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A new loop-punching mechanism for helium bubble growth in tungsten

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ABSTRACT

Growth of helium (He) bubbles with different initial sizes in tungsten (W) has been investigated by performing molecular dynamics simulations. Based on the simulation results a new loop punching mechanism for the large helium bubble growth is proposed. Different from the growth of small-size He bubbles by pushing out self-interstitial atoms and then rearranging into a prismatic dislocation loop, a large-size bubble grows by pushing out a dislocation, subsequently cross-slipping of its screw components and finally evolving into a prismatic dislocation loop. Such dislocations may react with each other to form a dislocation net around the bubble rather than to convert to prismatic dislocation loops.

1. Introduction

Because of its extremely low solubility in metals, helium (He) atoms introduced into metals tend to agglomerate into bubbles [1–4]. While numerous experimental studies have investigated He-metals interactions [5–11], it is still very difficult to *in-situ* observe the nucleation and growth process of He bubbles with the present experimental techniques because of their small size (no more than 10 nm in diameter [10,11]). Thus modeling and simulations become useful complementary tools to study the underlying nucleation and growth mechanism of He bubbles. The theoretical works can be further divided into two categories: the study of nucleation process [12–16] and the study of growth process [17–21]. For the latter case, molecular dynamics (MD) simulations have been used to investigate the underlying growth mechanism of He bubbles in tungsten (W) [17]. The simulation results show that these He bubbles grow by pushing out W self-interstitial atoms (SIAs), which orient along the <111> direction attaching to the bubble surface, then rearrange into a prismatic dislocation loop with a Burgers vector of $b = \frac{1}{2}\langle 111\rangle$, and move away from the bubble along the $\langle 111\rangle$ direction when the number of self-interstitial atoms exceeds the threshold. Using the same method, Wang and coworkers also studied the growth mechanism of He bubbles in W and obtained similar results [18]. Moreover, using MD and parallel replica dynamics method [19], the growth of He bubbles in W for the growth rates spanning 6 orders of magnitude was examined. The simulation results show that in spite of the enormous variation of the growth rate, the He bubble also grows by pushing out W self-interstitial atoms, and subsequently rearranging into a prismatic dislocation loop. Furthermore, it has been verified that this mechanism is also suitable for the He bubble growth in bcc Fe [20,21].

Theoretically, a He bubble can be considered as a hollow sphere containing He atoms embedded in material and subjected to the internal pressure; the stress distribution around it is similar to the stress distribution under the spherical indenter during the nano indentation simulation process. However, we notice that the deformation under the spherical indenter controlled by creating shear dislocations or emission of dislocation loops [22–24]. Therefore, it is quite interesting to consider the role of shear dislocation in the deformation mechanisms of these different

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processes. Considering the He bubble size in the previous simulations is much smaller than that of the spherical indenter, we naturally focus on the He bubble size that may be a key factor on the bubble growth.

To confirm our speculation, we investigate the bubble size effect on the growing mechanism of the He bubble by using the MD simulation method and using W as an example. We choose W because it is the main candidate material for plasma facing components in future thermonuclear fusion reactors, and will be exposed to high fluxes of He ions, which can lead to the formation of microscopic He bubbles.

2. Methods

The simulations are performed using the parallel MD code, LAMMPS [25]; the W–He inter atomic potential is described in detail in Ref. [26]. A simulation model of $40a_0 \times 40a_0 \times 40a_0$, (where a_0 is lattice constant of W) containing 128000 W atoms, is constructed to eliminate the possible size effect. The X, Y and Z-axes of the simulation box are taken to be in the directions of [100], [010] and [001], respectively; periodic boundary conditions are used in all three directions. To save CPU time, W atoms in a sphere region are replaced by He atoms to obtain the initial He bubble configuration. The model is relaxed to reach an equilibrium state, then more He atoms are introduced one by one into the bubble. After each He atom is introduced, the model is relaxed for 5 ps using the NVT ensemble. The temperature is 300 K.

