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Molecular dynamics study on the interactions between helium projectiles and helium bubbles pre-existing in tungsten surfaces

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ABSTRACT

Molecular dynamics simulations were performed to study the interactions between low-energy (⩽100 eV) helium (He) projectiles and helium bubbles pre-existing near tungsten (W) surfaces. It is observed that with increasing bubble size, the reflection coefficient of the He projectiles was reduced, and the channelling effect that could be observed with no pre-existing He bubble was depressed. The He projectiles can be captured by pre-existing He bubbles and also knock He atoms out of the bubbles. The spatial distribution of the single He atoms, including both the slowed-down projectiles and the knocked-out He atoms, was extracted. The single He atoms were found distributed around the bubbles in a region with the width of 3–5.5 in lattice lengths of W. Although the results were obtained for the interaction of He projectiles with isolated He bubbles pre-existing in W, they suggest that the reflection and retention status of He projectiles would change during the irradiation of high flux/fluence He on W surfaces due to the change of He bubbles coverage near W surfaces. The results can be coupled with Monte Carlo modelling in conditions closer to that in experiments of high flux/fluence He bombardments on W surfaces.

1. Introduction

The interaction of helium projectiles with plasma-facing materials (PFM) is a major concern in the research and development of magnetic confinement fusion devices, such as the International Thermonuclear Experimental Reactor (ITER). This issue is especially important in the divertor region, where the PFM surfaces are anticipated to suffer from low-energy (<200 eV) but high-fluence ($\sim 10^{27}$ m^{-2}) irradiation of hydrogen (H) and helium (He) plasma. Owing to the high temperature and good sputtering erosion resistance of tungsten (W), it has been considered to be the best candidate for the PFM of a divertor. However, many experiments have studied the radiation effect of He on W surfaces and shown that the plasma condition in the divertor region can induce the formation of He bubbles or even more complex structures on W surfaces [1–5]. These structural changes on W surfaces could lead to property degradation of the material and result in a source of potential unfavourable impurities in the fusion plasma.

The underlying physical processes involved in these experimental observations are still not well understood. The low-energy and high-flux condition mentioned above makes theoretical studies, including computer simulations, a difficult task. Because the incident energy of the He projectiles is low, the projectiles are slowed down within approximately 2 ps at a depth of few nanometres. Additionally, because the flux is high, the dose of He atoms near the substrate surfaces rapidly increases with irradiation time. Severe changes of the surface morphology continually occur in the experimental period owing to interplays of many various atomistic processes. Thus, a detailed atomistic description of the interactions between He projectiles and W surfaces with previously produced defects is one of the necessary topics to establish a knowledge base for understanding the morphological evolution of the surfaces. To address the problem, molecular dynamics (MD) simulation is an indispensable tool.

On the basis of MD simulations, the reflection and depth distribution of low-energy He projectiles on W surfaces have been studied by Li et al. [6,7], Borovikov et al. [8], and Hammond et al. [9]. Because the bombardments in these studies were simulated by a set of independent MD runs, these works are related to a situation of low irradiation fluence in which the interaction of a He projectile with the previously deposited He atoms and other types of defects is negligible. Aimed at studying the growth and burst of He bubbles on a W surface, MD simulations were conducted by Sefta et al. [10,11] by randomly placing He atoms on the periphery of pre-existing bubbles. This approach can accelerate the simulation of

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the growth process; however, the bombardment process of He projectiles was ignored. With an increased He dose near the surfaces, it is quite likely that a He projectile may interact with pre-existing He bubbles before the He projectile is slowed down to the environmental temperature. Cumulative bombardments of He on W surfaces were first simulated by Henriksson et al. [12] and later by Lasa et al. [13] and Li et al. [14]. The growth of He clusters and the response of W surfaces, such as the creation of <1 1 1> crowdion bundles and surface growth, were investigated. The interactions between the He projectiles and the defects produced in the previous bombardments were naturally included in these MD simulations. However, owing to the limited time scale achievable by MD simulations, the He flux in these studies was much ($\sim$3 orders of magnitude) higher and the fluence was much lower than that in the experiments. Moreover, these studies are very qualitative without distinguishing contributions of individual processes to what is observed.

To determine the impact of every process that may occur in high-fluence irradiation of He on W surfaces is onerous. Sefta et al. [15] and Ferroni et al. [16] conducted MD simulations on the sputtering of W surfaces that contain pre-existing He bubbles and are bombarded by He projectiles. Because sputtering was the major concern of these two works, the energy range (>200 eV) of the He projectiles was chosen above sputtering threshold of W. The He dose in the simulations of Ferroni et al. was still much low in comparison with that can be achieved in experiments. Higher He dose and larger He bubbles were considered in the work of Sefta et al. Both works came to the similar conclusion that the pre-existence of He bubbles had minor effect on the sputtering yield of W.

