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The behavior of small helium clusters near free surfaces in tungsten

A.V. Barashev [a,b], H. Xu [a,b,*], R.E. Stoller [a]

[a] Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6114, USA
[b] Department of Materials Science and Engineering, University of Tennessee, Knoxville, TN 37996, USA

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ABSTRACT

The results of a computational study of helium–vacancy clusters in tungsten are reported. A recently developed atomistic kinetic Monte Carlo method employing empirical interatomic potentials was used to investigate the behavior of clusters composed of three interstitial-helium atoms near {1 1 1}, {1 1 0} and {1 0 0} free surfaces. Multiple configurations were examined and the local energy landscape was characterized to determine cluster mobility and the potential for interactions with the surface. The clusters were found to be highly mobile if far from the surface, but were attracted and bound to the surface when within a distance of a few lattice parameters. When near the surface, the clusters were transformed into an immobile configuration due to the creation of a Frenkel pair; the vacancy was incorporated into what became a He_3–vacancy complex. The corresponding interstitial migrated to and became an adatom on the free surface. This process can contribute to He retention, and may be responsible for the observed deterioration of the plasma-exposed tungsten surfaces.

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1. Introduction

The divertors in a deuterium–tritium (DT) fusion reactor will operate at high temperatures while exposed to the high heat and charged particle fluxes arising from the DT fusion reaction. The plasma debris includes a high flux of He atoms which are a DT reaction product. Tungsten is an attractive candidate for this application due to its high melting point, low sputtering coefficient and high sputtering threshold energy [1]. A major potential impediment to successful operation of tungsten divertors is the surface erosion due to this He exposure and how He retention may influence the tritium inventory trapped in the divertor. The negative effects of the low energy (<100 eV) He atoms implanted from the fusion plasma include nucleation and growth of He bubbles and surface modification due to the formation of nanorod-like structures (known as 'fuzz') [2,3]. The atomistic mechanisms responsible for these phenomena are still not well understood and are the subject of considerable experimental and computational research.

The formation, stability, and mobility of small interstitial He clusters, and the initial stages of He bubble evolution are well suited for atomistic modeling. For example, previous work in bcc metals has demonstrated that small clusters of interstitial He atoms are highly mobile, but the lattice strain associated with helium clusters containing more than a few helium atoms can lead to the formation of Frenkel pair. The vacancy is incorporated into a He–vacancy cluster which is essentially immobile at relevant temperatures, and the ejected self-interstitial atom tends to be trapped by the He–vacancy cluster [4,5]. Similar studies devoted to this subject have recently been published on the tungsten–helium system, using both density-functional theory (DFT) [4,7] and molecular dynamics (MD) [8–11]. These efforts have resulted in a rather comprehensive understanding of the relative stability of various configurations of substitutional and interstitial He atom in the tungsten lattice [6], and small He–vacancy complexes He_kV_m ($k < 6$, $m < 5$) [7]. This knowledge has facilitated development of new interatomic potentials for the W–He system [12], which has made it possible to perform MD modeling of the effects of helium implantation on tungsten surfaces [8–11].

Clusters containing different numbers of He atoms can be created and contribute to the radiation-induced microstructural evolution both in the bulk and near free surfaces. In this paper we present the results of atomistic simulations involving small, and thus frequently-formed, highly mobile clusters of three interstitial He atoms located near low-index {1 1 1}, {1 1 0} and {1 0 0} free surfaces, as an initial phase of a larger investigation. It is found that the number of helium atoms required to create Frenkel pair in clusters near the surface is much smaller than that in the bulk, which indicates that surface may play an important role in helium retention. The simulations employed the self-evolving atomistic kinetic Monte Carlo (SEAKMC) method [13,14]. Like MD, this method describes the interatomic interactions using a set of

* Corresponding author at: Department of Materials Science and Engineering, University of Tennessee, Knoxville, TN 37996, USA. Tel.: +1 865 974 6183.
E-mail address: xhx@utk.edu (H. Xu).

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empirical potentials; but unlike MD it does not account for atomic vibrations. This enables the simulation of much longer physical times and it has been demonstrated to provide good fidelity to the results of MD simulations [14,15]. We demonstrate that although small interstitial He clusters are highly mobile in bulk material far from free surfaces, there is a short-range attraction to surfaces. If trapped by the surface, the clusters reduce their energy by producing a Frenkel pair. The incorporation of the vacancy transforms the mobile interstitial He cluster into an immobile He_3–vacancy complex. The corresponding interstitial migrates to and becomes an adatom on the free surface. This loss of mobility constitutes an additional mechanism for increasing He retention in tungsten, and adatom formation may contribute to the subsequent surface modification that produces tungsten fuzz at longer times. The presence of small vacancy–He clusters in the near-surface region may also increase tritium retention by trapping this otherwise mobile species.

