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Effects of Fe–He potential on primary damage formation in Fe-1%He

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ABSTRACT

The effects of different Fe–He interatomic potentials on primary damage formation in Fe-1%He are investigated using molecular dynamics (MD) methods. Simulations of cascades produced by primary knock-on atoms (PKA) of energy E_p = 0.5–10 keV were performed at an irradiation temperature of 100 K. It is found that the Fe–He potentials have significant effects on the point defect creation and the formation of Fe–He interstitial clusters, whereas small effects on the formation of He–vacancy clusters.

1. Introduction

It is well known that in fusion reactor environments helium atoms produced internally by (n,α) reactions in materials can easily precipitate into clusters or bubbles due to very low solubility and high mobility, which would significantly degrades the mechanical properties of materials [1,2]. Understanding of the fundamental behavior of helium in metals is one key issue in the research and development of fusion reactor materials.

Recently, we have investigated quantitatively the effects of displacement cascades on the formation of He–vacancy (He–V) clusters [3] and the stability of He clusters [4]. In those simulations the interactions of Fe–Fe, Fe–He and He–He were described by the Ackland et al. [5], Wilson–Johnson [6] and Beck [7] potentials, respectively. However, these potentials give the octahedral position of a He interstitial as the most stable interstitial configuration in Fe, which is in contrast to the results obtained recently by ab initio calculations [8]. Recently, a new empirical Fe–He potential developed by Seletskaia et al. gives the tetrahedral position of a He interstitial as the most stable configuration in Fe [9]. Previously, a new set of interatomic potentials for Fe–He, Fe–Fe and He–He interactions [9–11] has been employed to study the formation and nucleation of He–V clusters induced by displacement cascades [12], and the results were compared with an old set of the potentials [3]. However, the formation of point defects and He interstitials created by displacement cascades needs to be further studied. As the first step to address the effects of the potentials on defect production and He interstitial clustering, a number of displacement cascades have been simulated using two different Fe–He potentials, but with the same Fe–Fe and He–He potentials, in Fe with the 1 at.% He concentration (Fe-1%He) at 100 K.

2. Simulation procedure

In the present simulations, the Fe–Fe and He–He interactions are described by Ackland et al. [5] and Beck potentials [7] respectively, but the Fe–He interaction is described either by Wilson potential [6] or by Seletskaia potential [9]. For the Seletskaia's Fe–He interaction, the three-body term was introduced to improve the fitting for a single He interstitial, and the potential gives the tetrahedral position of a He interstitial as the most stable configuration in Fe. However, the octahedral position is the most stable configuration for a He interstitial calculated using the Wilson's Fe–He pair potential. Table 1 summarizes some He defect formation energies in Fe obtained by the two different Fe–He potentials. We found that although there exist some differences in the stable configurations of He interstitials, their migration energies obtained using the two Fe–He potentials are very similar. Furthermore, the formation energies of different He–V and He–He clusters obtained using the two Fe–He potentials are also similar. It is not clear how these two Fe–He potentials affect the formation of point defects and He interstitial clusters in α-Fe, which will be investigated in the

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Table 1
Summary of He defect formation energies (eV) in Fe obtained using the different Fe–He potentials.

Defect	VASP[a]	Fe–He potentials	
		Wilson–Johnson	Seletskaia
He octa	4.60	5.25	4.70
He tetra	4.37	5.34	4.33
He_{i-mid}	4.43	5.37	4.37
He sub	4.08	3.25	3.70
He–He–vac	6.29	6.31	6.42
He–He–He–vac	9.09	9.47	9.34
He–He interaction	8.72	9.78	8.33

[a] [8,9].

present work. For convenience, in this paper the Ackland, Wilson and Beck potentials for the Fe–Fe, Fe–He and He–He interactions will be referred to as P-I, and the Ackland, Seletskaia and Beck potentials as P-II.

All the simulations were performed using the molecular dynamics code MOLDY with P-I and P-II potentials. To generate the corresponding He concentrations in the simulation cells, Fe atoms were randomly replaced by He atoms, forming 1 at.% substitutional He atoms in bcc Fe. The primary knock-on atoms (PKAs) with energies, E_p, from 0.5 to 10 keV were considered. The detailed simulation method is same as that in the [3] and a total of 120 cascades were simulated using the P-I and P-II potentials.

3. Results and discussion

The present simulations indicate that the general features of these cascades are the same for both sets of potentials, i.e. there are a great number of defects produced in the ballistic phase, some of the formed point defects are gathered in small clusters and others remain isolated in the cooling phase. Fig. 1 shows the defects remaining in a 10 keV cascade of Fe-1%He after 10 ps with different potentials: (a) the P-I and (b) the P-II. It can be seen from Fig. 1 that the vacancy-rich He_nV_m ($n \leqslant m$) clusters tend to form within the cascade core, and the interstitials (including Fe and He interstitials) and helium-rich He_nV_m ($n > m$) clusters tend to form at the periphery of the original cascade volume for the two Fe–He potentials. However, big differences can be observed between the two potentials, which will be discussed in details in the following sections.

