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Dislocation climbing mechanism for helium bubble growth in tungsten

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ABSTRACT

Molecular dynamics simulations were used to study the growth process of a He bubble on an edge dislocation in W, and the results indicated that the growth was controlled by a dislocation climbing mechanism. Unlike the well-known loop punching mechanism, the bubble grew by punching out interstitial atoms, which were immediately absorbed into the dislocation core, causing the edge dislocation to climb. Moreover, the dislocation climbing mechanism was shown to be more energetically favorable than the loop punching mechanism for the He bubble growth.

Because of their extremely low solubility in materials, He atoms tend to agglomerate into bubbles after their introduction into not only nonmetallic materials (such as SiC [1] and Si [2]) but also metallic materials, such as Al [3], Au [4], Cu [5, 6], Fe [7], and W [8]. These nanosize He bubbles have a marked impact on the mechanical properties of materials, such as leading high-temperature embrittlement and deteriorating toughness; therefore, it is critical to explore their growth mechanism to enable control of their growth. The dislocation loop punching mechanism has long been regarded as the dominant mechanism for He bubble growth [9]. In this mechanism, an over-pressurized He bubble can grow by punching out an interstitial dislocation loop along the glide plane.

Experimental results have revealed that He bubbles tend to accumulate at internal preexisting lattice defect sites such as vacancies, grain boundaries, and phase interfaces [10–12]. The validity of the loop punching mechanism for He bubble growth at vacancies and grain boundaries has been verified by many experimental and computational works [13–15]. Dislocations are another lattice defect that facilitates He bubble formation. For example, He bubble growth at a twist grain boundary in Au was studied using transmission electron microscopy (TEM) [16, 17], with the results revealing the preferred nucleation of the bubbles at screw dislocation intersection junctions. The response of nanocrystalline W to low-energy He^+ ion irradiation at high temperature was also investigated using in situ TEM, and it was observed that the He bubbles could be nucleated on the dislocation line [18]. Moreover, thin foils of high-purity iron were irradiated in situ in a TEM using 1-MeV Fe^+ and 15-keV He^+ ions, revealing that the heterogeneous formation of He bubbles occurred mainly inside the large dislocation loop [19, 20]. Although these experimental works demonstrated that dislocations are also important sites for the nucleation of He bubbles, they failed to provide further details on the mechanism of the He bubble growth. It is therefore unclear if the loop punching mechanism is valid for this case.

In the present work, molecular dynamics (MD) simulation was used to investigate the He bubble growth process on edge dislocations in W. The results revealed that the bubble growth was controlled by the edge dislocation climbing mechanism rather than by the dislocation loop punching mechanism. W was selected as an example because it is the most promising candidate material for plasma facing components for future thermonuclear fusion reactors, which would be exposed to high fluxes of He ions, and leading to microscopic He bubble formation.

The simulations were performed using the parallel MD code LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) [21]; the W–He interatomic potential is described in detail in Ref. [22]. The *X*, *Y*, and *Z* directions of the edge dislocation model were set along [111], $[1\bar{1}0]$, and $[11\bar{2}]$, respectively. Three (111) atomic planes were removed from the middle of the model to the top surface to introduce a $1/2\langle 111\rangle(1\bar{1}0)$ edge dislocation. The three dimensions of the dislocation model were 9.85, 8.06, and 10.81 nm along the *X*, *Y*, and *Z* directions, respectively, and the model contained 53,676 W atoms. Periodic boundary conditions were applied along the *X* and *Z* directions, whereas a

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fixed boundary condition was applied along the *Y* direction. The dislocation model was then relaxed using the conjugate gradient method to obtain an equilibrium model. Considering the dislocation core to be a trapping center could facilitate He atom accumulation [4, 23, 24]; to reduce the simulation time, He atoms were introduced one by one into the tensile part of the dislocation core rather than into the region around the dislocation. After each He atom was introduced, the model was relaxed for 50 ps under 300 K using the constant-temperature, constant-volume (NVT) ensemble; 200 He atoms in total were introduced into the dislocation core during the simulation process. Another He bubble growth rate (adding 1 He atom per 100 ps) was also tested and found the bubble growth rate had little effect on its growth mechanism. For comparison, the He bubble growth mechanism in bulk W was also studied using the same method as for He bubble growth at an edge dislocation core. The visualization of the simulation results was performed using the Open Visualization Tool (OVITO) program [25]. Dislocation Extraction Algorithm (DXA) [26] method (which was embedded in OVITO) was used to visualize dislocation.

Fig. 1 shows the growth process of a He bubble on the $1/2\langle 111\rangle(1\bar{1}0)$ edge dislocation. After the He atoms were introduced into the edge dislocation core, they gathered around the dislocation to form an elongated He bubble along the dislocation line by 3.5 ns (Fig. 1B). After more He atoms were introduced, part of the edge dislocation near the He bubble climbed to form a pair of jogs and simultaneously slipped along [111] direction under the effect of the stress field of the He bubble (Fig. 1C). By 6.56 ns, the W self-interstitial atoms, which were pushed out by the He bubble, and attached to the He bubble surface, the boundary of which was a curved dislocation (Fig. 1D). Then, W self-interstitial atoms and the $1/2\ 111(1\bar{1}0)$ edge dislocation attracted with each other, leading the $1/2\ 111(1\bar{1}0)$ edge dislocation to slip toward the W self-interstitial atoms. Finally, the W self-interstitial atoms were absorbed into the $1/2\ 111(1\bar{1}0)$ edge dislocation, leading to part of the $1/2\ 111(1\bar{1}0)$ edge dislocation climbing again (Fig. 1E). During the growth of the He bubble, this process was repeated, with the edge dislocation constantly climbing (Fig. 1F).

