Computational Materials Science 117 (2016) 40–44

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Molecular dynamics simulation of temperature effect on tensile mechanical properties of single crystal tungsten nanowire

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ARTICLE INFO

Article history:
Received 1 June 2015
Received in revised form 16 December 2015
Accepted 1 January 2016

Keywords:
Temperature
Molecular dynamics
Mechanical property
Microscopic deformation mechanism
Single crystal tungsten nanowire

ABSTRACT

High-purity single crystal tungsten nanowire was prepared by the metal-catalyzed vapor-phase reaction method, which was firstly proposed by our research group. Its tensile stress–strain curves and microscopic deformed structures at different temperatures were simulated by molecular dynamics method, in order to study the effects of temperature on its tensile mechanical properties and failure mechanisms. Research results show that the stress–strain curves can be all divided into five stages: elastic, damage, phase transition (dominant), hardening and failure stages. Elastic modulus, tensile strength and strain of phase transition are decreased with increase of temperature, while hardening peak stress is first increased and then decreased. There exists a critical temperature T_c for its phase transition mechanism. When $T \leqslant T_c$, the phase transition occurs in one direction and leads to less damage and random failure in its damage zone. When $T > T_c$, the phase transition occurs in two directions and leads to more damage (twin plane) and failure in its twin plane. That is quite different from FCC metal, where there is only one direction of phase transition.

1. Introduction

Single crystal tungsten nanowire has better physical and chemical properties than macro tungsten. As a new metal nanowire, it has wider application prospect in aerospace, electronic machine, bio-pharmaceutical and other fields [1–4]. Currently, it is prepared mainly by methods of high-temperature gas-phase deposition [5], electrochemical etching [6] and RF sputtering [7], in which the growth process of nanowire cannot be well controlled. Our research group has proposed a new method of metal-catalyzed vapor-phase reaction to prepare single crystal tungsten nanowire of high purity and complete body-centered cubic structure (BCC) successfully [8]. It is very important to study mechanical properties and failure mechanisms of this metal nanowire. Up to now, there are only elastic modulus and hardness available by the nano indentation or bending test [9,10].

Due to limitation in test conditions, computational methods are usually adopted, e.g., molecular dynamics simulation, Monte Carlo simulation and discreteness simulation methods, in which the molecular dynamics method is the most widely used [11]. Current literatures are mainly focused on mechanical properties of the metal nanowire of face-centered cubic structure (FCC), including tensile mechanical properties influenced by strain rate, temperature and surface defect [12–18], compressive [19,20] and bending properties [21]. However, there is short of study on single crystal tungsten nanowire of body-centred cubic structure (BCC), especially on its mechanical properties and failure mechanisms at different temperatures.

In this paper, molecular dynamics method was used to study stress–strain curves and microscopic deformations of single-crystal tungsten nanowire at different temperatures. Effects of temperature on its mechanical properties and failure mechanisms were investigated in order to provide theoretical basis for its wide application.

2. Calculation scheme

2.1. Calculation method

The molecular dynamics method with the Large-scale atomic/molecular massively parallel simulator (LAMMPS) software [22] is adopted to simulate tensile mechanical behaviors of the single-crystal tungsten nanowire. In nature, molecular dynamics is a particle method by calculating the space position of any particle to describe the systematical mechanical behaviors based on the Newton second law:

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http://dx.doi.org/10.1016/j.commatsci.2016.01.001
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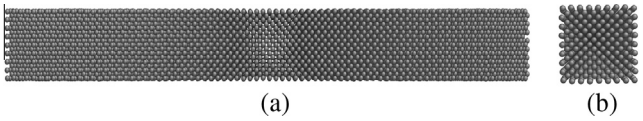

Fig. 1. Initial configuration of the single crystal tungsten nanowire (a) front view; (b) side view.

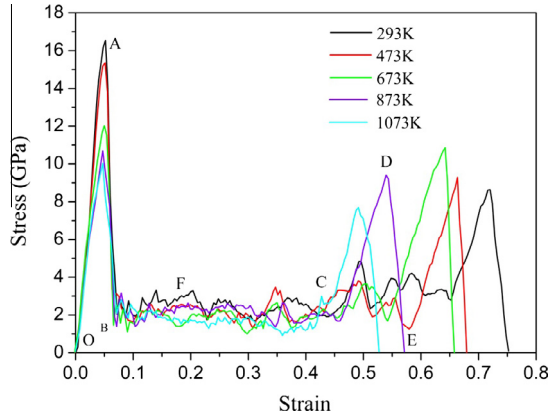

Fig. 2. Tensile stress–strain curves of single crystal tungsten nanowire at different temperatures.

