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The interaction of defects in titanium: A molecular dynamics study

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Abstract Behaviors and properties of helium in titanium were explored by molecular dynamics (MD) simulation in this study. The influence of He number, vacancy number and He density (ratio of helium to vacancy) on the thermal stability of He_nV_m clusters (where n and m denote the number of He atoms and vacancies) were investigated. Meanwhile, interactions among He atoms, SIA atoms and vacancies were discussed. The results demonstrate that the binding energies of an interstitial helium atom primarily depend on He and vacancy numbers rather than the helium-to-vacancy ratio (n/m). It is different from the previous report of other researchers. The binding energies of an isolated vacancy and a self-interstitial titanium atom depend on both the number of helium atoms and the helium-to-vacancy ratio (n/m) of clusters. The thermal stability of clusters is decided by the competitive processes among thermal emissions of vacancy, SIA and helium atom.

Key words Molecular dynamics; Binding Energy; Helium-Vacancy cluster; Titanium

1 Introduction

Titanium, as the material in the first walls of a fusion reactor, is exposed to high energy neutron irradiations, resulting in a high rate of helium production by (n,α) reactions. Introducing helium atoms into materials can significantly change their microstructure and mechanical properties, e.g. surface roughening and blistering, and void swelling. Understanding the fundamental behavior of helium in titanium is beneficial to researching and developing fusion reactor materials, especially predicting the material lifetimes.

The energies of a helium atom at different cell sites determine its solubility, diffusion, and trapping in metal, and helium coalescence and growth of bubbles, and calculating energy parameters is fundamental to the study of helium behavior in metal[1–6]. Morishita K *et al*[7] and Ao B *et al*[8] reported that the binding energies of an interstitial helium atom, an isolated vacancy and a self-interstitial atom (SIA) to a helium-vacancy cluster do not depend much on the cluster size, but instead they depend primarily on the helium-to-vacancy ratio (n/m) of the clusters. However, this is different from what is observed in this paper.

2 Molecular dynamics methods

Molecular dynamics (MD) model was used to evaluate effects of He, SIA and vacancy on formation energy and binding energy in titanium. A general description of molecular dynamics can be found in a number of textbooks[9–12]. The concrete implementation of MD in this paper is as follows.

The simulation box is 10 monolayers thick and each layer contains 10×10 atoms arranged in *hcp* (001) planes. The simulation box with n helium atoms and m vacancies is relaxed at 300 K using an electron-phonon coupling model, followed by cooling down and quenching the system to 0 K[13,14].

Tight-binding potential, which is widely used to study the thermal and defect properties of metals

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and inter-metallic alloys, is employed to describe the Ti-Ti interaction[15]. The Lennard-Jones potential, which is well fitted to the interaction for inert gas atoms, is chosen for the He-He interaction [16]. For the He-Ti interaction, pair-wise potential is constructed by fitting the Lennard-Jones function from *ab initio* data. The detailed description of these potentials can be found in our previous papers[17–21].

3 Calculation of defect energies

The formation energy is calculated by comparing the energy of a crystal containing defects with perfect lattice sites having the same number of atoms. The formation energy of a $\mathrm{He}_n\mathrm{V}_m$ cluster with n He atoms and m vacancies is defined as:

$$E_f(\mathrm{He}_n\mathrm{V}_m) = E_{\mathrm{tot}}(\mathrm{He}_n\mathrm{V}_m) - n\varepsilon_{\mathrm{He}} - (N-m)\varepsilon_{\mathrm{Ti}} \quad (1)$$

where N is the number of perfect *hcp* lattice sites in the calculated cell and $(N-m)$ is the number of Ti atoms in the box. $E_{\mathrm{tot}}(\mathrm{He}_n\mathrm{V}_m)$ is the total energy of a Ti lattice containing a $\mathrm{He}_n\mathrm{V}_m$ cluster with n He atoms in a void of m vacancies, $\varepsilon_{\mathrm{Ti}}$ is the cohesive energy of a perfect *hcp* Ti crystal, and $\varepsilon_{\mathrm{He}}$ is the difference in total energy between a perfect *hcp* Ti crystal and a Ti crystal containing a He atom. Here, the calculated results are $\varepsilon_{\mathrm{Ti}} = -4.84$ eV/atom and $\varepsilon_{\mathrm{He}(hcp)} = -0.00617$ eV/atom.

