Investigation of mechanical properties of twin gold crystal nanowires under uniaxial load by molecular dynamics method*

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Twin gold crystal nanowires, whose loading direction is parallel to the twin boundary orientation, are simulated. We calculate the nanowires under tensile or compressive loads, different length nanowires, and different twin boundary nanowires respectively. The Young modulus of nanowires under compressive load is about twice that under tensile load. The compressive properties of twin gold nanowires are superior to their tensile properties. For different length nanowires, there is a critical value of length with respect to the mechanical properties. When the length of nanowire is greater than the critical value, its mechanical properties are sensitive to length. The twin boundary spacing hardly affects the mechanical properties.

Keywords: molecular dynamics, twinned crystal boundary, gold nanowires, uniaxial load, mechanical properties

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1. Introduction

In recent years, metal nanomaterials, whose properties are different from macroscopic metal materials, have received a great deal of attention. The experiment of metal nanowires is uncontrollable, but by the molecular dynamics (MD) method their deformation can be observed under a certain condition.

Gleiter[1,2] investigated the deformation of nanostructure. Janusz *et al.*[3] used the molecular dynamics simulation method to calculate thermodynamic properties of the transition metal with face-centered cubic structure. Park and Zimmerman[4] discussed the mechanical properties of the gold nanowires in the yield condition, and summarized the plastic characteristics of gold nanowires by molecular dynamics simulation.

The current researches focus on the twin structure, whose load direction is vertical to the twin boundary orientation. The point defects in Au twin boundaries,[5] the fracture behavior and the ductility of the twinned Cu nanowires,[6] and the ductility of the magnesium nanowire[7] were studied under loads in the above direction.

In the present paper, we discuss the properties of gold twin crystal nanowires, whose directions are all parallel to the twin boundary orientation, under different conditions.

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

2. Simulation model

Some twin gold crystal models are given by the geometric construction method (Fig. 1). The nanowire models are rectangular columnar, whose x–y cross-section is the twin crystal section (Fig. 1(a)). The transverse section sizes of models are all $8a \times 8a$, of which a is the gold lattice constant and $a = 0.4078$ nm$= 4.078 \times 10^{-10}$ m. The other two cross-sections are shown in Figs. 1(b) and 1(c). The lengths of nanowires are all $19a$ and the atoms at both ends of the z axis are tool atoms, which are under loads and not involved in statistical computation.

The molecular dynamics simulation software NanoMD,[8] which is developed by Zhao's group in Nanjing University, are modified[9,10] for simulation. In this paper we adopt Johnson's EAM potential function[11] to describe the interaction between each two gold atoms. Cell list and Verlet list are combined with integration step $\delta t = 2.94$ fs$= 2.94 \times 10^{-15}$ s. At the beginning, atom initial velocity, which fits the Maxwell–Boltzmann distribution,[12] is generated randomly. The temperature of the model system keeps up 300 K by the Nosé-Hoover[13–16] method. Through 2×10^4 relaxation steps, the system achieves a thermal equilibrium state. The loads is exerted on the [110] orientation in the z-axial direction, whose stress is obtained by[17]

$$\sigma_\alpha^{zz} = \frac{1}{\Omega_\alpha}\left\{ -m_\alpha v_\alpha^z v_\alpha^z + \frac{1}{2}\sum_{\beta\neq\alpha}\left[\frac{\partial\phi}{\partial r_{\alpha\beta}} + \left(\frac{\partial F}{\partial \rho_\alpha}\right.\right.\right.$$

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$$+\frac{\partial F}{\partial \rho_\beta}\Big)\frac{\partial f}{\partial r_{\alpha\beta}}\Big]\frac{r^z_{\alpha\beta}r^z_{\alpha\beta}}{r_{\alpha\beta}}\Big\}, \tag{1}$$

where σ^{zz}_α is the zz component of the atomic stress tensor of atom α; Ω_α is its volume; m_α is the mass; v^z_α is the velocity component in the z direction of atom α; $r_{\alpha\beta}$ is the distance between atom α and atom β; ϕ, F, ρ, and f are parameters from EAM potential.

