Available online at www.sciencedirect.com
ScienceDirect
Journal of Nuclear Materials 374 (2008) 437–444
journal of nuclear materials
www.elsevier.com/locate/jnucmat

Multiple-interactions of displacement cascades with He–vacancy clusters in α-iron: Computer simulations

L. Yang [a,b], X.T. Zu [a,*], Z.G. Wang [a], F. Gao [c], H.L. Heinisch [c], R.J. Kurtz [c], X.Y. Wang [d], K.Z. Liu [d]

[a] Department of Applied Physics, University of Electronic Science and Technology of China, Chengdu 610054, China
[b] School of Physics and Electronics Information, China West Normal University, Nanchong 637002, China
[c] Pacific Northwest National Laboratory, MS K8-93, P.O. Box 999, Richland, WA 99352, USA
[d] National Key Laboratory for Surface Physics and Chemistry, China Academy of Engineering Physics, Mianyang 621907, China

Received 22 January 2007; accepted 24 September 2007

Abstract

Multiple-interactions of displacement cascades with He–vacancy (He–V) clusters are investigated using molecular dynamics simulations. The effects of a single displacement cascade on the stability of a He–V cluster depend on the He-to-vacancy (He/V) ratio and the primary knock-on atom (PKA) energy. Initial He–V clusters consist of 10 and 20 vacancies with He/V ratios ranging from 0.2 to 3 and the PKA energy, E_p, varying from 2 keV to 10 keV. The size of He–V clusters was found to generally increase with increasing He/V ratios for the same PKA energy, but the stability of He–V clusters decreases with increasing PKA energy. The results are compared with those for voids impacted by collisional cascades. During multiple 5 keV, cascade events, the final size of He–V clusters depends on only the initial He/V ratios. It is of interest to notice that the number of vacancies in a He–V cluster is determined by the first cascade event, while subsequent cascade overlap has a significant effect on its stability. These results are discussed in terms of the internal pressure of He–V clusters, the mobility of He atoms, the number of vacancies produced by cascades and the He/V ratio.
© 2007 Elsevier B.V. All rights reserved.

PACS: 02.70.Ns; 61.72.Ji; 61.82.Bg

1. Introduction

Based on their favorable long-term radioactivity burden and short-term radionuclide safety, as well as practical applications, ferritic/martensitic steels have been proposed as potential candidates for fusion reactor structure materials [1]. In a fusion reactor environment high rates of insoluble He are generated in steels due to nuclear (n, α) transmutation reactions, and these He atoms play a significant role in the radiation-induced microstructure evolution. Because of the extremely low solubility of helium in metals, helium atoms tend to be deeply trapped in small vacancy clusters, leading to the creation of helium-stabilized bubbles [2–6]. The formation of He bubbles in bulk or at grain boundaries (GBs) remains one of the most important issues in nuclear fusion technology, and He accumulation, both in the bulk and at GBs, has major consequences for the structural integrity of first-wall materials. Multiscale modeling provides a basis to obtain insight and general understanding of the complex radiation damage processes. Particularly, molecular dynamics (MD) methods have been widely employed to study the atomic-level processes of defects controlling microstructural evolution in advanced ferritic steels [7–9]. Recently, several computer simulations have been employed to yield important understanding of He behavior in bcc metals [10–12] and fcc metals [13,14]. Furthermore, atomistic calculations demonstrate the strong binding of He to GBs in α-Fe, and that

* Corresponding author.
E-mail address: xiaotaozu@yahoo.com (X.T. Zu).

0022-3115/$ - see front matter © 2007 Elsevier B.V. All rights reserved.
doi:10.1016/j.jnucmat.2007.09.060

both substitutional and interstitial He atoms are trapped at GBs [12]. The MD methods have also been utilized to study displacement cascades in α-Fe containing different concentrations of substitutional He atoms [15]. It is found that He bubbles can be nucleated directly within displacement cascades.

However, experimental observations have revealed that early-formed He bubbles in materials are subsequently subjected to bombardments of displacement cascades [16]. A simple model has been proposed by Trinkaus [17] to describe these experimental observations by assuming that the cascade-induced He resolution and the escape from existing bubbles depend on bubble size in relation to the He atom diffusion range reached in the thermal spike phase of a cascade. However, the recent computer simulations have shown that the stability of He–V clusters does not depend much on cluster size, but rather on the helium-to-vacancy (He/V) ratio in α-Fe [10], and within a displacement cascade [18]. In previous work, only the stability of He–V clusters containing 20 vacancies under a single cascade has been studied. In order to investigate the size effects on the stability of He–V clusters under a single cascade, we extended the simulations to those with 10 vacancies in this work. Particularly, the multiple interactions of cascades with the He–V clusters are systematically investigated to explore the possible mechanisms of cascade-induced He resolution and escape from existing bubbles. The results are discussed in terms of the internal pressure of He bubbles, the He/V ratio of He–V clusters, the mobility of He atoms and the PKA energy.