2. Methods

2.1. SEAKMC method

We use the SEAKMC method with its constituent static relaxations and the dimer method for identifying saddle points in the present research [13–15]. The SEAKMC framework consists of several components. First, individual defects in the system are identified and the active volumes (AVs) for each defect are selected. The concept of an AV was introduced in order to increase the computational efficiency by taking into account the localized nature of most defects, and excluding distant atoms from consideration. The AVs are currently defined by a maximum distance, r_{AV}, from any defect atom. Second, a specified number of searches, n, are carried out using the dimer method [16] to determine the saddle point energies for transitions between possible configurations, E_i ($i \leqslant n$) while considering only atoms in AVs. Third, a particular transition, i, is randomly chosen according to the list of probabilities, P_i, weighted by corresponding Boltzmann factors, $P \propto \exp(-E/k_BT)$, for a given temperature, T, where k_B is the Boltzmann constant. The system clock is advanced according to the residence-time algorithm [17] by $\Delta t = -\ln\xi/\Sigma\nu\exp(-E_i/k_BT)$, where ξ is a random number uniformly distributed on (0, 1], and ν is the attempt frequency, which is assumed here to be the same for all transitions. Fourth, depending on the nature of the defect, either local (within the corresponding AV) or global relaxation of the system is performed to move from the saddle point to another local energy minimum. This new state is the starting configuration for the next MC time step.

SEAKMC was developed to study defect evolution on the atomic level and compares well with MD when the harmonic transition state theory is applicable. Generally, it allows simulating physical processes on much longer time scales than MD, which enable the method to be used to resolve a long-standing question concerning ⟨100⟩-loop formation in bcc iron [18]. In the current implementation of the model, all the saddle points found are treated as independent. This may result in some errors in the estimates of physical time, but does not affect the interaction between defects.

2.2. Interatomic potential

The set of interatomic potentials for the W–He system proposed by Juslin and Wirth [12] has been used. This includes a short range modification to the Ackland–Thetford W–W potential [19], a new pair-type W–He potential, and the Beck pair potential for He–He interaction [20] modified at short distances by Morishita et al. [21]. Compared with older potentials, this combination demonstrates improved agreement with the DFT formation energies of He and self-interstitial atoms in W obtained in [6,7] and [22], respectively.

2.3. Calculation details

A box size of $20a_0 \times 20a_0 \times 20a_0$ with ~18,000 atoms was used, where $a_0 = 3.1652$ Å is the tungsten lattice constant. Periodic boundary conditions were employed along two (denoted as x and y) directions, with a free surface perpendicular to z direction as shown in Fig. 1. The AV size was defined by $r_{AV} = 2.7a_0$, based on saddle point energy convergence tests of He atom diffusion in bulk tungsten. The attempt frequency is an external parameter in the treatment of SEAKMC results and was assumed to be $\nu = 10^{12}$ s^{-1}. Unlike diffusion studies, in which the absolute value and temperature dependence of the attempt frequency are very important to the results, here it is just a scaling factor which influences the estimated time associated with a particular sequence of events but does not alter the events themselves. Therefore, the observations reported below do not depend on the chosen value. The number of dimer searches for transitions for each active volume was $n = 12$. A larger number of saddle point searches ($n = 48$) has been carried out for the diffusion of He clusters in tungsten and no significant difference was observed between the results obtained for $n = 12$ or 48. The 'atomTV' software (http://web.ornl.gov/sci/physical_sciences_directorate/mst/fusionreactor/index.shtml) was used for graphical representation and analysis of the results.

3. Results

3.1. Atomic configuration of cluster of three interstitial He atoms

In the tungsten lattice, a cluster of three interstitial He atoms forms a triangular complex with two He atoms near one face of the unit cell, and the third He atom near a perpendicular face as shown in Fig. 2. In Fig. 2, the pair of He atoms at the base are ~$0.013a_o$ above the (100) plane and the third is ~$0.044a_o$ to the right of the (001) plane. The habit plane of the triangle is close

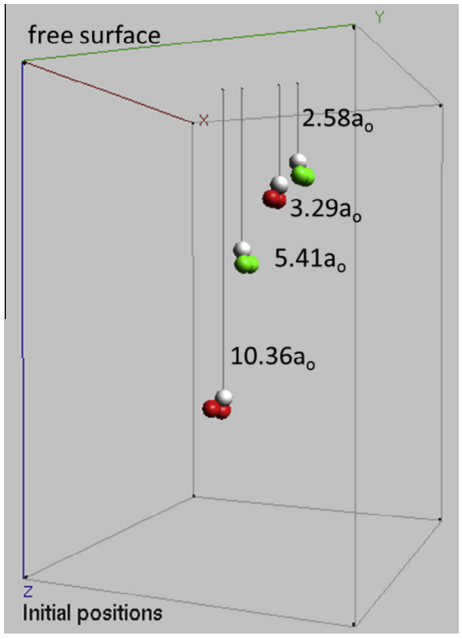

Fig. 1. Geometry for simulations: periodic boundary conditions along x and y directions, with a free surface perpendicular to z direction. Initial positions of typical He_3 interstitial clusters are shown with surface-to-cluster distances indicated; a_o is the W lattice parameter.

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