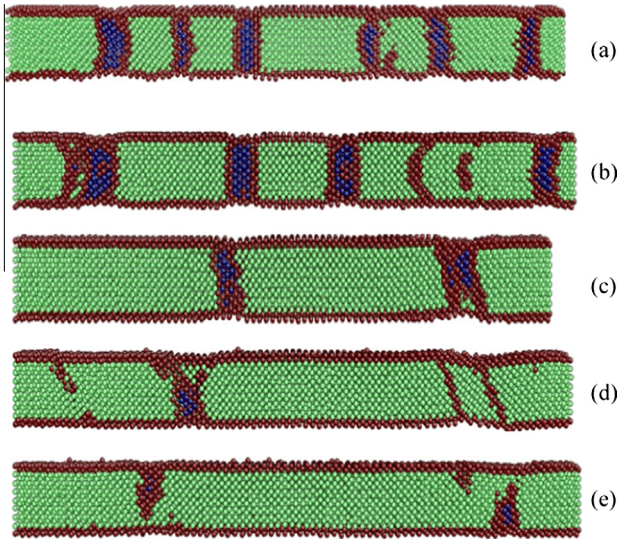

Fig. 3. Microstructures of single crystal tungsten nanowire at different temperatures (point B) (a) 293 K (ε = 8.8%); (b) 473 K (ε = 8.8%); (c) 673 K (ε = 5.6%); (d) 873 K (ε = 6.4%); (e) 1073 K (ε = 6.4%).

$$a_i(t) = \frac{d^2 r_i(t)}{dt^2} = \frac{F_i(t)}{m_i} \tag{1}$$

where $F_i(t)$, m_i, $r_i(t)$ and $a_i(t)$ are resultant force, mass, space position and acceleration of the particle i.

$F_i(t)$ can be obtained by a negative derivative of the potential function U with respected to $r_i(t)$:

$$F_i(t) = -\frac{\partial U}{\partial r_i(t)} \tag{2}$$

In molecular dynamics simulation, the choice of inter atomic potential function is very important. Currently, there are several potential functions available, such as LJ pair potential, Morse potential and embedded atom potential. A modified embedded atom potential proposed by Zhou et al. [23] has been successfully applied to simulate mechanical behaviors of metal multilayer systems [24,25] since it can better describe the physical and mechanical properties including lattice constant, elastic constant, cohesive energies, and the vacancy formation energy. In this study, the modified embedded atom potential function is adopted as follows.

$$U = \sum_i \left[\frac{1}{2} \sum_{j \neq i} \phi_{ij}(r_{ij}) + F(\rho) \right] \tag{3}$$

where $\phi(r_{ij})$ is potential term, representing the interaction between atom i and j separated by a distance r_{ij}, and $F(\rho)$ is correction term, corresponding to embedded energy of the atom i embedding into the electron density $\rho(r_{ij})$.

When the material is loaded in x-direction tension, the corresponding atomic tensile stress σ_i^{xx} in x direction can be calculated in terms of EAM potential function as follows [26]:

$$\sigma_i^{xx} = \frac{1}{\Omega_i} \left\{ -m_i v_i^x v_i^x + \frac{1}{2} \sum_{j \neq i} \left[\frac{\partial \phi}{\partial r_{ij}} + \left(\frac{\partial F}{\partial \rho_i} + \frac{\partial F}{\partial \rho_j} \right) \frac{\partial f}{\partial r_{ij}} \right] \frac{r_{ij}^x r_{ij}^x}{r_{ij}} \right\} \tag{4}$$

where Ω_i is the atom volume, m is the mass, and v_i^x is the velocity component in x direction. Φ, F, ρ and f are parameters of EAM potential function.

The tensile strain in x direction ε_{xx} is determined by

$$\varepsilon_{xx} = \frac{L_x - L_{x0}}{L_{x0}} \tag{5}$$

where L_{x0} and L_x are initial length and total length in x direction, respectively.

2.2. Calculation model

As shown in Fig. 1, the single-crystal tungsten nanowire is a cuboid of 25.28 nm × 2.528 nm × 2.528 nm. Its initial configuration is ideal lattice of BCC structure, where coordinate axes of X, Y, Z are along the crystal orientations of [100], [010], and [001],

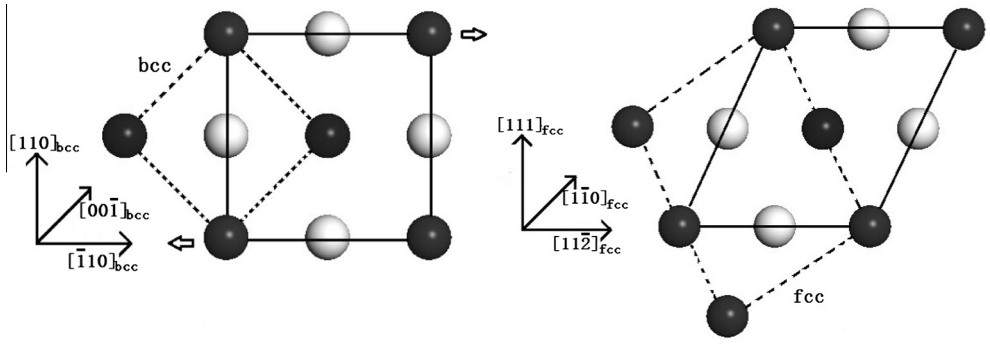

Fig. 4. Transition of BCC–FCC structures (the atoms in black and white are in the $[001]_{bcc}$ direction of the $\{001\}_{bcc}$ plane and in the $[110]_{fcc}$ direction of the $\{110\}_{fcc}$ plane, the dotted and solid line represent the lattice and the slip plane, and the arrow represents the slip direction.).