2. Simulation procedure

The interaction of single displacement cascades with small He bubbles and cascade overlap events in α-Fe was studied using MD. A modified version of the MOLDY computer code [7] was used in this study, employing the interatomic potentials of Ackland [19], Wilson-Johnson [20] and Beck [21] to describe the interactions of Fe–Fe, Fe–He and He–He, respectively. However, the He–He potential was refit to decrease the cut-off distance to 0.54857 nm to improve computational efficiency, and this leads to a small changes in cohesive energy of a perfect fcc He crystal (i.e. −0.005678 eV/atom, as compared with the value of −0.00714 eV/atom given by the original potentials). It should be noted that a new potential describing the Fe–He interaction has been recently developed [22], which is based on the stable configurations of a single He interstitial in Fe calculated by ab initio methods. However, the preliminary results of comparative studies of He–V clusters using both sets of potentials [23] indicate that there is no significant difference in the relaxed configurations of these He–V clusters. It is expected that the effects of this new He–Fe potential on the present study should be very small. All the simulations are carried out with periodic boundaries and constant volume conditions. The size of the MD block is chosen such that the results are not influenced by the periodic boundaries employed. A crystal of 128 000 atoms ($40a_0 \times 40a_0 \times 40a_0$, where a_0 is the lattice constant of Fe) is used to simulate the displacement cascades of 2 and 5 keV Fe recoil atoms, while 250 000 atoms ($50a_0 \times 50a_0 \times 50a_0$ unit cells) are employed to study 10 keV cascades. For example, 10 keV deposited among 250 000 atoms would lead to an increase in T of over 200 K, but the defects produced in cascades were in the core of the block, the cascade evolution was visually monitored in each event during the collisional and thermal spike phases to make sure that there was no self-interaction when boundary crossing occurred. We have simulated several cases with much larger block (500 000 atoms), but no significant effects are found. Therefore, 250 000 atoms ($50a_0 \times 50a_0 \times 50a_0$ unit cells) are large enough to study 10 keV cascades.

In the center of the simulation block, a He–V cluster was created by removing Fe atoms and filling the vacant sites with He atoms to a given He/V ratio. In order to study the effects of the size of a He–V cluster on its stability within displacement cascades, initial clusters with 10 and 20 vacancies were chosen, having He/V ratios varying from 0.2 to 3, as listed in Table 1. Prior to simulating a cascade event, the MD block containing the He–V cluster was equilibrated at 300 K for 10 ps under a constant pressure boundary condition, and it was then quenched to 0 K to archive the most stable configuration of the He–V cluster. Subsequently, the MD block was reheated to 100 K under a constant pressure condition and allowed to re-equilibrate for an additional 20 ps. Individual cascades from single primary knock-on atoms (PKA) with recoil energies of 2, 5, and 10 keV were initiated at distances of 0.887 nm and 1.183 nm from the center of the MD block along a high

Table 1
Summary of cascade-He–Vacancy cluster simulations

Simulation type	PKA energy (keV)	Number of vacancies in clusters	He/V ratio	Number of events[a]	Number of replicates[b]
Mono-irradiation	2,5	10	3	1	5
	2,5	10	2	1	5
	2,5	10	1	1	5
	2,5	10	0.5	1	5
	2,5	10	0.2	1	5
	2,5,10	20	3	1	5
	2,5,10	20	2	1	5
	2,5,10	20	1	1	5
	2,5,10	20	0.5	1	5
	2,5,10	20	0.2	1	5
	2,5,10	20	0	1	5
Isotropic multi-irradiations	5	20	3	6	3
	5	20	1	6	3
	5	20	0.5	6	3

A total of 28 different single event cascade-cluster conditions were simulated, with each condition replicated five times. Three multiple cascade events consisting of six consecutive cascades each were performed with each condition replicated three times.

[a] A single cascade event.

[b] Number of times entire sequence of events repeated.

index direction ⟨1 3 5⟩. The simulations were each continued for 15–20 ps at constant volume.

