Nuclear Inst, and Methods in Physics Research B 436 (2018) 51–62

Contents lists available at ScienceDirect

Nuclear Inst. and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb

Effect of the accumulated vacancies and interstitials on the tungsten surface on the surface's role as defect sinks

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ARTICLE INFO

Keywords:
Radiation damage
Surface
Segregation
Annihilation
Tungsten

ABSTRACT

Neutrons induce displacement damage to the tungsten-based plasma facing material by creating radiation-defects, e.g., vacancies (Vs) and self-interstitial atoms (SIAs). These defects will accumulate on the surface and further affect surface's role as defect sinks. In this work, by combining molecular statics (MS) and object kinetic Monte Carlo (OKMC) methods, we study the clustering of the V/SIA on the two typical low-index W surfaces (1 0 0) and (1 1 0) to uncover the effect of the agglomerated surface V/SIA on the segregation and annihilation of the V and SIA nearby. Results show that the V_n/SIA_n could form on the two surfaces via the agglomeration of the V/SIA on the surfaces with the energy release and the reduced energy barrier for the V/SIA diffusion near the V_n/SIA_n as respective energetic and kinetic driving force. Yet, the V_n/SIA_n is more easily formed on surface (1 1 0) compared to surface (1 0 0) due to the much larger binding energy of a V with a V_n (or a SIA with a SIA_n) and lower diffusion energy barrier of the V/SIA on surface (1 1 0) than that on surface (1 0 0). Long-term OKMC simulations of the V/SIA behavior near the surfaces at 1000 K show that surface (1 0 0) could develop to locally convex structures due to the SIA agglomeration, while surface (1 1 0) will evolve to locally concave-convex structures due to the V/SIA clustering. Meanwhile, the interaction mechanism of the V/SIA with the surface is changed from the fundamental segregation, annihilation and clustering of the V/SIA near a pure surface to the trapping for the V/SIA by the locally concave-convex structure and the junction.

1. Introduction

Tungsten (W) is a leading candidate material for the plasma facing material (PFM) of future fusion reactors due to its excellent properties of high melting point, good thermal conductivity, and low sputtering rate [1]. As a PFM, W will be exposed to high radiation fluxes of hydrogen isotopes and helium, and 14.1 MeV-neutrons that escape from the deuterium-tritium plasma. Irradiation of high fluxes of low-energy hydrogen and helium leads to bubble and fuzz formation near W surfaces [2–4]. The high energy neutrons colliding with W lattices will cause displacement damage and produce a large number of vacancies (Vs) and self-interstitial atoms (SIAs) in the material [5–8]. These defects will segregate to the surface and accumulate on the surface in addition to forming immobile defect clusters in the bulk, such as voids, bubbles and dislocation loops. The defects on the surface affect not only the interaction of the surface with the defects from the bulk, but also the hydrogen/helium behavior near W surfaces. Therefore, it is essential to understand the V/SIA driven surface structural evolution and the resulting change of the surface's role as defect sinks; these issues closely associate with interaction of the V/SIA with the surface.

It is well known that surfaces act as good sinks for radiation-created defects [9–15]. The typical experimental observation is the radiation-resistance of nano-porous metals due to the absorption of the V/SIA by the free surfaces prevalent in these metals [9,10]. Recent theoretical simulations suggest that there is tremendous energetic driving force for the SIA segregation to the surface [12]; the segregation energy for the SIA/V is over 6.9/1.3 eV [12]; the diffusion of the V/SIA near the surface is basically enhanced [12]. Molecular statics (MS) calculations by Duan et al. suggest that surface (1 0 0) could serve as a sink for small V clusters [11]. The SIA–V annihilation mechanism also depends on the surface orientation [12]. On surface (1 1 0), the annihilation of the SIA–V happens via the coupled motion of the V segregation towards the surface from the bulk and the two-dimensional diffusion of the SIA on

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https://doi.org/10.1016/j.nimb.2018.09.010
Received 30 June 2018; Received in revised form 5 September 2018; Accepted 5 September 2018

the surface; on surface (1 0 0), the annihilation of the SIA–V occurs via the V segregation and recombination [12].

