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Estimation of the lifetime of small helium bubbles near tungsten surfaces – A methodological study

Jiechao Cui, Zhangwen Wu, Qing Hou *

Key Lab for Radiation Physics and Technology, Institute of Nuclear Science and Technology, Sichuan University, Chengdu 610064, China

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ABSTRACT

Under low energy and high flux/fluence irradiation of helium (He) atoms, the formation and bursting of He bubbles on tungsten (W) surfaces play important roles in the morphological evolution of component surfaces in fusion reactors. Microscopically, the bursting of He bubbles is a stochastic process, and He bubbles have statistically average lifetimes. In the present paper, a molecular dynamics-based method was developed to extract, for the first time, the lifetime of He bubbles near tungsten surfaces. It was found that He bubble bursting can be treated as an activated event. Its frequency or, equivalently, the average lifetime of bubbles follows the Arrhenius equation. For a given bubble size, the activation energy exhibits a good linear dependence with the depth, and the pre-exponential factor obeys the Meyer–Neldle rule. These results are useful for establishing a model in multi-scale simulations of the morphological evolution of component surfaces in fusion reactors.

1. Introduction

As reviewed by a number of authors [1–3], the behavior of materials that are exposed to a complicated and extreme environment in a fusion reactor is a very challenging subject. Among these subjects, the interaction of tungsten (W) with plasma is especially relevant because W has been chosen as a plasma-facing-material (PFM) for the diverter in the International Thermonuclear Experimental Reactor (ITER). In the reactor, the W surface will suffer low energy (<200 eV) and high flux/fluence ($\sim 10^{27}$ m^{-2}) irradiation with hydrogen (H) and helium (He) plasma.

Many recent experimental researches [4–9] have been performed to study the low energy and high flux/fluence (LEHF) irradiation of He on W surfaces. It is well known from these experiments that the LEHF irradiation of He can induce severe morphological modifications of W surfaces (e.g., the formation of nano-scale fuzz). Morphological modifications can degrade the physical and chemical properties of surfaces and produce potential impurity sources that would affect the fusion plasma balance. Some either qualitative or phenomenological models have been proposed to explain the experimental observations [4,10–13]. Although these models were proposed from different viewpoints, it has been commonly recognized that the behavior of He bubbles that are formed in W surfaces plays a central role.

To understand the behavior of He bubbles near W surfaces and to establish the corresponding models, the knowledge of involved atomistic dynamic processes is essential. Atomistic dynamic processes relevant to LEHF irradiation of He on W are plentiful [14], and some of them were addressed by a number of authors based on the molecular dynamics (MD) simulations. For example, MD simulations have been performed by Henriksson et al. [15], Lasa et al. [16] and Li et al. [17,18] to study the growth of He bubbles and W surfaces under the cumulative bombardment of He on W surfaces. Because of the limited time scale that is achievable by the MD simulations, the He fluence in these studies was much lower, and the He bubbles were small compared with those in experiments. Before performing simulation investigations corresponding to real experimental conditions, it is necessary to clarify the contributions of individual processes and their rate information that should be coupled to models of larger time–space scales. The studies of individual processes have been conducted on the reflection of He projectiles on W surfaces [19,20], interaction of He projectiles with pre-existing He bubbles [21,22], and on migration and trap-mutation of He atoms and small clusters near W surfaces [23–27]. In this paper, we focus on the bursting of nano-scale He bubbles near W surfaces.

Because the solubility of helium in metals is very low, He bubbles in metal surfaces do not dissolve into metals [28], but can burst instead. Wang et al. [29] conducted MD simulations, in which the pre-created spherical cavities at a given depth below the surfaces were filled with different number of He atoms and the

* Corresponding author.
E-mail address: qhou@scu.edu.cn (Q. Hou).

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simulation boxes were then relaxed at one given temperature. They applied this method to extract the critical depth and inner pressure for bursting of He bubbles in palladium. Methodologically similar to the MD simulations of Wang et al. [29], the effects of He/vacancy ratio, temperature and film thickness above the bubbles on the burst of He bubbles near W surfaces were studied by Ito et al. [30]. In the simulation procedure of these two studies, the growth process of He bubbles was omitted. Simulations on the growth and bursting of He bubbles near the W surface were performed by Sefta et al. [31,32]. The growth process of He bubbles was included by successively adding He atoms to He bubbles every 5 ps. However, the growth rate of the He bubbles so generated was significantly higher than in the experiments. As noted by Sandoval et al. [33], based on the simulations of parallel replica molecular dynamics, the artificial high growth rate may lead to the overestimation of threshold conditions of He bubble bursting, i.e., the bursting of He bubbles should occur at a He/Vacancy ratio that is lower than what was predicted by the overrated growth rate of He bubbles. From the MD simulations of cumulative bombardment of He on W surfaces [17], it has been observed that the number of He atoms in He bubbles is approximately twice the number of interstitial W atoms that are produced in the growth of bubbles. Thus, it is most probable that bursting of He bubbles, if it happens, occurs at a He/Vacancy ratio of approximately two. As discussed in what follows, from the viewpoint of statistical physics, the He bubble bursting is a stochastic process that can eventually happen with a certain probability after the bubbles are formed at a He/Vacancy ratio. The probability is temperature- and size-dependent. Thus, the He bubble bursting frequency, or equivalently the average lifetime of He bubbles, should be a more appropriate parameter that can be used to characterize the bursting of He bubbles. Especially for the LEHF irradiation of He on W, the lifetime of He bubbles determines the evolution of bubble density that influences the morphological evolution of surfaces [22].