After the first cascade ended, the crystal containing the defects and He–V cluster was then quenched to 0 K, following which it was re-equilibrated at a given temperature. A second cascade was then introduced to interact with the He–V cluster, which initiated at a random location at the same radius and directly impacted on the He–V cluster. This maximized the effects of cascade-induced He resolution and escape from the He–V bubble. Once a cascade was introduced, the simulation continued for another 20 ps at constant volume, following which a relaxation of the lattice was performed at constant pressure for an additional 10 ps. All the subsequent cascades were introduced using a similar approach, and a total of six cascade overlap events were simulated. A summary of the simulated events is provided in Table 1.

3. Results and discussion

3.1. Interaction of a single cascade with He–V clusters

The stability of He–V clusters and voids (consisting of only vacancies) within displacement cascades was firstly examined. Fig. 1 shows the atomic arrangements of a cluster with a He/V ratio of 3. The (a) initial state, where the numbers of He atoms and vacancies in this cluster are 60 and 20 and (b) final damage state after a 5 keV cascade collision are shown, where the large and small spheres indicate He atoms and Fe interstitials, respectively and the medium spheres represent vacancies. In the initial configuration after relaxation, He atoms form a close-packed configuration at the center of the MD block, as shown in Fig. 1(a), but the internal pressure produced by the collective motion of He atoms in the cluster is not large enough to push iron lattice atoms off their normal sites to form Fe interstitials. Fig. 1(b) shows the final damage state after a displacement cascade. It can be seen that the cascade produces some single interstitial and large interstitial clusters at the periphery of the cascade, a similar behavior to those in pure α-Fe. The largest self-interstitial atom (SIA) cluster consists of 14 interstitials. However, it is surprising to note that there is a very small number of vacancies distributed at the core of the cascade, and almost all the vacancies produced by the cascade are swept into the He–V cluster, which results in an increase in the number of vacancies in the cluster. The total number of vacancies in this cluster is 41, as compared to 20 vacancies in its original state, which decreases the He/V ratio to 1.46. The He atoms in the cluster are not dissolved from the He–V cluster.

Fig. 2 shows the He–V cluster configuration with the He/V ratio of 1. The initial relaxed state, where the numbers of He atoms and vacancies in this cluster are 20 shows that the He atoms in this cluster are located very near substitutional sites, as shown in Fig. 2(a). After a cascade event, the number of vacancies in the He–V clusters remains almost the same, but two He atoms are dissolved from the cluster, forming a substitutional and an interstitial atom, respectively, as shown in Fig. 2(b).

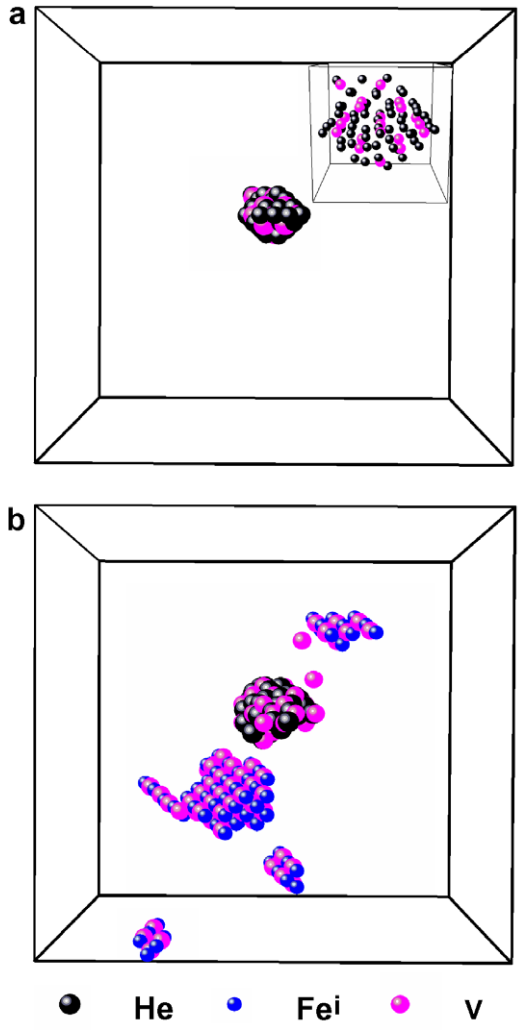

Fig. 1. Atomic structures of a cluster with a He/V ratio of 3: (a) the initial configuration, (b) the final damage state after a 5 keV cascade collision, where the largest and smallest spheres indicate He atoms and Fe interstitials, respectively, and the medium spheres represent vacancies. The inset on the left corner of (a) shows more clear arrangement of He atoms and vacancies in the initial He–V cluster.

