductility of the magnesium nanowire [8] have been well investigated by domestic and foreign scholars.

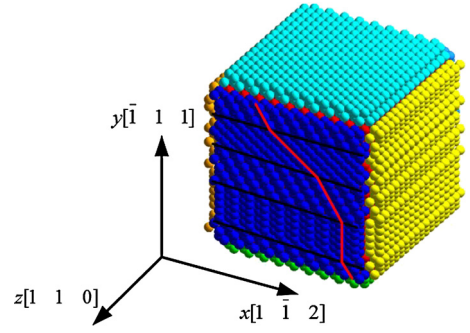

Fig. 1. The gold twin nanocube model sketch map. (For interpretation of the colors in this figure, the reader is referred to the web version of this article.)

Uniaxial tensile loading is dissatisfactory for complex stress states. The mechanics properties of gold twin nanocubes under different triaxial tensile rates are derived in this paper.

2. Model and simulation

The models are made by the geometrical generation method, whose sizes are $12a \times 12a \times 12a$, where a is the gold lattice constant and $a = 0.4078$ nm. The direction of twinning planes is perpendicular to [1 1 0] orientation, while the other directions are [1 $\bar{1}$ 2] and [$\bar{1}$ 1 1] orientations (Fig. 1).

* Corresponding authors.
E-mail addresses: yangzailin00@163.com (Z. Yang), zhaojianweicn@hotmail.com (J. Zhao).

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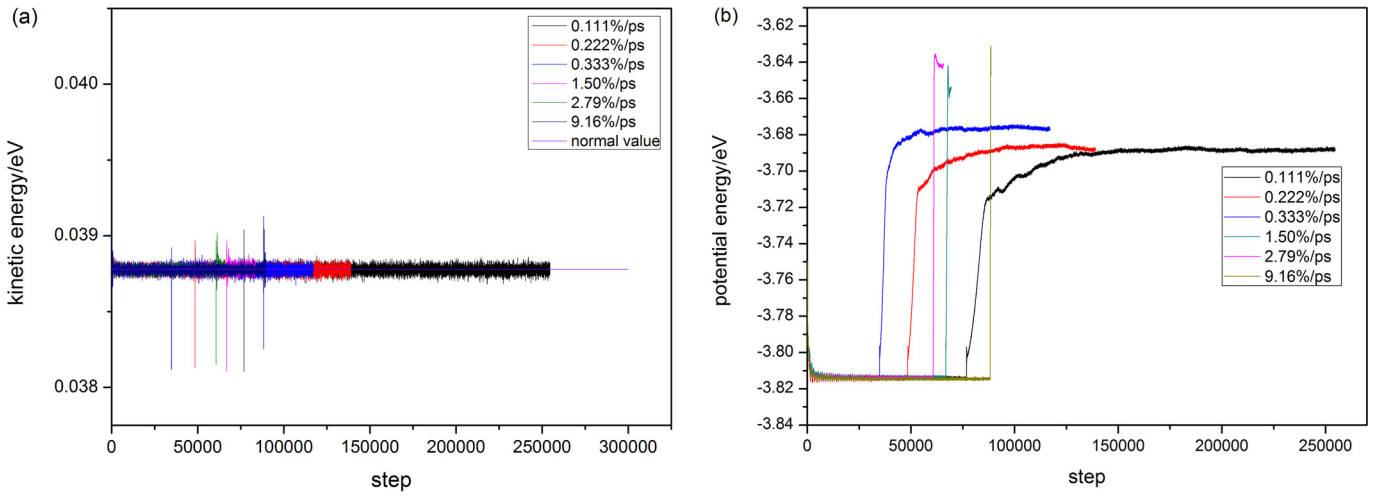

Fig. 2. The average energy curves of nanocubes under different tensile rates: (a) kinetic energy; (b) potential energy.

The simulations are accomplished with the help of NanoMD [9], which was developed by Zhao's group in Nanjing University. By modified NanoMD [10] the boundaries of models are free in three directions. The systems are kept at around 300 K by the Nosé–Hoover temperature-control method [11–14]. Johnson's analytical EAM potential function [15] is adopted to describe the relationship between two gold atoms. The systems are relaxation at initial velocity, which meet Maxwell–Boltzmann distribution [16], until the systems achieve thermal equilibrium state. After relaxation the energies are computed and numerical integration proceed combining Cell and Verlet chained list with integration step $\delta t = 2.94 fs = 2.94 \times 10^{-15}$ s. Then the models are loaded in three directions with same tensile velocity and some parameters are recorded in each tensile step, such as energy, atom position and stress. The stresses in different direction are calculated by the virial scheme [17], which is the average of all atomic stresses.

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

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 strain is defined as

$$\varepsilon = (l - l_0)/l_0 \tag{2}$$

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

Due to the triaxial stresses, the hydrostatic stress σ_m and Mises stress σ_{eq} are defined as following:

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

$$\sigma_{eq} = \sqrt{\frac{1}{2}\left[(\sigma_x - \sigma_y)^2 + (\sigma_y - \sigma_z)^2 + (\sigma_z - \sigma_x)^2\right]} \tag{4}$$

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

3. Result and discussion

The models are loading at three directions with same tensile velocity rates. Table 1 gives the values of tensile rates and their corresponding absolute velocities.

Table 1
The relationship between tensile rates and absolute velocities.

Tensile rate	Absolute velocity
0.111% ps^{-1}	0.0430 m/s
0.222% ps^{-1}	0.0860 m/s
0.333% ps^{-1}	0.129 m/s
1.50% ps^{-1}	0.582 m/s
2.79% ps^{-1}	1.08 m/s
9.16% ps^{-1}	3.55 m/s

3.1. Energy discussion

The kinetic energy of nanocubes only depends on the systems temperature when the models are invariant as following:

$$K.E. = 3/2 k_B N T \tag{5}$$

where $K.E.$ is abbreviation of kinetic energy; N is the atomic number of nanocube; k_B is the Boltzmann constant; T is the system's temperature.

Fig. 2 gives the energy curves of nanocubes in different tensile rate with tension. Fig. 2(a) shows the average kinetic energy is around normal value 0.038778 eV, because the temperature of models is controlled around 300 K by the Nosé–Hoover method. Also, the temperature is not checked each step, so the curves of average kinetic energy are shocks. At the beginning of loading, the average kinetic energies rise and fall gravely. Then they return to normal until break.

The potential energies begin to increase with the tensile loading after relaxation and the curves have the tendency to reduce when the simulation stop. With tensile rate increasing, the increasing range of average potential energy augment and the increasing time decrease. When the tensile rate reach 1.5% ps^{-1}, the variation of average potential energies are different significantly.

3.2. Deformation discussion

Different deformation is showed in nanocubes under different tensile rate. Different color atoms represent different deformation behavior hereinafter: yellow atoms are immobile atoms; blue atoms are dislocation atoms; red atoms are crack atoms.

Twin boundaries are existing as the dislocation, which are the special atomic layers. Also, in the process of relaxation, the crack atoms are transformed into relatively stable dislocation atoms, which meets relaxation process (Fig. 3).

The bigger tensile rate, the less tensile step and the faster nanocubes break (Fig. 4). However, the values of tensile step mul-