To enable clearer visualization of the edge dislocation climbing mechanism for He bubble growth, the detailed atomic configuration of the edge dislocation climbing process is shown in Fig. 2. Initially (6.557 ns), the edge dislocation was located at the left side of the He bubble (Fig. 2A). After 1 ps, the W self-interstitial atoms were pushed out by the He bubble and were located in the red circle in Fig. 2B. With the attraction between the edge dislocation and W self-interstitial atoms, the edge dislocation slipped along [111] direction and approached the self-interstitial atoms; meanwhile, the configuration of the W self-interstitial atoms also changed (Fig. 2C). Finally, the W self-interstitial atoms were absorbed into the edge dislocation core, leading the edge dislocation to climb (Fig. 2D).

For comparison, the He bubble growth process in a perfect W lattice was also studied, and the simulation results are presented in Fig. 3. Before 2.44 ns, the He bubble grew homogeneously, and no W self-interstitial atom was pushed out from the He bubble. After 2.44 ns, W self-interstitial atoms were gradually pushed out from the He bubble. At 4.0 ns, several W self-interstitial atoms had been pushed out and attached to the He bubble surface, the boundary of which was a curved dislocation, as shown in Fig. 3B. With the growth of the He bubble, more W self-interstitial atoms were pushed out, causing the curved dislocation to become larger (Fig. 3C). By 4.76 ns, the curved dislocation had evolved into a prismatic dislocation loop and was pushed out from the He bubble along the $\langle 111\rangle$ direction (Fig. 3D). This is the well-known loop punching mechanism for He bubble growth, which has been verified to be the dominant mechanism for He bubble growth in many experimental and simulation works [13–15]. With the growth of the He bubble, the prismatic dislocation loops were constantly punched out from the He bubble surface. By 10.26 ns, another prismatic dislocation loop had been pushed out (Fig. 3F).

By now, there were two mechanisms for the growth of the He bubble: the well-known loop punching mechanism and the dislocation

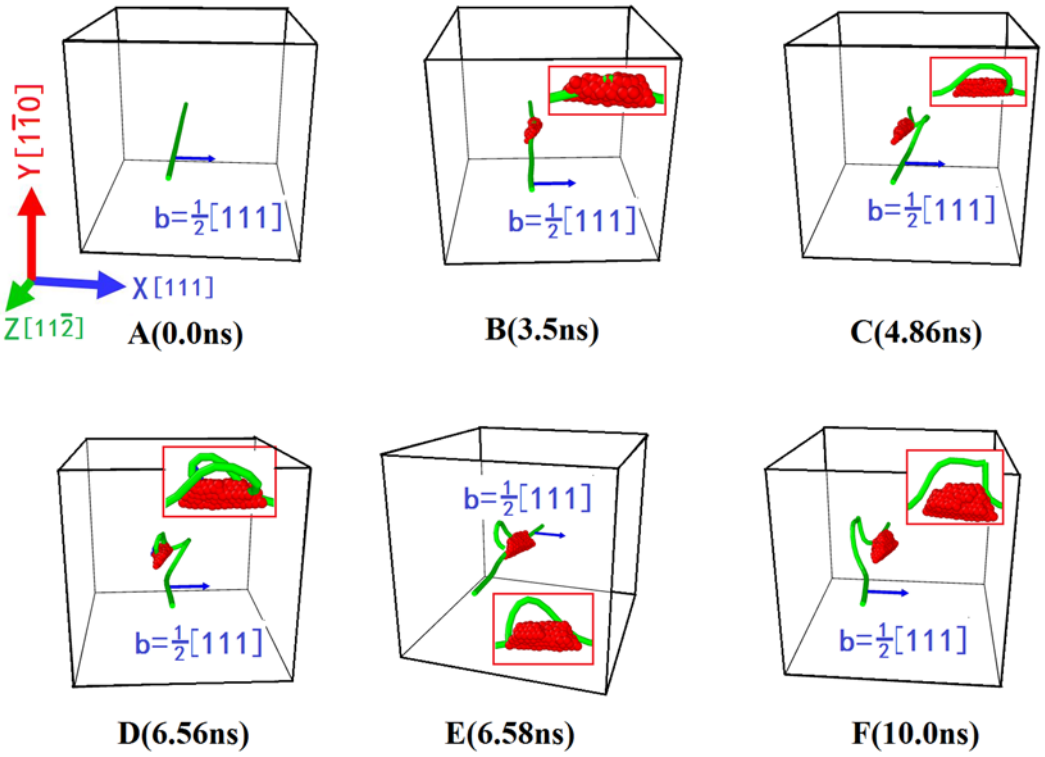

Fig. 1. Dislocation climbing mechanism for He bubble growth. The green line represents the dislocation, and the blue arrow indicates its Burgers vector direction. The red balls represent He atoms. To enable clearer visualization of the He bubble, a view from [111] direction of the He bubble is inserted in each figure. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)