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Numerical study of the effect of hydrogen on the crack propagation behavior of single crystal tungsten

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HIGHLIGHTS

- Hydrogen facilitates dislocation emission from crack tip.
- There are three mechanisms of hydrogen effect on crack propagation.
- Hydrogen can either improve or reduce the ductility of single crystal tungsten.

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ABSTRACT

An atomic model of single crystal bcc tungsten containing a pre-existing crack was built and molecular dynamics simulations were performed to investigate the crack propagation behavior with and without hydrogen atoms under uniaxial tensile load. Two kinds of crystal orientation were analyzed to study the effect of hydrogen on different crack propagation patterns. The results show that hydrogen can either improve or reduce the ductility of tungsten. High hydrogen concentration could result in the rearrangement of tungsten atoms ahead of the crack tip and reduce the stress concentration in the neighboring area around the crack tip. This will prevent the crack from propagation temporarily and therefore increase the fracture strain. Besides, hydrogen atoms can also facilitate the dislocation emission from the crack tip, which is accompanied by a larger plastic deformation. Both the mechanisms improve the ductility of tungsten. However, a void could be nucleated in a local hydrogen-rich area under tensile load. Its growth and link-up with the main crack will accelerate the crack propagation and speedup the fracture process, which diminishes the ductility of tungsten.

1. Introduction

Magnetic confinement fusion reactors, such as ITER and DEMO, require advances in both plasma physics technology and materials science, including structural materials and the materials surfaces exposed to the plasma. Tungsten is one of the most important candidates to satisfy the varied demands of the plasma facing materials (PFM) due to its high melting point, low sputtering yield and good thermal properties [1,2]. As a PFM, W is supposed to withstand intense heat loads and bombardment of high fluxes of hydrogen (H) isotope ions. The heat loads could induce high thermo stresses therefore result in fatigue and surface cracking [3,4]. Being the lightest element, H atoms can easily diffuse into the bulk, be immobilized by point defects and lead to blistering on W surface. Experimental observation confirms that the thickness of the blister covers is orders of magnitude larger than the projected range of H atoms [5], which shows evidence of the high mobility of H atoms in W.

Meanwhile, many metals absorbing hydrogen show the reduction of mechanical properties which is known as hydrogen embrittlement. Various theories have been developed to explain this phenomenon. Among them, hydrogen-enhanced decohesion (HEDE) [6] and hydrogen-enhanced local plasticity (HELP) [7] are well accepted. The HEDE model assumes that H causes a weakening of the bonds of metal atoms and leads to planar (cleavage) failure. In the HELP theory, H tends to form a Cottrell atmosphere [8] around dislocation cores that facilitates dislocation motion, causing an increase in local plasticity. Despite the extensive works concerning hydrogen embrittlement, the micro mechanism is still not fully understood. The interaction between H and dislocations is a complex process. Atomic simulations of Fe show that H atoms trapped at screw dislocation cores can either increase or decrease the mobility of screw dislocations, depending on H concentration, strain rate and temperature [9]. As for W, research work of the effect of H is very

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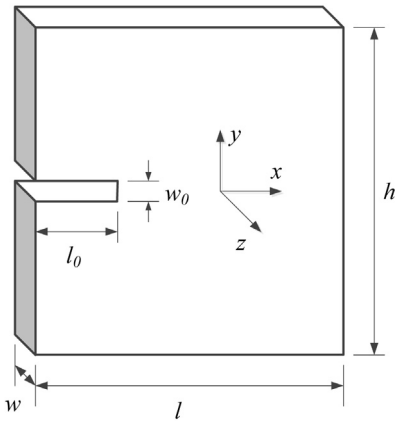

Fig. 1. The sample geometry of single crystal bcc W with a crack.

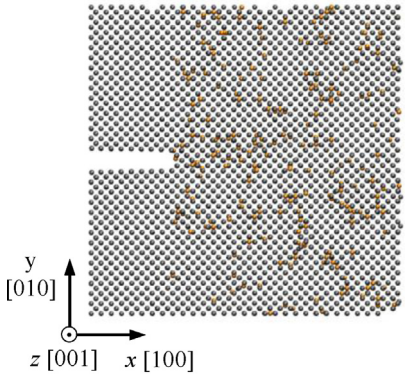

Fig. 3. Atomistic configuration of crystal orientation (B) with 200 H atoms (black dots represent W atoms and orange ones H). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

limited. Although our previous simulations indicate that the elastic modulus and yield stress of bulk W decrease due to the retention of H [10], further investigation need to be done to accurately predict the mechanical response of W in real fusion environment and understand the micro mechanism.