Figs. 1 and 2 clearly demonstrated that the effect of a cascade of a given PKA energy on a He–V cluster depends on the He/V ratio. Fig. 3 shows the number of vacancies in clusters as a function of PKA energy for different He/V ratios after one cascade impacting on the He–V clusters with the initial vacancy number of 20. It can be clearly seen that the change in the number of vacancies in the He–V clusters strongly depends on the initial He/V ratio and the PKA energy. When the He/V ratio is larger than 1, the size of He–V clusters increases after the displacement cascade, but it decreases when the ratio is less than 1. The clusters with the He/V ratio of 1 are relatively stable, which is independent of the PKA energy. In addition, it can be seen from Fig. 3 that for the same PKA energy, the size of voids decreases more significantly than that of

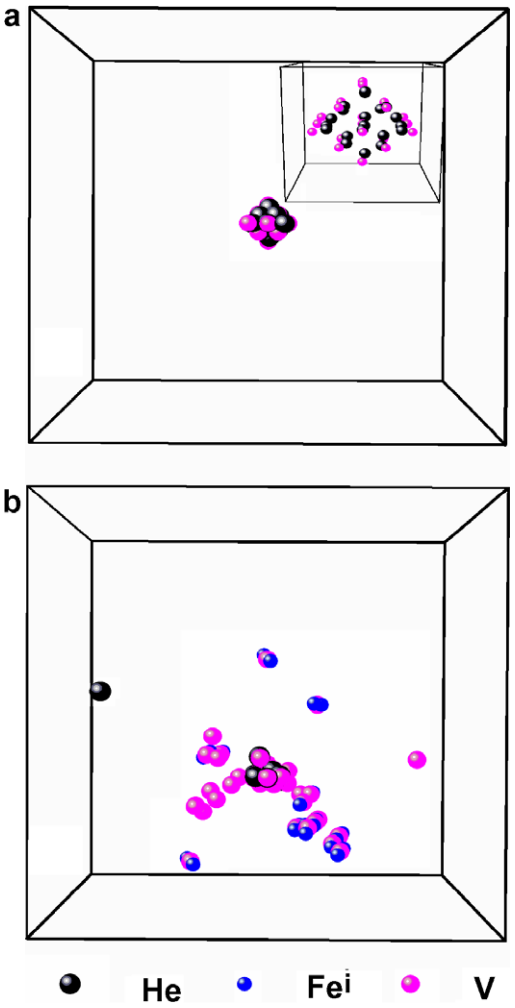

Fig. 2. Atomic plots showing (a) the initial He–V clusters with a He/V ratio of 1 and (b) the final damage state by a 5 keV cascade, where atoms representations are same as those in Fig. 1.

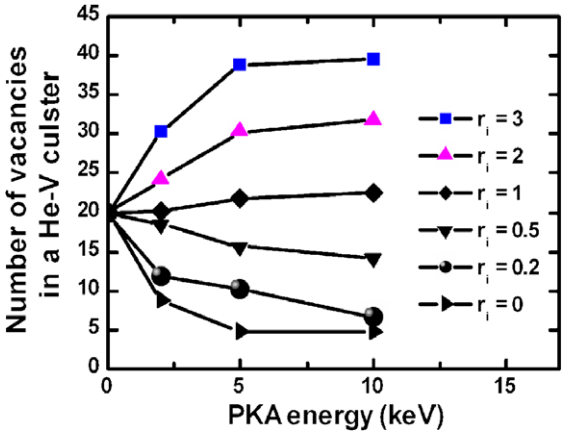

Fig. 3. The number of vacancies in the clusters as a function of the PKA energy for different He/V ratios after a single cascade event.

the He–V clusters, which suggests that the extra He atoms in voids may be important to enhance the stability of voids.

