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Atomistic simulations of the effect of embedded hydrogen and helium on the tensile properties of monocrystalline and nanocrystalline tungsten

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HIGHLIGHTS

- Uniaxial tensile behavior of monocrystal tungsten (C-W) and nanocrystalline W (NC-W) have been investigated.
- Dislocation-based activities dominate the plastic deformation of MC-W.
- Grain boundary-based activities dominate the plastic deformation of NC-W.
- H/He atoms have significant impacts on the tensile behavior of MC-W and NC-W.
- Strong strain enhanced He cluster growth has been revealed.

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ABSTRACT

Uniaxial tensile properties of monocrystalline tungsten (MC-W) and nanocrystalline tungsten (NC-W) with embedded hydrogen and helium atoms have been investigated using molecular dynamics (MD) simulations in the context of radiation damage evolution. Different strain rates have been imposed to investigate the strain rate sensitivity (SRS) of the samples. Results show that the plastic deformation processes of MC-W and NC-W are dominated by different mechanisms, namely dislocation-based for MC-W and grain boundary-based activities for NC-W, respectively. For MC-W, the SRS increases and a transition appears in the deformation mechanism with increasing embedded atom concentration. However, no obvious embedded atom concentration dependence of the SRS has been observed for NC-W. Instead, in the latter case, the embedded atoms facilitate GB sliding and intergranular fracture. Additionally, a strong strain enhanced He cluster growth has been observed. The corresponding underlying mechanisms are discussed.

1. Introduction

During the operation of fusion reactors, plasma facing materials (PFMs) will be damaged through plasma/surface interactions. The damage, for example, can be caused by the D-T fusion phase reaction: $D + T \rightarrow \alpha + n$ (14 MeV), wherein the PFMs will be subjected to low energy, high flux hydrogen (H) isotopes and helium (He) in addition to high energy neutrons (n). The plasma irradiation of the PFMs causes significant modification of their crystal structure and morphology, leading to adverse material behaviors. Therefore, it is critical to select suitable PFMs that can withstand the specific environment of fusion reactors. Tungsten (W) has been regarded as one of the most promising candidates for PFMs [1].

Experimental and theoretical research efforts to study the H/He irradiation response of W have been extensively undertaken for decades. Many experimental results show that microstructural damage, including point defects, dislocation loops, bubbles, pinholes, "fuzz", etc. [2–5], can be formed due to the exposure to H/He irradiation. For the case of low energy, high flux He irradiation at

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elevated temperatures, formations of pinholes and "fuzz" are the major microstructural changes [2,6]. In contrast, when W samples are subjected to high energy He irradiation above a certain fluence [7,8], surface blistering and exfoliation are the major morphological changes. Recent research efforts have been focusing mainly on the low energy, high flux H/He irradiation which is similar to the conditions that PFMs experience in a fusion reactor. Various models and mechanisms based on theoretical simulations including density functional theory (DFT) and Molecular Dynamics (MD) have been proposed and used in order to describe the degradation mechanisms of W exposed to irradiation by H and He. For example, several models have been proposed for the mechanism of "fuzz" formation. Observation of He plasma induced nanostructures called "fuzz" was first reported by Takakmura et al. [9] Such nanostructures are severely deformed W with sizes of several tens of nanometer. The detailed TEM analysis revealed that there exist nanometer-sized helium bubbles inside the nanostructure [10]. "Fuzz" can be formed at temperatures between 1000 K and 2000 K, and when the helium ion energy is over 20–30 eV [6]. These models have been summarized in the work of Ito [11]. Accumulation of He ions and the formation of bubbles which can easily grow leading to localized plastic deformation have been regarded as a plausible explanation. Based on MD simulations, Krasheninnikov et al. [12,13] suggested that the enhanced flow of W atoms by creep and helium cluster formation with large inserted He concentration be responsible for the growth of "fuzz" at high temperatures. Additionally, experimental results indicate that irradiation by H and He causes different kinds of morphological changes on the W surface. Surface blistering with micrometer depth is the main morphological change caused by the bombardment of H isotope ions [14,15]. However, it is pinholes and "fuzz" that form right at nanometer depths for He irradiation, and there are bubbles in the as-formed nanostructures [2,6]. This indicates that there are different damage evolution mechanisms between H induced damage and He induced damage. However, relevant research efforts on this issue are scarce.

