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Molecular dynamics simulations of cumulative helium bombardments on tungsten surfaces

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ABSTRACT

Molecular dynamics simulations were performed to study the cumulative bombardments of low-energy (60–200 eV) helium atoms on tungsten surfaces. The behaviour of helium and the response of tungsten surface were investigated. The helium incident energy and tungsten temperature play important roles on the formation and growth of helium clusters. The temperature can promote the coalescence of helium clusters and increase the size of the helium clusters. The rupture of the helium clusters has also been observed. During the formation of helium clusters, the interstitial tungsten atoms are produced and evolve into bundles of <1 1 1> crowdions, which would be constrained around the helium clusters for a long time. However, they will finally move onto the top surface along the <1 1 1> direction, which results in stacking the tungsten atoms on the surface. The complex combination effects of the helium clusters and the interstitial atoms result in the growth of the surfaces. Besides, several tungsten atoms were ejected from tungsten surfaces.

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1. Introduction

Tungsten (W) has been chosen as a promising candidate for the plasma-facing material (PFM) in controlled nuclear fusion reactors (CNFRs) [1,2], especially for the divertors, where the PFM will face irradiation of high-flux particles and intense heat flow [3]. For example, in the International Thermonuclear Experimental Reactor (ITER) [4], the estimated flux of the helium with energy ranging from 20 eV to 200 eV is $(0.1–1)\times10^{23}$ ions m^{-2} s^{-1}, and the temperature of the PFMs is 300–3000 K [5]. For the demo or commercial CNFRs in the future, the particle flux and heat flow would be more intense. Thus, interactions between low energy and high fluence helium beams and tungsten surfaces at various temperatures have been the focus of many experimental studies [6–9]. There has been evidence that the condition of high fluence, high temperature and low energy can invoke complex physical processes that are not well understood, such as nanostructure formation on tungsten surfaces [10]. To understand the underlying atomistic processes, theoretical studies are needed. Because a large number of atoms are involved in the processes and many-body effects therein act, molecular dynamics is the most suitable method of simulating at an atomistic level the bombardment of low-energy atoms on surfaces.

Using the molecular dynamics, we have studied in a previous paper the damage to tungsten surfaces by the bombardment of low-energy helium atoms in which the bombardments were independent of each other [11], a situation that approximates low fluence irradiations. In the present study, we focus on the cumulative bombardment of helium atoms on a tungsten surface where a projectile and the defects induced by it will interact with the defects, such as helium bubbles that are produced by previous bombardments.

Sefta et al. have studied the behaviour of helium bubbles in tungsten by molecular dynamics [12]. The helium bubble was created by carving out a tungsten volume and replacing it with helium atoms. Although the method can save computer cost, it ignores the bombardment process of helium atoms, the slowing-down and diffusion processes of helium atoms in tungsten substrate and the interactions between defects, such as the coalescence of helium bubbles. Henriksson implanted helium atoms cumulatively into tungsten surfaces and gave the very basic information of defects produced in early stage of helium bombardments, such as helium cluster formation [13]. However, the interactions between defects were also not considered. Besides, the tungsten substrates in Ref. [13] was set below 300 K, in our previous work, surface temperature has proved to influence helium retention in tungsten substrates [14], thus the formation and evolution of defects would be different at different temperatures. Lasa based on the work of Henriksson, mainly gave some talk on the effect of the high fluence,

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Table 1
The box sizes, the number of tungsten atoms N_W in the boxes and the corresponding helium fluences that were reached in our simulations for each considered combination of incident energy E_i and substrate temperature T_s.

E_i (eV)	T_s	Box size (Å^3)	N_W	Fluence (10^{20} m^{-2})
60	1500 K/2100 K	63.3 × 63.3 × 63.3	16800	0.50
80	300 K/1500 K	94.9 × 94.9 × 83.9	48600	1.33
100	1500 K/2100 K	94.9 × 94.9 × 94.9	54000	1.11
200	300 K/1500 K	94.9 × 94.9 × 94.9	63000	1.11

the temperature and the impurities on tungsten surface growth, aiming to explain the onset of a fuzz-like nanostructure formation on tungsten surfaces [15,10]. However, the damage evolution below the surface, such as the emission and diffusion of damage and the helium behaviour were not given.

