4 - 12 Mechanical Properties of Monocrystalline Tungsten Simulated with Molecular Dynamics

Wang Dong, Gao Ning, He Wenhao, Cui Minghuan, Gao Xing and Wang Zhiguang

Due to its unique properties, *e.g.* high melting temperature, high thermal conductivity and low sputtering erosion, tungsten (W) has been selected as one of the most promising candidate materials for the divertor in ITER and future fusion devices[1]. In fusion reactors, tungsten will suffer from radiation damages by energetic particles, leading to the degradation of material properties, affecting the life time of components. Void is one of important typical radiation defects. It changes the local stress field, which influences the dislocation behaviors and the mechanical properties of materials. In this work, the mechanical properties of monocrystalline (mc) tungsten and the influence of void on it are studied with molecular dynamics method using LAMMPS code[2]. This study will not only improve our understanding of radiation damage, but also provide important information for the upgrading of material properties.

The potential fitted by Bonny[3] was used to describe the W-W interaction. Tensile tests were applied on mc W along $<100>$, $<110>$ and $<111>$ directions with strain rate of 1×10^8/s at 300 K. Fig. 1(a) shows the stress-strain curves of mc tungsten. It can be found that the mechanical properties of W is anisotropic. The tensile strengths in $<100>$, $<110>$ and $<111>$ are about 26.68, 40.84 and 46.63 GPa, respectively. Comparing with DFT results[4] the tensile strengths are in good agreement in $<100>$, lower in $<110>$ and higher in $<111>$. In addition, the Young's moduli are about 430.93 GPa in $<100>$ and 545.26 GPa in $<110>$ and $<111>$ directions. It is found that $<100>$ is the weakest direction of tungsten, and $<111>$ to be the strongest. Since the deformation of BCC metal in $<100>$ direction will experience the "Bain Path", changing from BCC to FCC structure, leading to the decrease of strength in this direction. However, $<111>$ is the close packed direction of BCC lattice, and the interaction of each atoms along $<111>$ is strong, making it the strongest direction.

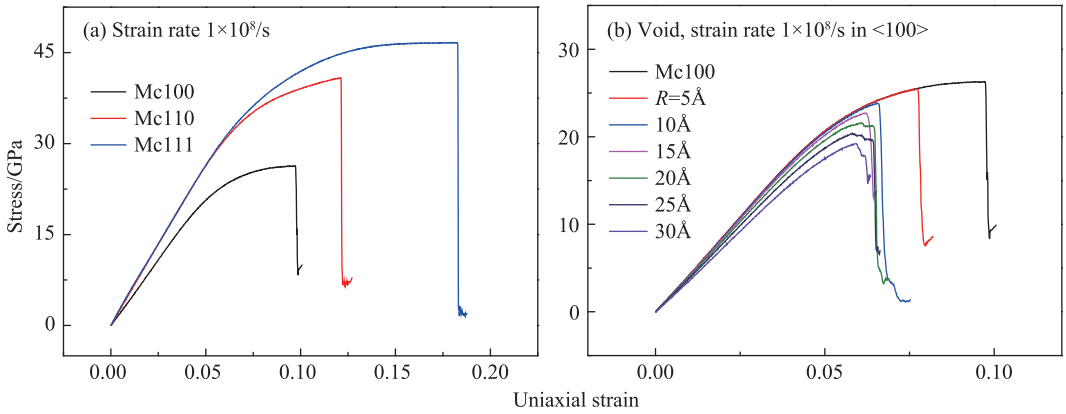

Fig. 1 (color online) The stress strain curves of mc tungsten at a strain rate of 1×10^8/s at 300 K. (a) pure mc W deformed along $<100>$, $<110>$ and $<111>$ directions, denoted as mc100, mc110 and mc111 respectively. (b) mc W containing a void deformed along $<100>$ direction. The void radius ranges from 5 to 30Å.

To study the effect of void on the mechanical properties of mc W, tensile tests were applied to get the stress-strain response of mc W containing a void at 300 K. The radii of considered void range from 5 to 30Å. The strain was applied with a rate of 1×10^8/s in $<100>$ direction. Results are shown in Fig. 1(b). It is indicated that the existence of void decreases the tensile strength and Young's modulus of mc W, which decrease with the increasing of void radius. The reason is that the void decreases the critical shear stress for crystal sliding, leading to the occurrence of sliding near the void. Then the tensile strength and elastic modulus decrease when void exists. This result is in agreement with the results of Ni[5] and Cu[6,7], except that the elastic moduli are not changed in the literatures. This difference is due to that the ratios of void size to simulation box are not kept constant in our work. It is indicated that the presence of void, especially large void, will degrade the mechanical properties of mc tungsten. In the application of mc W, voids should be diminished to strengthen it.

References

[1] G. Federici, C. H. Skinner, J. N. Brooks, et al., Nucl. Fusion, 41(12r)(2001)1967.