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The influence of crystal defects on the elastic properties of tungsten metals

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HIGHLIGHTS

- The energy of FCC structure generated during the plastic deformation was higher than that of the BCC structure, thus the system energy was consumed.
- The energy of HCP lattice was higher than that of FCC lattices. The two kinds of lattices form the twin belt with a long range periodic order, and so the system stress changed periodically with the strain.
- The growth of the disordered structure not only destroyed the long range periodic structure of the twin belt, but also produced a cavity, which absorbed a large amount of energy and finally made the system fractured.
- The effect of temperature on the fracture was equivalent to the effect of the vacancy, and the correlation between temperature and vacancy was quadratic.

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ABSTRACT

The four stretching process stages of the elastic, plastic, stalemate, and fracture were represented for the metal tungsten by using molecular dynamics method. The young's modulus, yield strain and yield stress were calculated. The microscopic mechanics of the stretching process is analyzed. The energy of FCC and HCP generated was higher than that of BCC, so that the energy of the system increased, and the stress level was lower in the plastic deformation stage. In the late stage of plastic deformation, the growth of the twin belt was of long range ordered periodic structure, which made the system stress change periodically. In the Stalemate Stage of deformation, the other disordered structure, setting in the HCP structure of the twin belt, growed to absorb energy and generate cavity under stress and makes the lattice fracture. The yield stress of metal tungsten decreases monotonically with temperature and vacancy. The effects of temperature and vacancy on the lattice fracture were discussed.

1. Introduction

Tungsten is one of the most likely candidates used as the first wall materials facing the plasma in the future Tokamak of nuclear fusion, with its high melting point, high conductivity and low sputtering [1–3].

The failure and fracture of material is a typical feature of its brittleness, which is usually closely related to the lattice breaking and plasticity. The growth and connectivity of cavity in the lattice are the nature for the fracture, and the growth of the cavity is often attributed to the movement of dislocations. The defects, existing in the crystal, can sometimes reduce and sometimes improve the material properties [4–7]. It is important, for the design of the candidate materials used as the first wall facing the plasma, to study the relationship of the fracture with the plastic of tungsten and the effect of defects.

In this paper, the molecular dynamics is used to simulate the stretching process of single crystal tungsten. The microscopic

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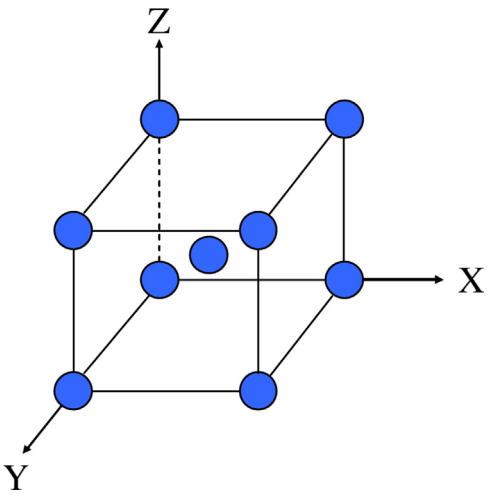

Fig. 1. Lattice of tungsten, which was a body centered cubic (BCC) crystal structure. A super cell with size of $50 \times 10 \times 10$ was provided with periodic boundary conditions in the X, Y and Z directions, in the numerical simulation.

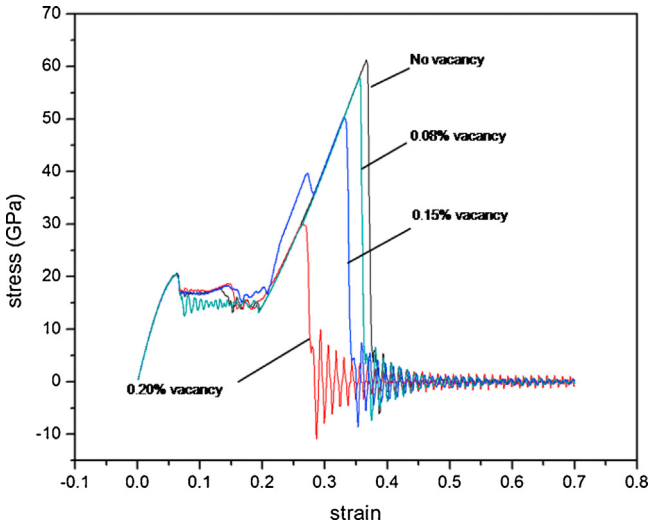

Fig. 2. The relationship between strain and stress of tungsten with the different vacancy concentration in the case of 300 K temperature.

mechanism of plastic and fracture in stretching process is analyzed. The effects of vacancy and temperature on the plasticity and fracture are studied. The relationship between the vacancy and temperature is discussed.