3.1. Point defect

Fig. 2 shows the number of Frenkel pairs, N_F, created by the cascades in Fe-1%He versus the kinetic energy of the PKA, E_p, including

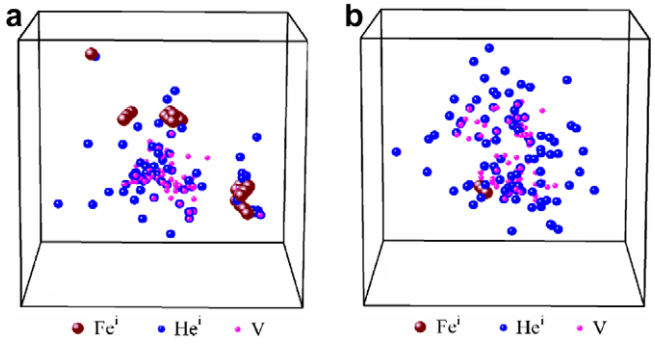

Fig. 1. Typical defect configurations of a 10 keV cascade at 100 K after 10 ps in α-Fe with 1 at.% He for different potentials: (a) the P-I and (b) the P-II, where the largest and medium spheres indicate Fe and He interstitials respectively, and the smallest spheres represent vacancies.

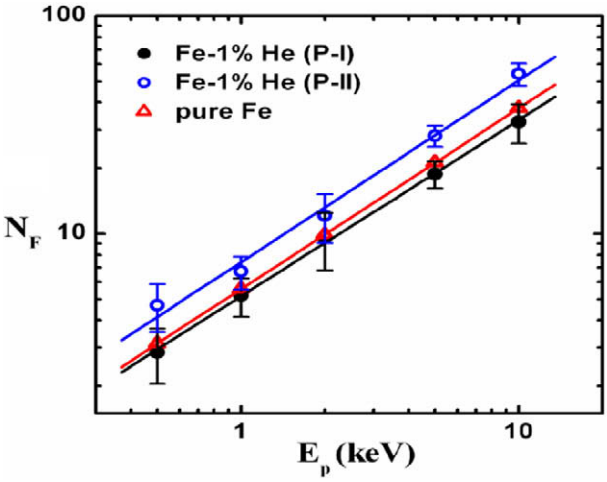

Fig. 2. Log–log plot of N_F versus E_p in α-Fe with 1 at.% He concentration for different potentials and in pure α-Fe at 100 K. The error bars show standard deviation.

He and Fe interstitials. From the Fig. 2, it can be clearly seen that the value of N_F given by the P-I is slightly smaller than that in pure α-Fe without helium [13] for the same PKA energies, but N_F obtained by the P-II is significantly higher than that of pure Fe. The differences of the formation energies of He point defects given by the two Fe–He potentials may account for the observed difference in the present simulations. In the P-II the Seletskaia's Fe–He potential gives much lower formation energies of He interstitials, but higher formation energy of a substitutional He atom, as shown in Table 1. This may suggest that the more He interstitials can be formed within a cascade.

Number of He interstitials at peak time versus PKA energy (E_p) was shown in Fig. 3 for the two sets of potentials used in this work. Clearly, the P-I potential provides less He interstitials at peak time than the P-II potential, i.e. more substitutional He atoms are displaced from their sites within cascades with the P-II than with the P-I. Furthermore, the detailed analysis of these cascades indicates the contribution of He interstitials to the total N_F is significantly larger than that of Fe interstitials for the two sets of potentials.

In Fig. 1, it is of interest to find that a few Fe–He interstitial dumbbells can be formed in the cascades simulated with the P-I,

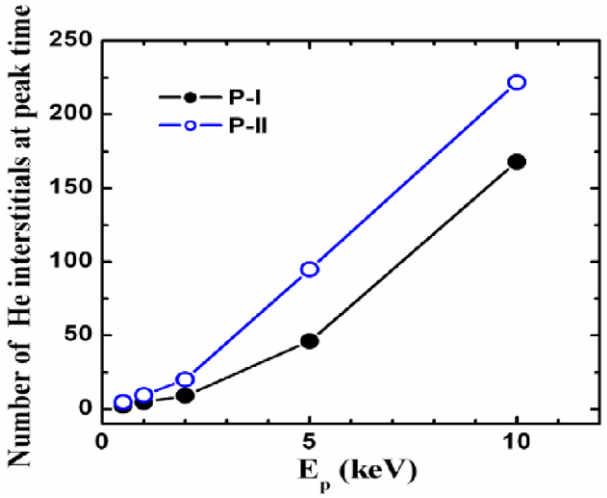

Fig. 3. Number of He interstitials at peak time versus PKA energy for different potentials.