In order to investigate the size effect of He–V clusters on their stability, the interactions of displacement cascades

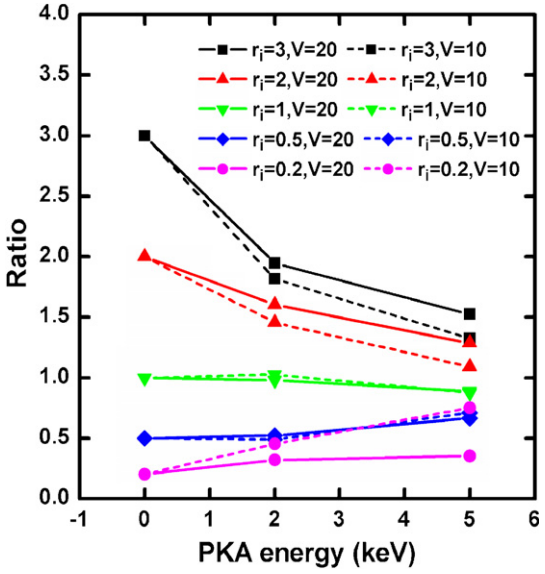

Fig. 4. The ratios of different size He–V clusters as a function of PKA energy after a single cascade event, where solid and broken lines represent the ratios of the initial clusters with 20 and 10 vacancies, respectively.

with the He–V clusters containing 10 and 20 vacancies were comparatively simulated for the PKA energies of 2 and 5 keV. Fig. 4 shows the He/V ratio for the different sizes of the clusters as a function of PKA energy after a single cascade event. For the clusters with the initial He/V ratio larger than 1, a single displacement cascade decreases the He/V ratio from its initial value for the clusters containing 20 or 10 vacancies, but the decrease for the clusters with 10 vacancies is greater than that for the clusters with 20 vacancies. In contrast, for the clusters with the initial He/V ratio less than 1, interaction with a displacement cascade leads to an increase in the He/V ratio, and the increase for the clusters with 10 vacancies is larger than that with 20 vacancies. These results may indicate that large clusters are more stable than small clusters for the same He/V ratio. Furthermore, the clusters containing both 10 and 20 vacancies, with the initial He/V ratio of 1, are very stable, and the effects of single displacement cascades on the size and ratio of these clusters are negligible.

All these behaviors are mainly associated with the initial He/V ratios and the internal pressures in clusters. To demonstrate these effects, Fig. 5 shows the internal pressure for the different sizes of the clusters as a function of PKA energy after a single cascade event. After a cascade event, the MD block was quenched to 0 K, and then, the stress components of each He atoms in the cluster were determined. The total stress components of the He–V cluster were summarized over all the He atoms in the cluster, and the pressure was evaluated using the formula of $P = [\text{stress}(1,1) + \text{stress}(2,2) + \text{stress}(3,3)]/(3.0 * V)]$, where V is the volume of the He–V cluster. It can be seen that the initial pressure in the clusters with 20 vacancies is generally higher than that with 10 vacancies, particularly for large He/V ratios. During the cascade process, it is

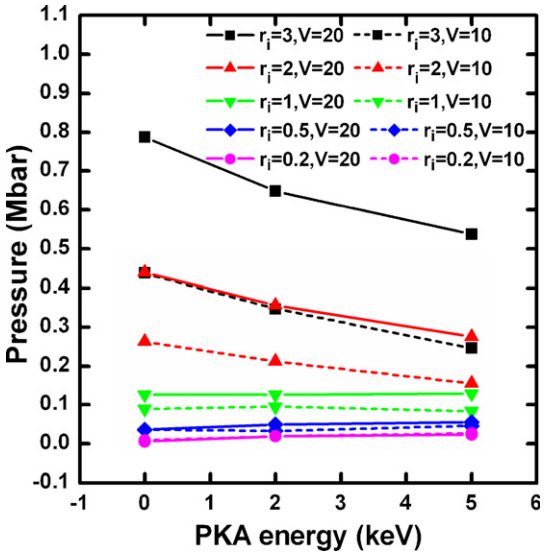

Fig. 5. The pressure of different size He–V clusters as a function of PKA energy after single cascade event, where solid and broken lines represent the ratios of the initial clusters with 20 and 10 vacancies, respectively.

observed that high He gas pressure in the clusters resists displacement cascade-induced convective flow into the cluster, and the clusters with higher pressure are, therefore, more stable. However, for the clusters with the initial He/V ratio of 0.2, the internal pressures in the clusters with both 10 and 20 vacancies are comparatively small. The effects of displacement cascades on these clusters are essentially the same, and no significantly different behavior is observed. These results suggest that for the cluster with the initial He/V ratio of 0.2, the 2 He atoms remain in the cluster after 2 or 5 keV cascade impacting, but the number of the vacancies in the cluster decreases significantly, leading to an increase in the He/V ratio (Fig. 4). However, the internal pressures of two clusters with different size remain almost the same before and after the cascade collision, and thus, the two clusters appear to behave similarly under single cascade condition.