In our paper, large-scale molecular dynamics simulations were performed to gain a comprehensive picture of the whole process of the slowing-down of the incident helium atoms and the migration, coalescence, dissociation and release of helium and interstitial clusters, and the evolution of tungsten damage produced. After an outline of our simulation method is given in Section 2, in Section 3.1, the effects of the incident energy, surface temperature on the nucleation and the release of helium will be presented. In Section 3.2, the damage of the tungsten surface will be discussed.

2. Simulation methods

The molecular dynamics simulation of cumulative bombardments of atoms on surfaces requires computations that are very time consuming. To improve the computational efficiency, a molecular dynamics package MDPSCU (Molecular Dynamics Package of SiChuan University) using graphics processing units (GPUs) for parallel computing was used [16]. With respect to the physical models, a Finnis–Sinclair-type potential obtained by Ackland et al. [17] was adopted to describe the interactions between the

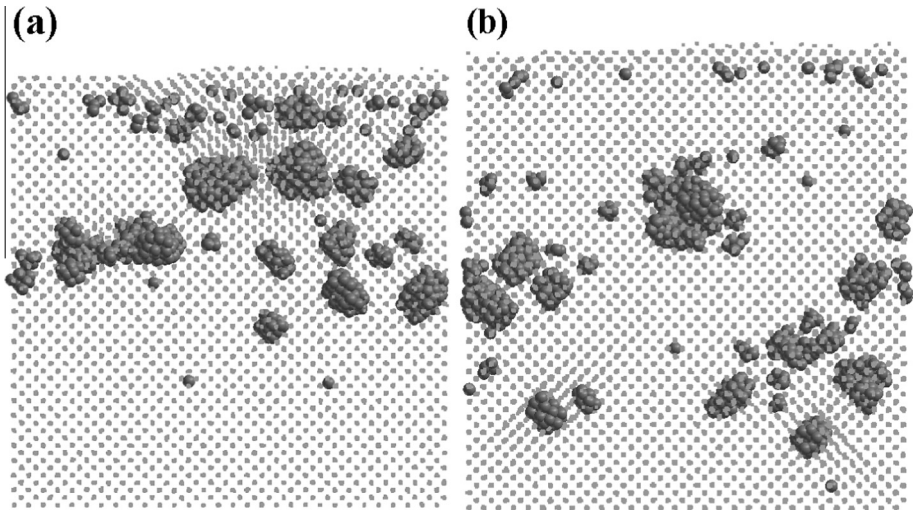

Fig. 1. Side view of the tungsten substrates with the same number of retained helium atoms. T_s = 1500 K. (a) E_i = 100 eV; (b) E_i = 200 eV. Gray dots: tungsten atoms; dark balls: helium atoms.

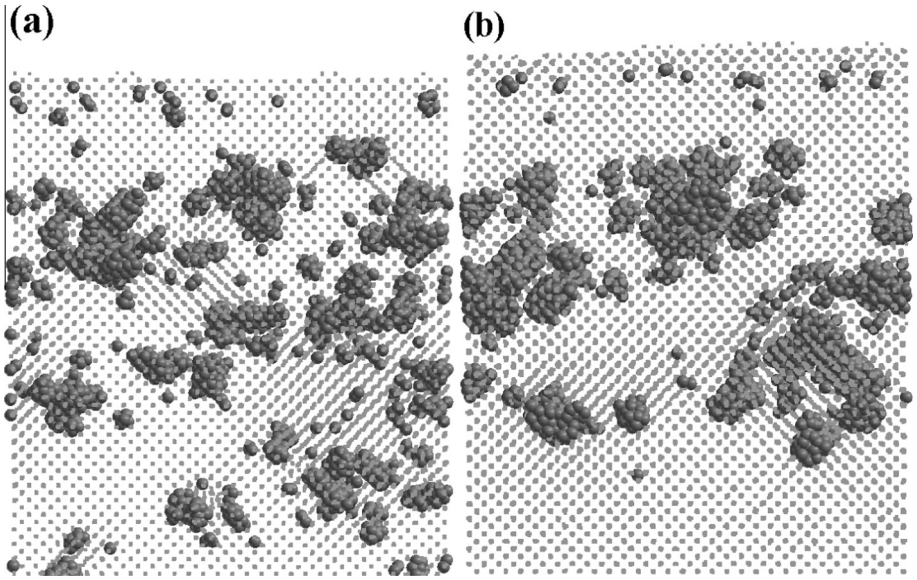

Fig. 2. Side view of the tungsten substrates with the same number of retained helium atoms. E_i = 200 eV. (a) T_s = 300 K; (b) T_s = 1500 K.

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