In the present paper, we report our MD simulations of low energy ($\leqslant$100 eV) He projectiles bombarding He bubbles pre-existing in W. In contrast to the MD simulations of cumulative bombardments [12–14] and sputtering of He on W surfaces [15,16], we focus on the direct bombardment of He projectiles over isolated pre-existing He bubbles. The influence of He bubbles, on the reflection and depth distribution of He projectiles and the dissociation and bursting of He bubbles caused by He projectiles were studied. Considering that to conduct full MD simulations of high flux/fluence He bombardments on W surfaces is too difficult, the results of the present paper can be used for model establishments in more computationally efficient Monte Carlo methods.

2. Simulation methods

2.1. MD simulation

Our MD simulations were performed using the graphics processing unit (GPU)-based MD package MDPSCU [17]. On the interatomic potentials, an N-body semi-empirical potential of the Finnis–Sinclair type modified by Ackland and Thetford was employed for W–W interaction [18]. This W–W potential has been widely used in the literature to study radiation effects of W [8,10,19–22]. For the interactions between the He and W atoms, we adopted a pairwise potential that was obtained by fitting to *ab initio* data and could reproduce the correct order of stability for interstitial He in W. Because collisions between He and W atoms were involved, this He–W potential was smoothly connected to Ziegler–Biersack–Littmark (ZBL) potential in the short He–W distance. Considering that the pressure inside the He bubbles is high, we used the exponential-six potential [23], which was well fitted to the equation of state of high-pressure He, for He–He interaction. Again, we modified the exponential-six potential for a short distance by connecting it to the ZBL potential.

For the initial configurations of the simulation boxes, bcc W substrates of size 15 $a_0 \times 15$ $a_0 \times 15$ a_0 were first created with the normal direction of their surfaces in (1 0 0) crystal orientation, where a_0 = 3.1652 Å is the lattice constant of W. MD simulations of He bubble growth in metals [10,24] have indicated that interstitial metal atoms caused by accumulated pressure of He bubbles would move away from the bubbles accompanying the release of the bubble pressure and restoration of the crystal structure surrounding the bubbles. The number of He atoms in the bubbles was found to be approximately twice the number of the ejected metal atoms [14,24]. Based on this observation, we introduced a pre-existing He bubble to a simulation box by removing the W atoms in an approximate sphere of a given centre and then inserting a number of He atoms equal to twice the number of removed W atoms. The centre of the He bubbles was set as 3.5 a_0 below the top surfaces of the substrates, a depth approximately equal to the position where the depth distribution for 100 eV He incidence in W is maximum [6].

The simulation boxes prepared with initial configurations were relaxed to thermal equilibrium at temperatures of 300 K and 1500 K. Then, the MD simulations of He atom bombardments on W surfaces were run. The energies of the He projectiles were chosen to be 60 eV and 100 eV. Only the normal incidence of the projectiles was considered. The initial positions of the He projectiles in the z-direction were one interaction cutoff distance above the top surface of the substrates, whereas the positions in the x- and y-directions were randomly selected in the circle region formed by the projection of the He bubble shape on the surface. The periodic boundary conditions were applied in the x- and y-directions. The W atoms on the two bottom layers of the substrates were fixed. The time step size was adaptable to ensure that the maximum distance for the atoms to move in one time step was less than one-tenth of the lattice length of W. The total simulation time was approximately 2–3 ps.

In our previous study on the reflection and depth distribution of He [6], electron–phonon coupling (EPC) based on the model by Finnis et al. [25] was included in MD simulations. The inclusion of the EPC has an important effect on the calculation results which is different from that obtained by Borovikov et al. [8] without considering EPC. To avoid such confusion, in the present paper, we had no EPC included in our MD simulations, although the impact of the EPC is an issue deserving of investigation.

2.2. Analysis method

The reflected He projectiles and He atoms (pre-existing in substrates) escaping from the substrates were identified when their z-positions were above the top surface of the substrates. The transmitting He atoms were also identified by their z-positions. As shown by the MD simulation results, there are possibilities for the projectiles to knock out He atoms or small He clusters from the pre-existing He bubbles and to induce bubble bursts. We identified the He clusters (bubbles) and isolated atoms by the connectivity of He atoms. To automatically detect the connectivity of the He atoms, we implemented an algorithm based on the three-dimensional Voronoi tessellation [26]. The Voronoi tessellation divides the space into polyhedrons that fully fill the space. Using Voronoi tessellation to detect connectivity of atoms has the advantage that no additional artificial control parameter must be introduced. According to the mathematical definition of Voronoi tessellation, the Voronoi polyhedron of an atom is constructed by the planes drawn perpendicular to the vectors joining the atom with its surrounding atoms at the midpoints of the vectors. However, not all planes are the faces of the Voronoi polyhedron. The faces of the Voronoi polyhedron are the only planes which ensure that no atom beyond the central atom exists in the polyhedron. We