3.2. Stability of He–V clusters under cascade overlap

Under irradiation conditions, particularly in fission and fusion reactor environments, He–V clusters would be continuously bombarded by displacement cascades. It is important to investigate the interaction of multi-displacement cascades with He–V clusters, and to see if these clusters are stable or dissociate into small clusters under cascade overlap conditions. As described above, the stability of He–V clusters with the initial He/V ratios of 3, 1 and 0.5 are considered to interact with multiple 5 keV cascade events. Fig. 6 shows the change of atomic configurations of a He–V cluster with the initial He/V ratio of 3 due to cascade overlap. The multiple PKA positions were repeatedly initiated at random locations for cascade events, but at a same radius and directed towards the He–V cluster such that the thermal spike had the maximum effects on these

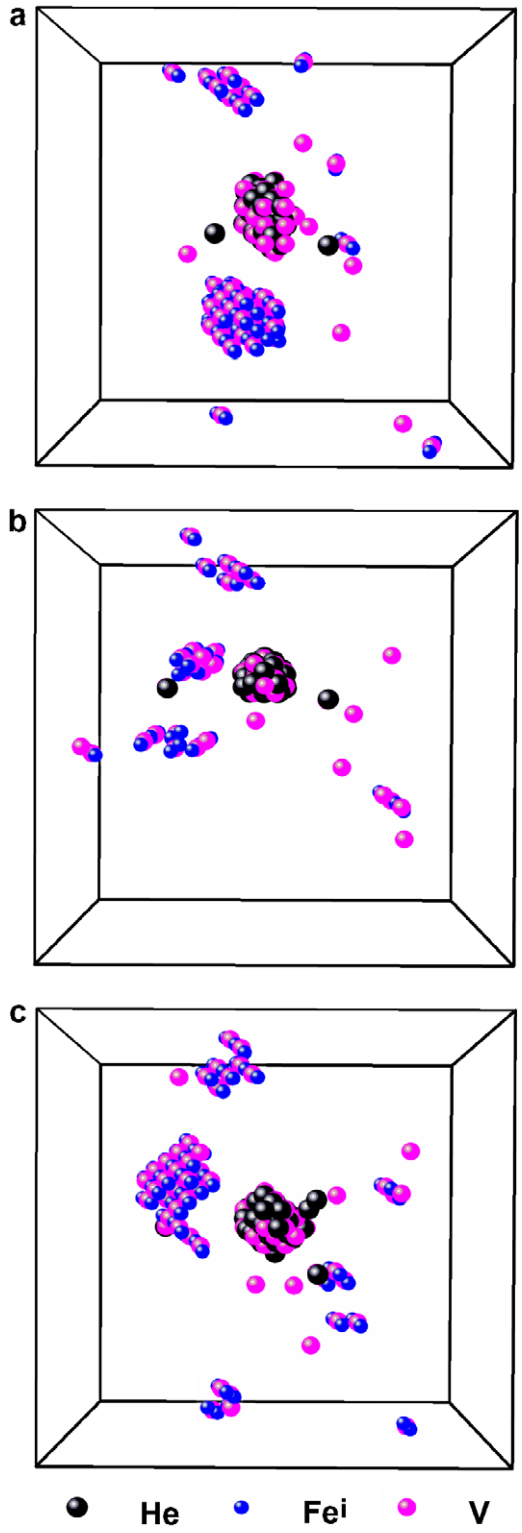

Fig. 6. The change of atomic configurations of a He–V cluster with the initial He/V ratio of 3 due to 5 keV cascade overlap: (a) after the third cascade event, (b) after the fourth cascade event, (c) after the sixth cascade event, where atoms representations are same as those in Fig. 1.

clusters. After the first displacement cascade, the total number of vacancies in the He–V cluster is 41, which decreases the He/V ratio to 1.46. The He atoms in the cluster are not dissolved from the He–V cluster, shown as in