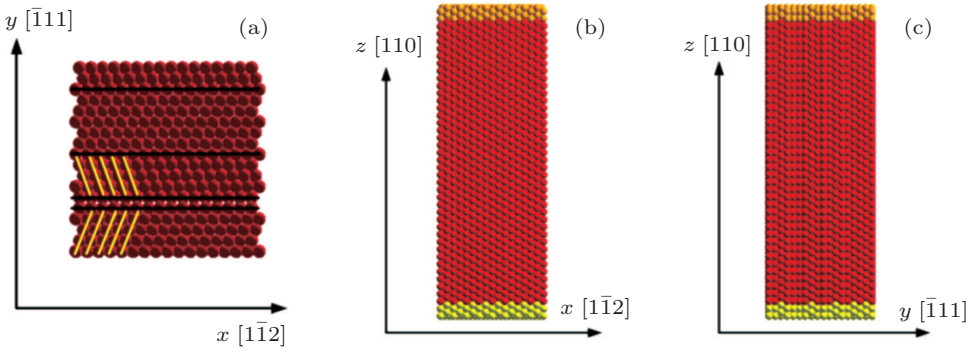


Fig. 1. (color online) Three view drawings of the simulation model.

3. Result and discussion

The nanowires under tensile or compressive loads and different lengths are simulated respectively. Their mechanical properties are different under different conditions.

3.1. Properties of twin crystal nanowires under different load styles

The models deform at 0.129 m/s tensile or compressive velocity rate in the z-axial direction on the basis of the above mentioned models.

3.1.1. Energy discussion

The average energies of models under different load styles are different (Fig. 2). The average kinetic energy (KE) of the system is as follows:

$$\mathrm{KE} = \frac{3}{2}k_\mathrm{B}NT, \tag{2}$$

where k_B, N, T are the Boltzmann constant, the number of atoms, and the temperature of the system respectively. When the system is definite, the average kinetic energy is only depending on the temperature of the system. The kinetic energies of models are almost the same, whose error is less than 1×10^{-5} under tensile or compressive load (Fig. 2(a)).

The average potential energies in different steps under tensile and compressive loads are shown in Fig. 2. With ignoring the accidental error of the computer simulation, both relaxation processes are the same. After relaxation, the potential energy increases with load. Under tensile load the potential energy of the system is almost constant until the 10^5-th step, however under compressive load the potential energy increases in an oscillatory manner.

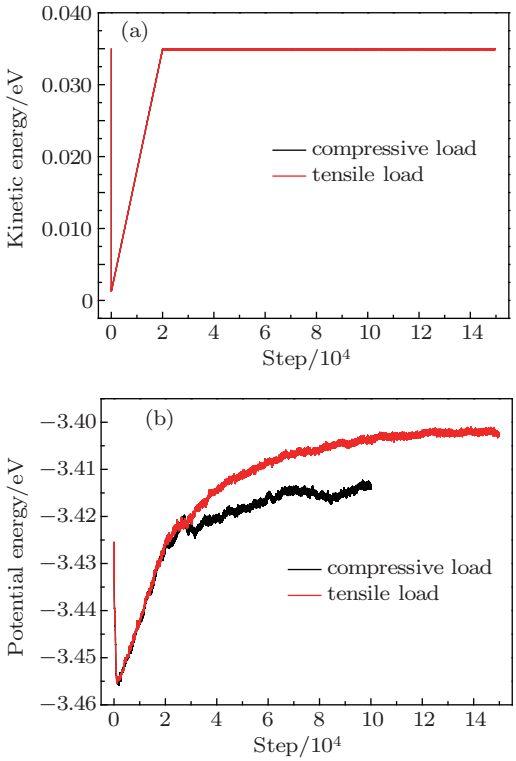


Fig. 2. (color online) Kinetic energy (a) and potential energy (b) of nanowires under tensile and compressive loads.

3.1.2. Mechanical properties discussion

Figure 3 shows that with the strain increasing each of the curves is almost a line like that in the elastic stage of macroscopic material at the beginning of deformation. Then the system arrives at the yield stage and the stress at the peak of the curve is defined as the yield stress σ_s. After yielding, system stress decreases rapidly and its speed is faster under tensile load than under compressive load.

