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A multiscale approach to defect evolution in tungsten under helium irradiation

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ABSTRACT

We have studied He irradiation in tungsten from a multiscale point of view: Density Functional Theory (DFT) to obtain the binding energies of He to vacancy clusters, Binary Collision Approximation (BCA) and Molecular Dynamics (MD) to produce defect cascades and Object Kinetic Monte Carlo (OKMC) to study their evolution in larger temporal and spatial scales. A comparison between BCA and MD cascades produced by PKA at different energies has been done at different temperatures: at high temperature and at high PKA energies the OKMC results clearly depend on the defect cascades. 625 keV pulsed He ion irradiation has been simulated with cascades obtained by means of BCA and MD. The results show that in the case of ion irradiation, BCA results can provide good OKMC results. However, in the case of neutron irradiation producing high energy PKAs, BCA cascades clearly overestimate the number of FPs, which may have a strong influence on the OKMC results.

1. Introduction

Tungsten is proposed as material for plasma facing components (PFC) in future fusion power plants due to its good properties: high melting point, high thermal conductivity, low sputtering coefficient and low tritium retention [1–3]. In direct-target Inertial Fusion Energy (IFE) the first wall will be irradiated by He ions, among others. The energy of He ions is on average ~2.5 MeV due to thermalization in the compressed target [4]. This energy is high enough to produce Frenkel Pairs (FP). He tends to nucleate inside vacancies because of its insolubility in metals, resulting under certain circumstances in dramatic He bubble formation [5,6], which can cause microstructural changes [7,8] that may develop into blistering, cracking and exfoliation of the material [9,10].

In this work we study He irradiation in tungsten with a multiscale simulation methodology: Density Functional Theory (DFT), Molecular Dynamics (MD), Binary Collision Approximation (BCA) and Object Kinetic Monte Carlo (OKMC). OKMC simulations provide quantitative data of damage distribution at large time and spatial scales, which allows to reproduce experiments and to obtain further information to the experimental results. However, this technique depends on initial damage cascades [11]. Damage cascades have been calculated with MD and BCA methods to produce input cascades for the OKMC simulations, with the aim to study their influence on the OKMC results. The role of BCA and MD cascades on the final results will be discussed.

2. Methods

MD simulations were carried out with LAMMPS code [12] with the Tersoff potential for tungsten, modified with ZBL [13]. Simulation box dimensions were $13.2 \times 13.2 \times 13.2\ nm^3$ (148176 W atoms) or $7.5 \times 7.5 \times 7.5\ nm^3$ (27648 W atoms). The boxes were thermalized at 300 K, 1000 K and 2000 K respectively. PKA energies from 0.2 to 2 keV were simulated with 1 fs time-step during 21 ps. For this purpose, the velocity (equivalent to the PKA energy) of an atom in the middle of the simulation box is set, while a thermal bath is set in a small region of ~1 nm thick on the box sides. The temperature were rescaled each 5 fs. The simulations were carried out in the supercomputer Magerit-CESVIMA (UPM), using 64 cores and a simulation time of about 5 h. Vacancies and interstitials were obtained by analyzing the results with the space-filling Wigner–Seitz cells methods [14,15].

BCA simulations were carried out with the SRIM [16] code. We set the displacement energy, $E_d = 90$ eV [17]. FP production with

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Table 1
Attempt frequencies ($\nu_0 = 6 \times 10^{12}\ s^{-1}$) and migration energies for single objects: He atom, SIA and single vacancy [20].

Object	Attempt frequency (s^{-1})	Migration energy (eV)
He	$10^{-2}\ \nu_0$	0.01
I (SIA)	ν_0	0.013
V	ν_0	1.66

PKAs from 0.2 to 2 keV was studied to build a defect (FP) cascade database. As SRIM does not provide the position of self interstitial atom, we assumed a thermalization distance following a Gaussian distribution with the range and straggle obtained by SRIM. In this way, we generated another defect cascade database with BCA. The defect cascades obtained by MD or BCA were introduced in MMonCa, an Open Source OKMC code [18,19], at a rate of $10^{13}\ cm^{-2}\ s^{-2}$, up to $10^{15}\ cm^{-2}$ in the case of continuous irradiation or the same fluence ($10^{15}\ cm^{-2}$) but in one single pulse at the beginning of the simulation in the case of pulsed irradiation. The PKA energies were 200 eV, 300 eV, 1 keV and 2 keV at 300 K and 1000 K. At 300 K we have simulated also pulsed irradiation, i.e., we have introduced all the MD or BCA cascades at the same time, at the beginning of the simulation.