Fig. 1(b). After the second cascade, the number of vacancies in the He–V cluster grows to 45, which brings the He/V ratio down to 1.31, and one He atom escaped from the cluster, forming a substitutional atom. The number of Fe atoms in the largest interstitial cluster increases up to 24, which is consistent with the results of cascade overlap in α-Fe [24]. In general, two cascade overlap increases the probability of forming clusters in comparison with the value of well-separated cascades. This effect arises mainly because pre-existing clusters at the edge of the second cascade act as sinks for newly-formed interstitials. The final damage state after the third cascade overlap is shown in Fig. 6(a). Although more vacancies are produced during the third cascade overlap, the number of vacancies in the He–V cluster remains to be 45. However, the number of interstitial atoms in the largest interstitial cluster reduces to 19, and this may be due to the direct impact of cascade on the interstitial cluster, leading to its dissociation. It is observed that these dissociated interstitials consist of single interstitial or interstitial clusters, and they are very mobile during thermal spike phase. These mobile interstitials and small clusters can easily recombine with vacancies, which decreases the number of surviving Fe interstitials and vacancies. Fig. 6(b) shows the final damage state after the fourth cascade event, where the largest SIA cluster is completely dissolved due to the very high temperature (the maximum temperature being about 4000 K at the core of cascade, which is averaged in the shell of mean radius of a_0 from the center of the cascade and thickness $a_0/4$, where a_0 is the lattice parameter. This is an effective temperature) in the thermal spike phase. Some dissolved Fe atoms recombine with vacancies, and others return to vacant lattice sites close to the edge of the He–V clusters, resulting in the decrease in the size of the He–V cluster. After the sixth cascade event, the number of vacancies in the He–V clusters increases again, and single interstitials and some large SIAs clusters are formed at the periphery of the cascade, as shown in Fig. 6(c). During the six cascade overlap, the number of vacancies in the He–V clusters increases up to 43, but the configuration of the He–V cluster change significantly. A few He atoms at the periphery of the cluster are temporarily knocked off by cascade collision, but most of the resolved He atoms soon return to their mother clusters during the thermal spike phase.

For the initial He/V ratio of 1, the He–V cluster under cascade overlap is more stable than the cluster with the He/V ratio of 3. Fig. 7 demonstrates the changes of the atomic configurations of a He–V cluster with the He/V ratio of 1 due to cascade overlap. After the first cascade event, shown as in Fig. 2(b), the number of vacancies in the He–V clusters remains the same, but two He atoms are dissolved from the cluster, forming a substitutional and an interstitial atom, respectively. After subsequent two cascade events, not shown, the number of vacancies in the He–V cluster increases slightly, but the significant change in the cluster size appears in the fourth cascade event, Fig. 7(a), with an increase in the number of vacancies up to 30. In addition, three He atoms are dissolved from their mother cluster, which leads to the He/V ratio to be 0.57. As noted above, the higher the He/V ratio is, the more stable the cluster is. It is expected that the surviv-