Table 1 gives some mechanical values of twin gold crystal nanowires under two load styles, where σ_s, ε_s, E are yield stress, yield strain and Young modulus respectively. The

nanowires yield more easily under compressive load than under tensile load, however the Young modulus in the former case is twice as great as that in the latter case.

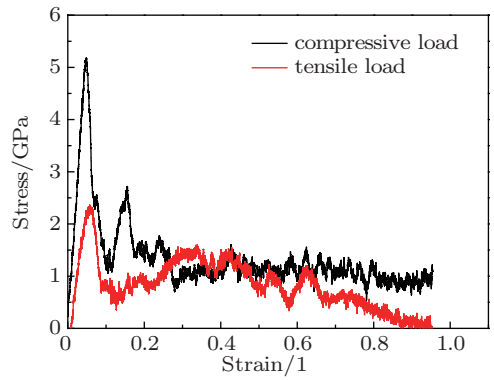


Fig. 3. (color online) Relationship between stress and strain of nanowires under compressive load and tensile load.

Table 1. Mechanical values of nanowires under different load styles.

Load	σ_s/GPa	ε_s	E/GPa
Tensile	2.35975	0.05752	41.02
Compressive	5.17801	0.04852	106.72

3.1.3. Micro-deformation discussion

In the paper, we discuss the micro-deformations by using colored atom balls, where blue atoms are the twin boundary or dislocation atoms and yellow atoms are stable.

Relaxations under tensile and compressive loads are similar due to the fact that models are not applied loads. In the process of compression, compressive instability leads to the fact that dislocations appear, which come into slip planes. The models will be broken in the form of pileup along slip planes. Nevertheless, there are different statuses in the models under tensile loads. Slip planes break the twin crystal structure, around which the non-crystallizing of the atoms is acute and the necking phenomenon turns up until it is broken. The directions of dislocations are both 45 angle and twin boundaries prevent the dislocation from developing.

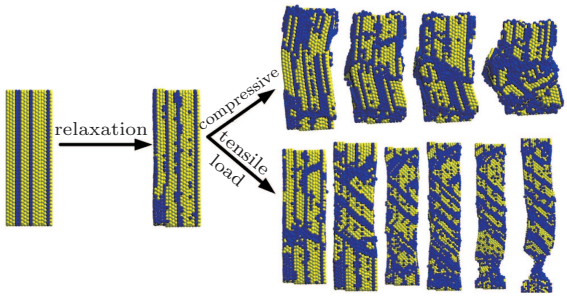


Fig. 4. (color online) Micro-deformations of nanowires under compressive load and tensile load.

3.2. Properties of different length nanowires

On the basis of the above mentioned models, different length twin gold nanowires are simulated. Different mechanical properties are obtained.

3.2.1. Energy discussion

The energy increases linearly during the relaxation. The system's average kinetic energy is dependent only on temperature (Eq. (2)), so the average kinetic energies of different length models are coinciding with each other in the process of the whole simulation. The potential energy curves are different while their tendencies are similar. Also, the longer the nanowire, the lower the potential energy curve is (Fig. 5(a)). Figure 5(b) shows the potential energy at a certain step, where E_f is the potential energy at the final step of the simulation. All certain potential energies are small with the length increasing, and the final step potentials are biggest, which verifies the fact that the potential energy of the steady state is smallest.