In the present paper, we propose and evaluate an MD simulation method for calculating the He bubble bursting frequency, or equivalently, the average lifetime of He bubbles. The method is a type of emulation of thermal desorption experiments. Although the method had been used to calculate the escaping rate of single He atoms trapped near W surfaces [27] and the dissociation rate of W clusters [34], it is for first time applied to He bubble bursting, which consists of more complex atomistic processes. We will show that the triggering of He bubble bursting can be equivalently considered as an activated event of certain activation energy, and the dependence of the frequency on temperature can be described using the Arrhenius equation.

2. Method

2.1. Simulation method

Before running the MD simulation, we prepared the initial simulation boxes with the size of $30a_0 \times 30a_0 \times 30a_0$, where a_0 represents the lattice constant of W. The surface orientation was (100) crystal orientation and defined as the z-direction. To create an initial He bubble in the substrate, we created a cavity by removing a given number of W atoms that were closest to a point, which was regarded as the center of the bubble, in the substrate and then filled the cavity with helium atoms. The z-coordinate of the point was a given value, but The x- and y- were randomly set. According to our previous simulations of the He bubble growth in metals [17,35], the accumulated pressure of He bubbles may induce dislocation loop punch, accompanying the release of the bubble pressure and the restoration of crystal structure surrounding the bubbles. The number of He atoms in the bubbles after dislocation loop punch was found to be approximately twice the number of the ejected metal atoms [17,35]. Thus, in the present paper, we chose 2 for the ratio $r_{He/v}$ of the number of filling He atoms (n_{He}) and the number of the removed W atoms (n_W). Fig. 1 shows the initial simulation box, with d_b denoting the layer thickness above the He bubble, and R_b denoting the initial bubble radius. For each combination of d_b, R_b, $r_{He/v}$ and surface orientation, we prepared $Q_b^{(0)}$ (=100) replicas for the purpose of statistical analysis to be presented in the Section 2.2.

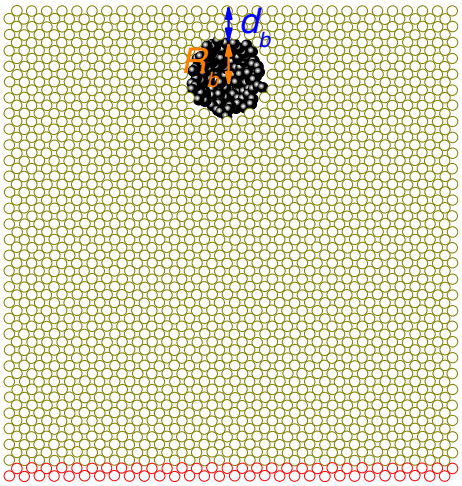

Fig. 1. Schematic graph of the initial simulation box. The dark spheres are He atoms, the circles are W atoms. The two bottom layers of W atoms are fixed (red circle). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

With the prepared initial simulation boxes, the MD simulations were run using the graphics processing unit (GPU)-based MD package developed in our group [36]. We used the many-body semi-empirical potential of the Finnis–Sinclair type proposed by Ackland et al. for the W–W potential [37]. This W–W potential has been used in our previous work [18,38,39] and is widely used by other research groups [26,31,33]. For the He–W interaction, we adopted a pairwise potential that was obtained by fitting to the *ab initio* data. The pairwise potential reproduces the correct order of stability for the interstitial He in W [40]. For the He–He interaction, we used the exp-6 potential that was obtained by fitting to the state equation of high pressure He [41]. Throughout all MD runs, the periodic boundary conditions were applied only in the x- and y-directions. To avoid the displacement of substrates during the burst of He bubbles, two bottom layers of the substrates were fixed at their original positions.

Each MD simulation run consisted of three stages. In the first stage, because the initial simulation boxes that were generated above were not in equilibrium, we quenched the boxes to zero temperature. In the second stage, the boxes were firstly thermalized to a temperature $T^{(0)}$ (for example 300 K) and then relaxed for enough time steps to bring them to thermal equilibrium at this temperature. The thermalization of a simulation box was conducted by assigning the atoms in the box with velocities that were generated by the Monte Carlo sampling of the Maxwell distribution of atom velocity. The boxes were relaxed by numerically integrating the dynamics equation of atoms, using a finite difference scheme that can be written as [42]:

$$\mathbf{r}_i^{(n)} = \mathbf{r}_i^{(n-1)} + \delta t \mathbf{v}_i^{(n-1)} + \frac{1}{2}\delta t^2 \mathbf{a}_i^{(n-1)} \quad (1.a)$$

$$\mathbf{v}_i^{(n)} = \mathbf{v}_i^{(n-1)} + \frac{1}{2}\delta t(\mathbf{a}_i^{(n-1)} + \mathbf{a}_i^{(n)}) \quad (1.b)$$