In the present study, molecular dynamics (MD) simulations were performed to investigate the effect of H on the crack propagation behavior inside single crystal W under uniaxial tensile load. The simulation methods and the model are detailed in Section 2. The results are described and analyzed in Section 3. Conclusions are presented in Section 4.

2. Simulation method and atomistic model

In this work, a rectangular sample of single crystal bcc W containing a pre-existing central crack is considered. Considering the symmetry of the problem, only half of the sample is modeled, as shown in Fig. 1. The initial crack was introduced by removing certain lays of W atoms on the left side so that the crack opening is beyond the cut-off of W—W bonds employed in the potential (3.8 Å). Due to the symmetry, the atoms lying in the left border plane (see the shaded surface in Fig. 1), of the model, which is also the middle plane of the entire sample, are fixed in x direction while other atoms are free to move in all three directions. Periodic boundary conditions were applied in the y and z directions and free boundary condition in the x direction.

Crack propagation analyses were performed for two kinds of crystal orientation. In orientation (A), as shown in Fig. 2, the axes were chosen to be x-[1 1 0], y-[$\bar{1}$ 1 0] and z-[0 0 1]. The model has a size of $21\sqrt{2}a \times 21\sqrt{2}a \times 6a$ where a is the lattice constant of bcc

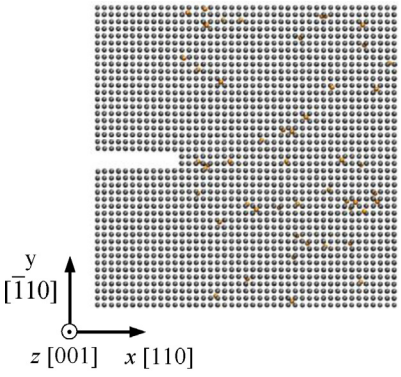

Fig. 2. Atomistic configuration of crystal orientation (A) with 50 H atoms (black dots represent W atoms and orange ones H). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

W and was taken as 3.165 Å (angstrom) [11]. The initial crack has a length of $6\sqrt{2}a$ and lies in the (1 1 0) plane. In this case, there is no slip plane in the x–y plane. We can expect no dislocation emission from the crack tip. In orientation (B), as shown in Fig. 3, the coordinate system is chosen as the basic cubic orientation, i.e. x-[1 0 0], y-[0 1 0] and z-[0 0 1]. The dimensional parameters are $l = 30a$, $h = 30a$ and $w = 6a$. The length of the crack is $8a$. In this case, there exists the {1 1 0} slip planes in the x–y plane and we can expect dislocation emission from the crack tip.

H atoms were deposited in the area from the crack tip to the right end of the crystal randomly and uniformly without consideration of the existing W atoms. Thus, some H atoms might be very close to or even overlap with W atoms, which could cause enormous repulsive forces between H and W atoms and therefore blow atoms out of the simulation box at the beginning. To avoid this we started the simulations with a constant NVE updates of position and velocity for all atoms. Meanwhile, a limit was imposed on the maximum distance that an atom can move in each time step. The value of the maximum distance was chosen to be 0.001 Å. When the displacement of an atom calculated in one time step integration is more than 0.001 Å, the limit value will be used. After a relaxation of 5000 time steps, all atoms were in reasonable sites. Then, the system was equilibrated at 300 K and 0 bar for 20 ps, which is long enough for the total energy of the system to arrive at a stable state. Figs. 2 and 3 illustrate the atomic configuration after equilibration.

For a W–H system, the most popular potential is the one developed by Juslin [12]. Previous work [13–15] shows that this potential can describe the interaction between W–W and W–H atoms properly. However, Li [15] reported that Juslin's potential may have some limits in describing the interaction between H atoms and vacancies in bulk W. Li developed a new potential [16] which is supposed to be more accurate in simulating systems containing defects like vacancies. However, the practicability of the new potential is yet to be verified and the enlarged cut-off makes the integration much more time consuming. In our simulations, the potential developed by Juslin was employed.

The tensile load was applied in a constant strain rate along the y direction. At each time step, the y coordinates of all atoms were rescaled according to the given strain rate. Zero pressure was applied in z directions so that they respond to the tensile strain dynamically. The given strain rate is $5 \times 10^8\ s^{-1}$. This high strain rate is inherent to MD simulation which includes dynamical information usually on ps or ns timescales. To catch the motion of H atoms, the time step was chosen to be 0.1 fs which is about 1/100 of the vibration time period of H atoms in interstitial sites of W lattice [10].