The defect binding energy is determined by comparing the difference in total energy before and after binding a point defect to a $\mathrm{He}_n\mathrm{V}_m$ cluster. The binding energy of an interstitial He atom, a vacancy and a self-interstitial Ti atom to a $\mathrm{He}_n\mathrm{V}_m$ cluster can be given by[7,22]:

$$E_{\mathrm{b}}(\mathrm{He}) = E_{\mathrm{f}}(\mathrm{He}) + E_{\mathrm{f}}(\mathrm{He}_{n-1}\mathrm{V}_m) - E_{\mathrm{f}}(\mathrm{He}_n\mathrm{V}_m) \quad (2)$$

$$E_{\mathrm{b}}(\mathrm{V}) = E_{\mathrm{f}}(\mathrm{V}) + E_{\mathrm{f}}(\mathrm{He}_n\mathrm{V}_{m-1}) - E_{\mathrm{f}}(\mathrm{He}_n\mathrm{V}_m) \quad (3)$$

$$E_{\mathrm{b}}(\mathrm{SIA}) = E_{\mathrm{f}}(\mathrm{SIA}) + E_{\mathrm{f}}(\mathrm{He}_n\mathrm{V}_{m+1}) - E_{\mathrm{f}}(\mathrm{He}_n\mathrm{V}_m) \quad (4)$$

where $E_{\mathrm{f}}(\mathrm{He})$ is the formation energy of He at an interstitial site, $E_{\mathrm{f}}(\mathrm{V})$ is the mono-vacancy formation energy, and $E_{\mathrm{f}}(\mathrm{SIA})$ is the self-interstitial Ti atom formation energy. The calculated $E_{\mathrm{f}}(\mathrm{He})$, $E_{\mathrm{f}}(\mathrm{V})$, and $E_{\mathrm{f}}(\mathrm{SIA})$ in *hcp* Ti were 3.19, 1.59 and 1.64 eV/atom, respectively.

4 Results and discussion

4.1 Formation energy

The formation energy of $\mathrm{He}_n\mathrm{V}_m$ (n=0–50, and m =1–7) was calculated using Eq.(1). We found that the formation energies of a $\mathrm{He}_n\mathrm{V}_m$ cluster grow quickly with the introduction of He atoms (not shown here).

Fig. 1 shows the formation energy of $\mathrm{He}_n\mathrm{V}_m$ as a function of the He density of the cluster. The He formation energy increases with the He density, and it grows faster for m=7 than m=1. By introduction of vacancies, the He formation energy increases for equal He density and it rises faster for n/m=7 than n/m=1.

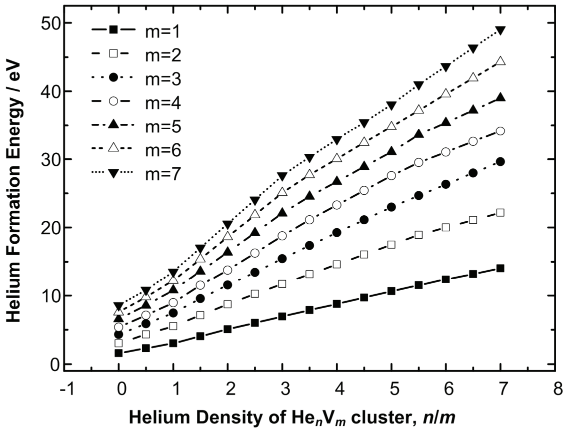

Fig.1 The formation energy of $\mathrm{He}_n\mathrm{V}_m$ versus the He density of the cluster.

4.2 Binding energy

The binding energies of a He atom, a vacancy, and an SIA Ti atom to a $\mathrm{He}_n\mathrm{V}_m$ cluster were calculated with Eqs. (2), (3) and (4). Binding energy represents the released energy of combining the $(n+1)$-th helium atom, the SIA atom and the vacancy with a $\mathrm{He}_n\mathrm{V}_m$ cluster, thus denoting the strength of the combination. For comparing the difference of the binding energy among helium atom, SIA atom and vacancy, and presenting clearly the influence of helium atom, vacancy and n/m on binding energy, all binding energies in Fig.2, 3 and 4 are average values. For n/m, both $\mathrm{He}_1\mathrm{V}_1$ and $\mathrm{He}_7\mathrm{V}_7$ are regarded as n/m=1.

Fig.2 shows a plot of the binding energy of a He atom, a vacancy and an SIA Ti atom to a $\mathrm{He}_n\mathrm{V}_m$ cluster as a function of the He number in the cluster. By introducing the He atom, the vacancy binding energy increases, but SIA binding energies decrease.

However, introducing the He atom causes the He binding energy to decline, followed by a slow rise when the He number of the cluster is greater than 10, which is consistent with previous experimental observations [23].

From Fig.2, it is found that helium and SIA atoms are more easily attracted by a He_nV_m cluster than a vacancy, when there are fewer helium atoms in the He_nV_m cluster. However, with increasing number of helium in the He_nV_m cluster, it is easier for a He atom and vacancy to be trapped by a He_nV_m cluster than an SIA atom. It denotes the continuous emission of self-interstitial atoms and growth of the He_nV_m cluster by trapping helium atom and vacancy.

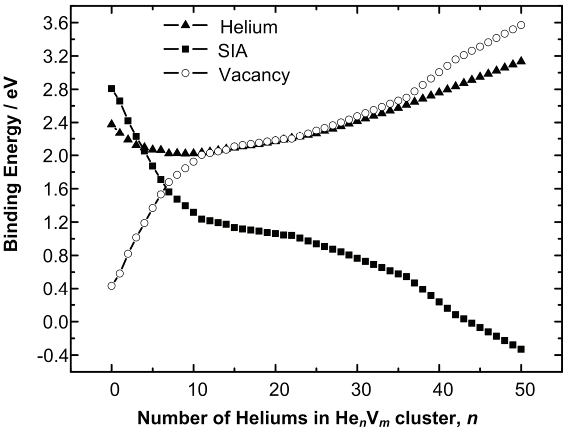

Fig.2 Binding energy of He atom, vacancy and SIA atom to a He_nV_m cluster vs the number of He atoms in the cluster.