Interestingly, the dependence of the displacement damage on the surface orientation was observed in ion-irradiation experiments of W [16–20]. Ran et al. studied the effect of crystal orientation on the behavior of a W surface under a 30 keV focused Ga+ ion beam irradiation [19]. They found that grains with a (1 0 0) direction parallel to the ion beam always maintain a much smoother surface morphology. The surface-orientation dependence of the blistering in W was also observed in experiments [17,18]. Blistering slightly occurs on the resolidified grains with surface orientation near (1 0 0), and it gets heavier on the grains near (1 1 0) [17]. The response of W surfaces to irradiation is via sputtering of surface atoms [21], interactions among the V, SIA and the surface and hydrogen/helium behavior near the surface [15]. Since the fusion neutron in a fusion reactor has a small cross-section and a large free path, it will not directly interact with the surface, but via the segregated V/SIA from the bulk displacement damage.

The present work is focused on the V/SIA clustering on the two typical low-index surfaces (1 0 0) and (1 1 0) by using the MS, molecular dynamics (MD) and long-term simulation techniques of object kinetic Monte Carlo (OKMC) [22]. The results reveal that both the V and SIA could be clustered on the two surfaces due to the attraction of the V with a V-cluster (V_n) and a SIA with a SIA-cluster (SIA_n). The surface with small defect clusters still act as sinks for the V/SIA. As radiation defects accumulate on the surface, the surface may develop into the locally concave-convex structure, which could trap the bulk V/SIA. Surface (1 0 0) may show better resistance to morphology change than surface (1 1 0) due to the much larger binding energy of a V with a V_n (or a SIA with a SIA_n) and lower diffusion energy barrier of the V/SIA on surface (1 1 0) than that on surface (1 0 0). Yet the fraction of the V/SIA survived on surface (1 0 0) is higher than that on surface (1 1 0).

2. Computational method

2.1. Interatomic potential and calculation models for MS calculations

The bond-order potential (BOP) [23] was used to describe interatomic interaction among W atoms. Tests suggest that the formation energy for a bulk V is 3.75 eV and 10.19 eV for a bulk SIA of ⟨1 1 1⟩ crowdion. The diffusion energy for the V and SIA is 1.80 and 0.002 eV, respectively. These values are consisted with reported ones in [23]. The potential has been widely used in studying radiation damage in bulk W and nano-structured W [11,12,24]. Note that, different empirical potentials could give rather different values for a certain defect property, e.g. V/SIA diffusion energy barrier.

Two typical low-index surfaces (1 0 0) and (1 1 0) with low surface energy were built to investigate the V/SIA behavior on the surfaces. The surface (1 0 0) model contains 2112 atoms with a size of $25.4 \times 25.4 \times 52.3$ Å^3; the surface (1 1 0) model contains 2016 atoms with a size of $25.4 \times 31.4 \times 50.4$ Å^3. Periodic boundary conditions were imposed in the two Cartesian directions parallel to the surface, while a vacuum layer with a thickness of 15 Å was added in the direction normal to the surface. The model size has been checked to be large enough to avoid the interaction of the defect with the other surface on the opposite side of the surface. In other words, there is a bulk region near the surface. The system was relaxed at 0 K by employing the steepest descent method. The surface structural stability was investigated by performing MD simulations at 1000 K. The time step was set 2.0 fs. The simulation lasts for 50 picoseconds. The temperature was maintained by rescaling the velocity of all the atoms. The velocity-Verlet algorithm was used for integrating Newton motion equations. The relaxed surface models are presented in Fig. 1(a) and (b).