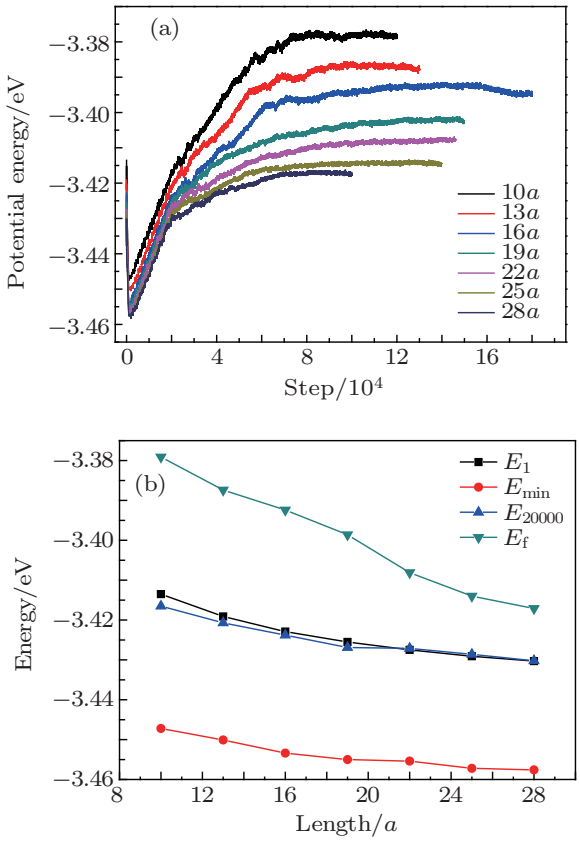


Fig. 5. (color online) (a) Average potential energies versus simulation step and (b) the particular step potential energies versus simulation step for different length nanowires.

3.2.2. Mechanical properties discussion

Although the lengths of gold nanowires are different, the variation trends of curves are similar (Fig. 6). The system begins with elastic deformation until the yield stage, then falls in an oscillatory manner until the break. The longer the nanowire, the more rapidly the break happens. Table 2 gives the mechanical values of different length twin gold crystal nanowires in the yield stage. When the length $L > 19a$, Young modulus E diminishes clearly and the curves (Fig. 6) have no secondary peak values.

Table 2. Mechanical values of different length nanowires in the yield step.

	10a	13a	16a	19a	22a	25a	28a
σ_s/GPa	2.6060	2.6590	2.66066	2.54622	2.18770	2.39526	2.26787
ε_s	0.04636	0.04578	0.04644	0.04451	0.04200	0.04664	0.06379
E/GPa	56.21	58.08	57.29	57.21	52.07	51.34	35.55

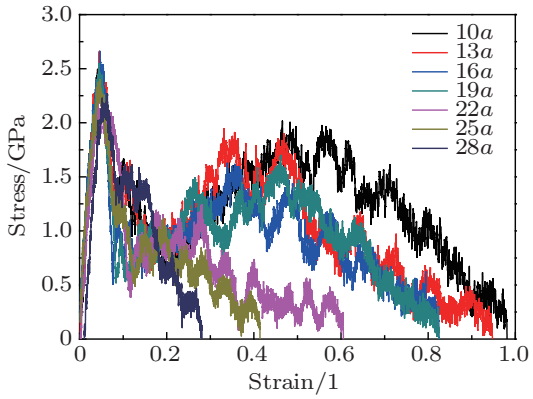


Fig. 6. (color online) Stress–strain curves of different length nanowires.

3.2.3. Micro-deformation discussion

Figure 7 shows representative microscopic structures of different length twin gold nanowires in broken stages. When the nanowires yield, low coordination number atoms of the system increase. Then slip planes come out immediately, at this point, stress decreases with the increase of strain. Twin gold nanowires with a shorter length form a stress well, because most of the atoms in the nanowires are in a non-crystallizing state and there are many low coordination number atoms. Through a combination of low coordination atoms and slip planes, a stress well appears in each of the stress–strain curves of the nanowires. As the simulation continues, the non-crystallizing atomic motion of the atoms around slip planes increases, which brings about the damage of the initial twin crystal structure. Then the necking phenomenon appears, resulting in the fracture of nanowires. Under the same tensile speed load, the longer