The visualization of the simulation results is done by using the OVITO program [27]. To clearly display the growing mechanism of the bubble, the simulation model is analyzed using common neighbor method (CNA) [28], and the perfect bcc W atoms are filtered out; therefore only those atoms in or at the neighbor of the bubble (He atoms and its surrounding W atoms) as well as atoms at lattice defect (self-interstitial atoms and its surrounding W atoms) are left and displayed in the following figures (Figs. 1, 3, 5 and 7). In these figures, the color from blue to red qualitatively designates the distance from the present atomic site to the center of the He bubble

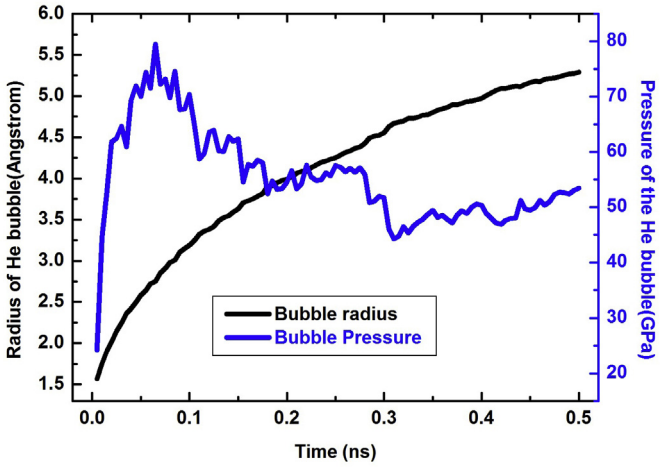

Fig. 2. The radius and pressure of the He bubble as a function of simulation time.

to further clearly show the lattice defects which are pushed out from the He bubble.

The pressure of a He bubble is calculated using the following two equations:

$$\sigma_{ij} = \frac{1}{V}\left(\frac{1}{2}\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N} U'\left(r^{\alpha\beta}\right)\frac{\Delta x_i^{\alpha\beta}\Delta x_j^{\alpha\beta}}{r^{\alpha\beta}} - \sum_{\alpha=1}^{N} m_\alpha \dot{x}_i^\alpha \dot{x}_j^\alpha\right), \quad (1)$$

$$\text{and } P = -(\sigma_{xx} + \sigma_{yy} + \sigma_{zz})/3, \quad (2)$$

where V is the current volume of the bubble, N is the total number of He atoms, $\dot{x}_i^\alpha$ is the ith component of velocity of He atom α, and m_α is its mass, $r^{\alpha\beta}$ is the distance between two He atoms α and β, $\Delta x_i^{\alpha\beta} = x_i^\alpha - x_i^\beta$, U is the potential energy function.

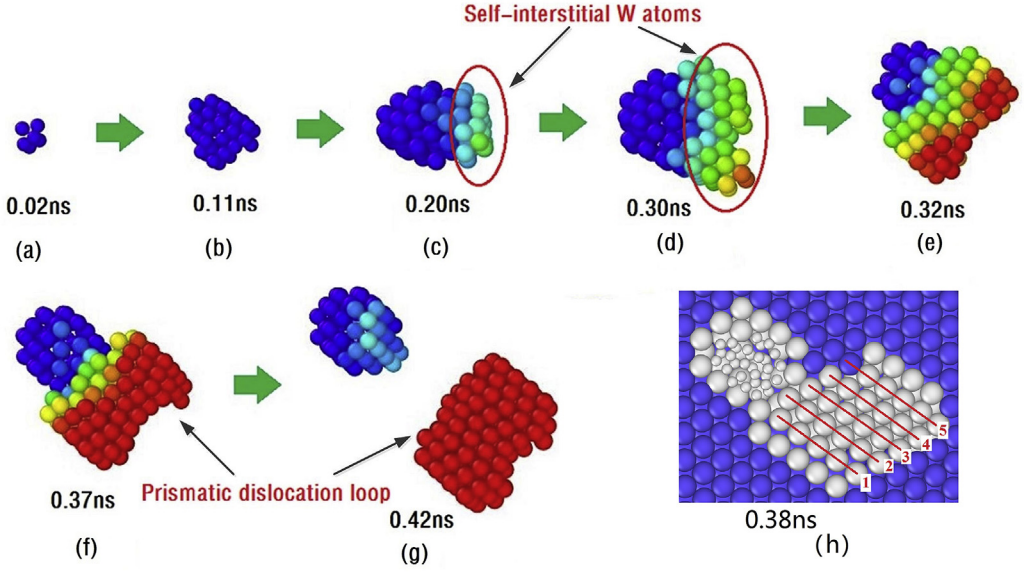

Fig. 1. The evolution of a He bubble with initial radius of 0.15 nm. The color from blue to red qualitatively designates the distance from the present atomic site to the center of the He bubble. For (a) and (b), the bubble grows homogeneously; for (c) and (d), self-interstitial W atoms have been pushed out and attach to the bubble surface; for (e)–(g) the self-interstitial W atoms evolve into a prismatic dislocation loop and then moves away from the bubble; (h) the atomic structure of the self-interstitial atom cluster. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)