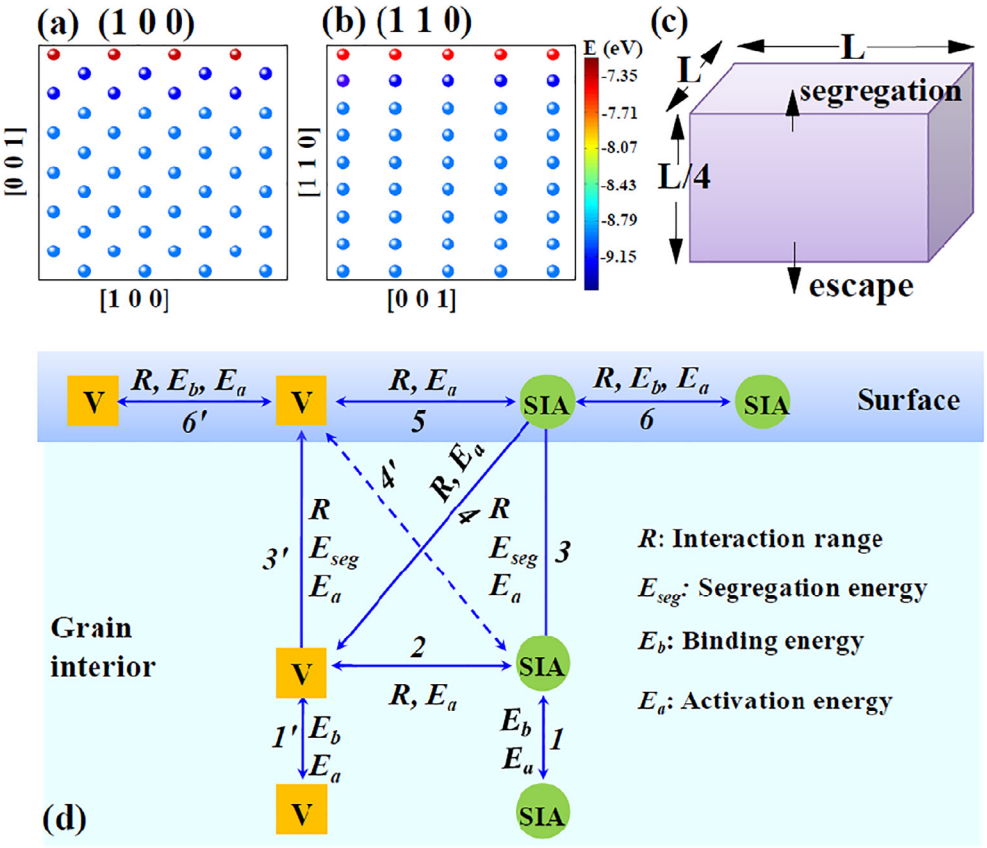

Fig. 1. The stable structures of pure surfaces (1 0 0) (a) and (1 1 0) (b). The atoms are colored with their potential energies as indicated by the color bar on the right side of (b). (c) Structural model for OKMC simulation of the V/SIA behavior near the surface. *L* is the model size in the direction parallel to the surface, while the size is *L*/4 in the direction normal to the surface. (d) Illustration of the fundamental interaction processes of the vacancy (V), self-interstitial atom (SIA) with the surface. Here, the yellow square and green sphere represents a V and SIA, respectively. Processes *1* and *1′* represents the clustering of the bulk SIA and V, respectively, while process *2* represents the annihilation of a bulk V-SIA pair. Processes *3* and *3′* denotes the segregation of the SIA and V, respectively. Processes *4* and *4′* are for the annihilation of the V with the SIA near the surface. Since the SIA generally preferentially segregates to the surface, the annihilation is mainly via process *4* where a SIA on the surface annihilates the V nearby. The V-SIA annihilation on the surface is denoted by process *5*, while processes *6* and *6′* represents the respective on-surface clustering of the SIA and V. The parameters characterizing theses processes include interaction range (R), segregation energy (E_{seg}), binding energy (E_b), and activation energy barrier (E_a). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)