2. Methods

The principle of molecular dynamics is that, according to the interaction potential of particles, Newton's equations of motion for multi-body system were established; the particle trajectories in space and the statistical macroscopic physical characteristics of system were calculated, under a certain condition of temperature and pressure [8–10].

The lattice of the metal tungsten, as shown in Fig. 1, is a body centered cubic (BCC) crystal structure, and the lattice constant $a = 0.3165$ nm. In Fig. 1, the X, Y and Z coordinate axes were corresponding to the [1 0 0], [0 1 0] and [0 0 1] directions of the BCC crystal. A super cell with size of $50 \times 10 \times 10$ was provided with periodic boundary conditions in the X, Y and Z directions, in the numerical simulation.

Nose–Hoover method [11] was used to adjust the temperature of the NPT ensemble, in which the amount of substance (N), pressure (P) and temperature (T) were conserved. And the relaxation of tungsten crystal was carried out in the NPT system, and the energy fluctuation was very small. Under the NPT ensemble, the stretching of the metal tungsten was simulated by the way of the X axis, with the strain rate 0.002/ps and the time step 0.005 ps. The interatomic potential function of tungsten was presented by Daw with the embedded atom potential EAM [12,13] . The calculations were completed using the classical molecular dynamics code LAMMPS which is designed for parallel computers and distributed under the GNU public license [14,15].

3. Results and discussion

Fig. 2 shows the relationship between the strains and the stress of the metal tungsten with the lattice defects of vacancies in the case of 300 K temperature. The BCC structure in the cell was transformed to the surface centered cubic (FCC), the hexagonal close-packed (HCP), and other lattice structures under the stress of the stretching process. Fig. 3 shows the ratio of the three kinds of lattice BCC, FCC, and HCP, under the tensile strains.

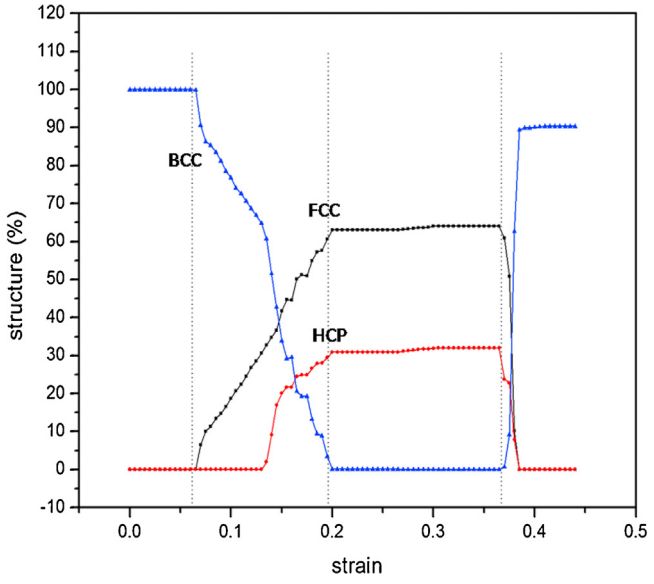

Fig. 3. The ratio of lattice BCC, FCC, and HCP.

Figs. 2 and 3 represent that the stretching process of the metal tungsten included four stages: elastic deformation, plastic deformation, strengthening and fracture.

Fig. 4 shows the structure of the super cell in the stretching process. The tensile strain range of the stage of the reversible elastic deformation was between 0 and 0.063. At this stage, the stress was proportional to the strain, and the whole system was maintained as the BCC lattice structure as shown by Fig. 4(a). The Young's modulus was obtained as 328 GPa by fitting the elastic line. By comparison, the Young's modulus of annealed tungsten is 411 GPa [16], those of single crystal tungsten nano-whiskers are from 300 to 414 GPa [17], and that of 375 GPa calculated for single crystal tungsten nano-whiskers [18] . So the calculated Young's modulus in this work is in the range of those reported in the literatures and acceptable.

The second stage of the stretching process was a plastic deformation stage. At the beginning of plastic deformation, the yield strain was 0.063 and the yield stress was 20.65 GPa. By comparison, the yield stress of annealed tungsten is from 550 to 620 MPa [16], but the calculated yield strain of single crystal tungsten nano-whiskers was 0.072 and the yield stress 25.4 GPa [18]. It indicates

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