Also from Fig.2, the variation range for vacancy and SIA binding energies are greater than that of He. This suggests that the influence of the He number on SIA and vacancy binding energy may be greater than on He binding energy.

Fig.3 shows the relationship of binding energy with He density. The binding energy of an SIA atom to a He_nV_m cluster decreases gradually with He density, but increases at He density of >5.5. The binding energy of a vacancy to a He_nV_m cluster gradually rises with He density, but declines at He density of >5.5. The change at the He density of > 5.5 originates from SIA emissions associated with the vacancy increase in number. This finally results in the rise of SIA binding energy and the decline of vacancy binding energy. However, there is little fluctuation for He binding energy.

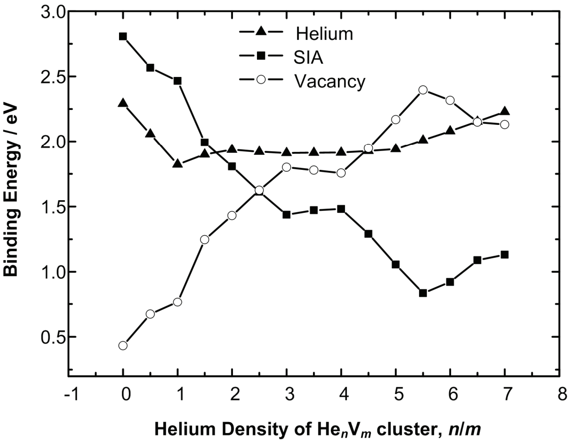

Fig.3 Binding energy of He atom, vacancy and SIA Ti atom to a He_nV_m cluster versus He density of the cluster.

Fig.3 shows that it is easier for SIA atom than vacancy to be trapped by a He_nV_m cluster in lower He density. However, with the increase of He density, a vacancy is more easily trapped by a He_nV_m cluster than an SIA atom. This indicates that the SIA and vacancy binding energy depends on the He density. However, the He density has little influence on the He binding energy.

The dependencies of the binding energy on vacancy numbers in the He_nV_m cluster are shown in Fig. 4.

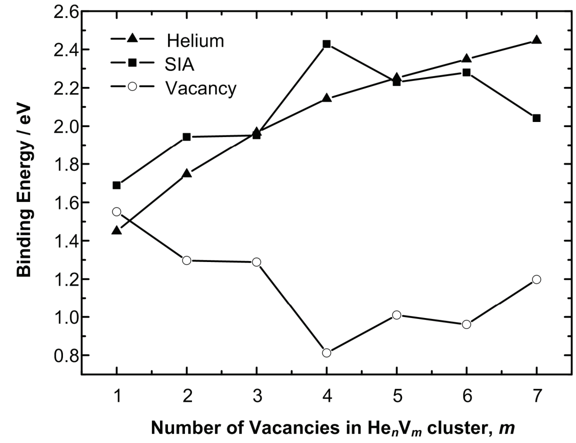

Fig.4 Binding energy of He atom, vacancy and SIA Ti atom to a He_nV_m cluster versus the number of vacancies in the cluster.

From Fig. 4, one can find that the He binding energy increases with the vacancy number. Comparing Figs.(2)–(4), we note that He binding energies depend primarily on the number of He and vacancy. With increasing vacancy numbers, however, the SIA and vacancy binding energy changes little. Moreover, He and SIA binding energies are larger than vacancy binding energy generally. This indicates that He and SIA atoms are more easily trapped by a $\mathrm{He}_n\mathrm{V}_m$ cluster than vacancies. We can imagine that the ratio of n/m in a cluster gradually increases with the growth of helium bubble and that there are SIA atoms in the $\mathrm{He}_n\mathrm{V}_m$ cluster. The growth process of a He bubble is a competitive process among He, SIA and vacancies which are trapped by a $\mathrm{He}_n\mathrm{V}_m$ cluster.

5 Conclusion

The formation energies and binding energies of a $\mathrm{He}_n\mathrm{V}_m$ cluster in Ti have been studied by using molecular dynamics. The main conclusions of in this paper are that He binding energies primarily depend on the number of He and vacancy. Furthermore, the binding energies of vacancy and SIA atom depend on both helium number and He density. In general, the order of the influence on binding energy from big to small is He number, He density and vacancy number. With the growth of helium bubbles, the ratio of n/m in a cluster gradually increases. Helium bubble grows by a competitive process among vacancies, SIA and helium atoms to be trapped by a $\mathrm{He}_n\mathrm{V}_m$ cluster.

Formation energy and binding energy are important parameters for kinetics calculations and long-term and multi scale simulations. This conclusion is instructive for further research into the influence of defects on materials.

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