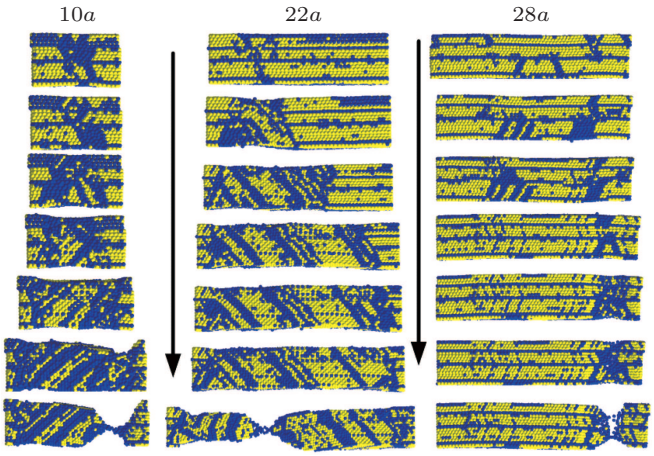


Fig. 7. (color online) Micro-deformations of different length nanowires.

the nanowires, the smaller the influence of non-crystallizing atomic motion of the atoms around slip planes on the whole system after yielding.

Also, in the progress of tension it is verified that the dislocations destroy the prevention of a twin boundary and keep developing along the length direction.[18]

3.3. Properties of different twin boundary nanowires

The twin boundary spacing has an effect on the mechanical properties when the tensile direction is vertical to the twin boundary orientation.[19] There appear different properties when the loading direction is parallel. The other two twin boundary models are simulated (Fig. 8). Because only twin boundary spacings are different, the average energies are all the same.

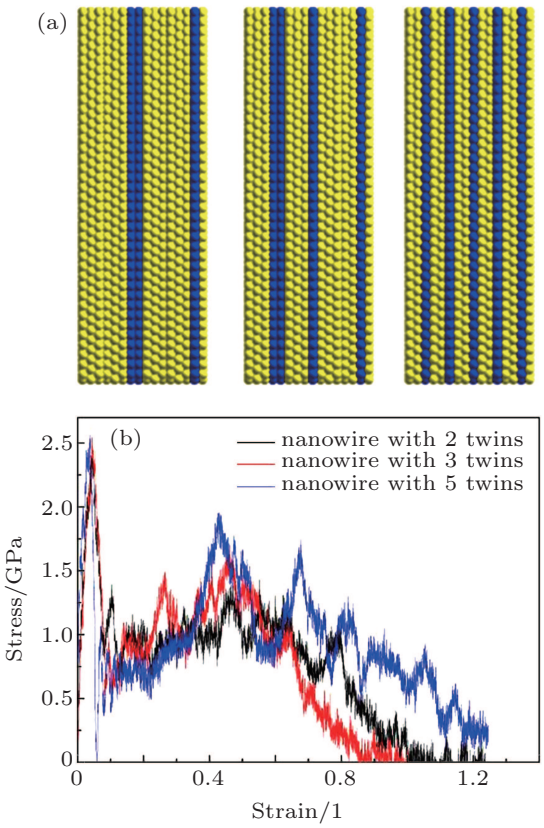


Fig. 8. (color online) Three twin boundary nanowires (a) and their stress–strain curves (b).

Figure 8(b) shows that the yield stresses of nanowires under tensile loading, whose directions are parallel to the twin boundary, are the same, which is different from the scenario under vertical tensile loading. Only the stress of the 5 twin

nanowire decreases faster after yielding. The twin boundary spacing affects only the rate of dislocation developing.

4. Conclusions

In this work, we investigate the mechanical properties of twin gold crystal nanowires by the molecular dynamics method through controlling variables. The nanowires under tensile or compressive loads, different length nanowires, and different twin boundary nanowires are simulated respectively. The micro-deformation is the progress of dislocation developing by breaking twin boundaries.

When the models are under different style loads, the mechanical properties are different. The Yong modulus under a compressive load is about twice that under a tensile load. The compressive properties of twin gold nanowires are superior to its tensile properties.

The length of nanowires also affects the mechanical properties. When the length of nanowires is short: $L = 10a$, $13a$, $16a$, the nanowires length changes hardly affect the mechanical properties of twin gold nanowires; when the length turns long with the increase of the nanowire length, system yield stress and Young modulus decrease and the yield strain increases. The longer the nanowires, the less the influence of non-crystallization is.

When the loading direction is parallel to the twin boundary, the twin boundary spacing hardly affects the mechanical properties.

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