Experimental examinations of irradiation resistance have been mainly performed on polycrystalline W [16–18]. However, computational simulations carried out so far are oriented to study H/He behaviors including diffusion, trapping and clustering in very ideal systems such as single crystals and bicrystals [19–21]. In realistic material systems, a large variety of defects, i.e. dislocations, grain boundaries (GBs), impurities, etc. are present which can be very different from such ideal systems. Moreover, it is predicted that nanocrystalline tungsten (NC-W) has better irradiation resistance compared to the coarse-grained counterparts due to the high density of dislocations and GBs that can act as sinks for the implanting ions and irradiation induced defects [22,23]. Therefore, it is crucial to investigate the irradiation resistance and damage evolution mechanism considering the above mentioned defects. In particular, the effect of GBs which plays important roles in the properties of polycrystalline materials should be examined in more depth.

Voronoi tessellation is a popular scheme to create a nanocrystalline structure, and the resultant as-constructed nanocrystalline structure is totally random, representing a non-textured bulk polycrystalline material. NC-W constructed by this method has been used to investigate the behavior of H embedded in W. For example, diffusion and trapping behaviors of H in NC-W have been studied using MD with a bond order potential (BOP) for the W-H system [24]. Results show that H preferentially diffuses toward the GBs, substantiating the notion that GBs can act as strong trapping sites. Even though the mechanical properties (e.g., shear strength) of a single crystal W with embedded He have been investigated [13], the effects of embedded He on the plastic deformation mechanism have not been reported so far. Therefore, in the present study, using an NC-W that was constructed by Voronoi tessellation, we will investigate the influence of embedded H and He atoms on the tensile properties of NC-W and MC-W. The effect of strain on H/He cluster growth in W will also be discussed. As such, it is intended that this work could serve as a preliminary step forward towards the design of advanced irradiation resistant W materials with the assistance of defect sinks (e.g. GBs).

2. Simulation method

The open-source MD code LAMMPS [25] was used to study the effects of embedded H and He atoms on the tensile properties of W. An embedded atom method potential (EAM) for large scale atomistic simulation in the ternary W-H-He system developed by Bonny et al. [26] was used. This potential has been proven to accurately reproduce the key atomic interactions between H, He and point defects in the W-H-He system. The detailed validation of the potential including point defect properties of H and He in W, binding energy between H-H, He-He and H-He pairs, binding energy of various VHHe clusters, etc., can be found in Ref. [26].

Two different types of simulations have been performed. In the first case, uniaxial tension of the MC-W (lattice parameter $a = 0.316$ nm) block with periodic boundary conditions in all three dimensions was simulated. The domain has 50 unit cells in each dimension. A number of H and He atoms (H/He = 1:1) determined by an atomic percentage (0.5% < [H and He] < 15%) relative to the number of W atoms are then randomly distributed in the simulation slab. A similar He atom introduction method has been used by Smirnov et al. [13] to investigate the shear strength of W with embedded helium. To equilibrate the system, the total potential energy was first minimized using the conjugate gradient relaxation method and then thermal equilibrium was established by selecting velocities at 300 K and running for 0.1 ns with a 1-fs time step using temperature re-rescaling every 100 time steps. An annealing process was further performed for the isothermal-isobaric NPT equations of motion to zero pressure for 0.1 ns with the same time step. After initial equilibration, uniaxial tensions at five strain rates: 1.0×10^8 s^{-1}, 5.0×10^8 s^{-1}, 1.0×10^9 s^{-1}, 5.0×10^9 s^{-1} and 1.0×10^{10} s^{-1} were applied. The simulation cell was deformed in the y-direction, while the lateral boundaries were controlled using the NPT equations of motion to zero pressure. The simulations continued with a 1-fs time step until 20% strain was reached. In the second case, the mechanical properties of NC-W were investigated as a function of H/He concentration. NC-W with grain size of ~5 nm was created using an in-house Voronoi tessellation code provided by Piaggi [24]. This sample contains 60 randomly oriented grains and is cubic with a box side of 50 lattice constants. The grain size distribution was calculated, and the results were described by a log-normal distribution with a mean grain size of ~5 nm. Parameters for the equilibration procedure and tensile loading conditions used in the second case were the same as those for the MC-W. It should be mentioned that all the simulation were performed at 300 K, which is lower than the PFMs operational temperature (e.g. 550–800 °C for the first wall of a fusion reactor [27]).

3. Results and discussion

In this section, we will first describe the simulated results of the mechanical properties of MC-W and NC-W, including the elastic modulus, stress-strain behavior, etc. Deformation mechanisms of both MC-W and NC-W will be described and discussed. Secondly, the effects of embedded atoms on the mechanical properties of both MC-W and NC-W will be presented. Finally, the evolution of H/He clusters in W during uniaxial tension will be discussed.