In the case of OKMC simulations for He in tungsten, we used a parametrization combining our own DFT data with previously published data [20–22]. Details on the He parameterization will be given elsewhere (see migration values for single objects in Table 1). We have simulated pulsed He (625 keV) irradiation, following the experimental conditions published by Renk et al. [23]. In a simulation box of $1500 \times 50 \times 50\ nm^3$ we introduced 80 pulses (10^{13} He cm^{-2} per pulse) at ~773 K, which leads to a sudden temperature raise to ~1500 K during ≈500 ns. One set of He cascades were obtained with SRIM and the second one was calculated as follows: the PKA position and energy were obtained with SRIM and in those positions we used the defect cascades obtained with MD corresponding the PKA energy.

3. Results and discussion

In Fig. 1(a), a comparison between our MD results with previously published data [24–26] is shown. The trend is similar, however, our results show a higher FP production comparing to those of Setyawan et al. [26] and lower values comparing with the results of Troev et al. [24]. These differences could be due to using different potentials and methodologies. As shown in Ref. [20], the lowest formation energy of a vacancy is given by the potential we have used. This leads to the highest FP production rate as observed in Fig. 1(a). Caturla et al. [25] obtained the highest values. This is

Table 2
Energy distribution of PKA due to He ions (625 keV) irradiation in tungsten [16].

PKA energy (eV)	Fraction
<150	0.38
150 ⩽ energy < 250	0.25
250 ⩽ energy < 400	0.14
400 ⩽ energy < 750	0.11
750 ⩽ energy < 1500	0.06
1500 ⩽ energy < 2500	0.02
Energy < 2500	0.01

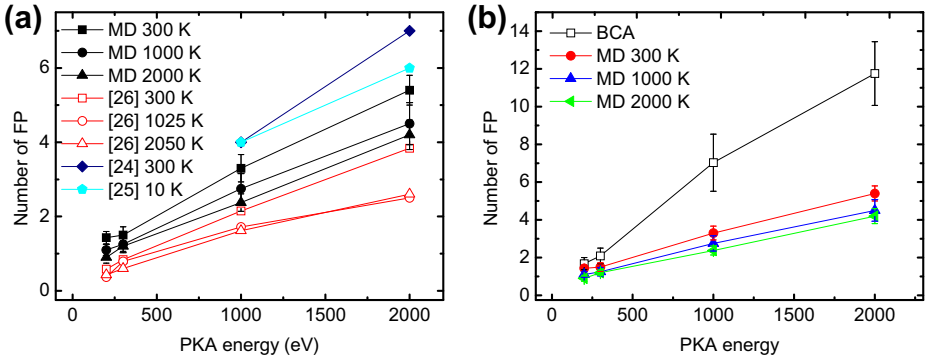

Fig. 1. Average number of created FPs as a function of the PKA energy at different temperatures. We compare our results obtained by Molecular Dynamics with previously published data (a) and with our Binary Collision Approximation results (b).

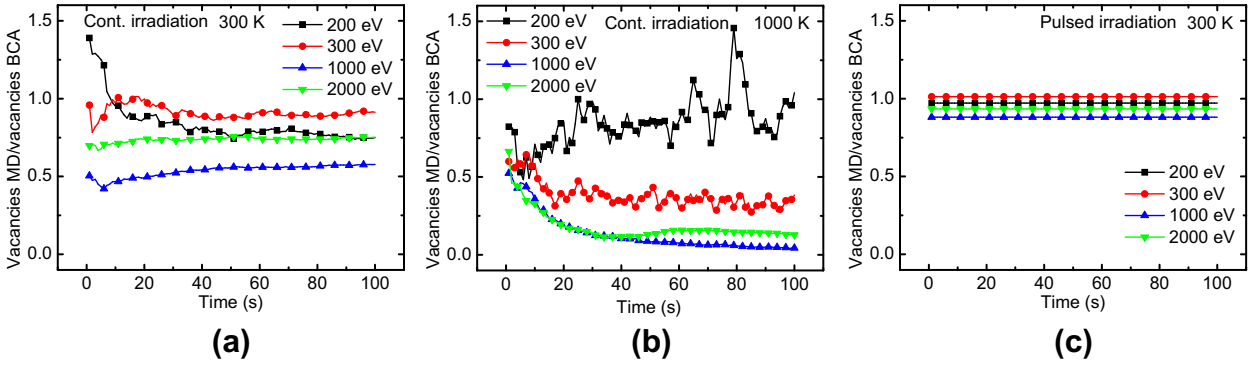

Fig. 2. Temporal evolution of the number of remaining vacancies obtained with MD cascades divided by the number of vacancies obtained with BCA cascades in the case of (a) continuous irradiation at 300 K; (b) continuous irradiation at 1000 K and (c) pulsed irradiation at 300 K, as a function of the PKA energy.