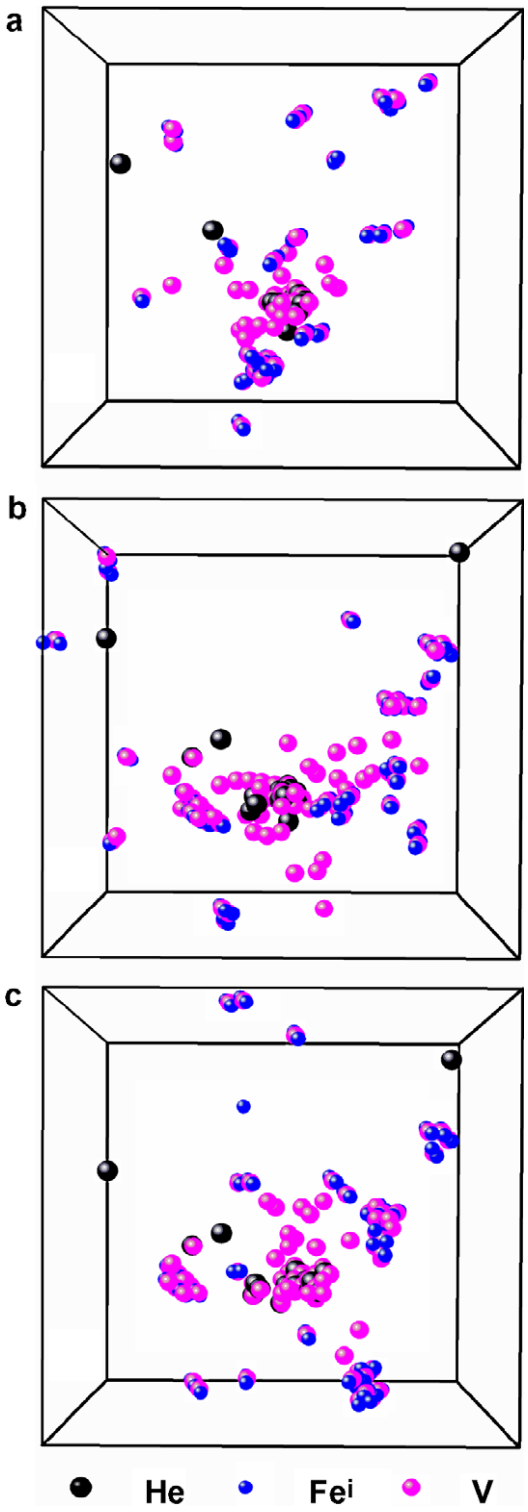

Fig. 7. The change of atomic configurations of a He–V cluster with the initial He/V ratio of 1 due to 5 keV cascade overlap: (a) after the fourth cascade event, (b) after the fifth cascade event, (c) after the sixth cascade event, where atoms representations are same as those in Fig. 1.

ing probability of this cluster should be much smaller than the initial structure. In fact, more He atoms are dissolved from the mother cluster during subsequent cascade overlap, and the cluster is dissociated into two small clusters in the center of the cascade. The single He interstitials are very mobile, with relatively low migration energy of 0.078 eV [10], and they can diffuse far away from their mother cluster, as shown in Fig. 7(b). After the sixth event, Fig. 7(c), the number of vacancies in the large He–V cluster increases, but it decreases in the small cluster, which brings their He/V ratios to be about 1.

From Figs. 6 and 7, it has been clearly demonstrated that the effect of multiple cascade events on a He–V cluster depends on the He/V ratio. The high He/V ratio of the He–V clusters leads to an increase in the number of vacancies in the clusters, whereas the lower ratio exhibits higher possibilities for the clusters to be dissolved. Fig. 8 shows the number of vacancies in the He–V clusters with the He/V ratios of 3, 1 and 0.5 versus the number of cascade events simulated. After the first three cascade events, the number of vacancies in the He–V clusters, with the He/V ratio of 3, increases significantly, but remains almost constant during subsequent cascade overlap. For the He/V ratio of 1, the He–V cluster is relatively stable after the first three cascades overlap, but the number of vacancies increases significantly after the fourth cascade event, and the He/V ratio decreases. Therefore, the cluster becomes unstable, and is partially dissolved by the subsequent cascade overlap. For the He/V ratio of 0.5, the number of vacancies in the cluster decreases after the first three events, and this leads to an increase in the He/V ratio, as expected. It can be seen from Fig. 8 that the number of vacancies in the He–V clusters strongly depends on the He/V ratios.

When the He/V ratio of the cluster is 3, its initial pressure is relatively large, about 0.787 mbar. Furthermore, the simulation cell is initially equilibrated at 100 K and the temperature spike within the first picosecond of the displacement cascade significantly increases the pressure within the He–V cluster, by perhaps a factor of 0.5. Consequently, He atoms can be piled out from the cluster by the large pressure, and these He atoms may attract the neighboring vacancies produced in cascades (the average number of vacancies produced at 5 keV cascades is about 21 in α-Fe), resulting in the growth of the He–V cluster and the decrease in its internal pressure. This process provides a pathway to obtain new balance between the internal and external pressures of the cluster. After several cascade events, the number of vacancies in the He–V cluster increases to a saturated value, and remains for the rest of cascade overlap events. For the cluster with the initial ratio of 1, the He atoms are almost located on substitutional sites, and this configuration represents the most stable atomic arrangements of the He–V cluster. After the interaction of the first displacement cascade with the He–V cluster, the number of vacancies in the core of the cascade increases slightly, as seen in Fig. 8, and some vacancies produced by the cascade are swept into the He–V cluster, which increases the number of vacancies and decreases the internal pressure in the He–V cluster. During the next cascade event, the internal pressure in the cluster is too small to resist displacement cascade-induced convective flow into the cluster, which leads to the He–V cluster partially dissolved in the collisional phase, and a small He–V cluster re-nucleated near its mother cluster in the thermal spike phase. Thus, the number of vacancies in the mother He–V cluster decreases, but the internal pressure increases. During the subsequent events, the cluster continues to grow by capturing more vacancies, releasing the internal pressure of the He–V cluster.

All the simulations have shown that the stability of He–V clusters does not depend much on cluster size, but rather on the He/V ratio in α-Fe. Fig. 9 shows the He/V ratio of clusters versus the number of simulation events. During the first cascade event, the ratio decreases rapidly for the initial He/V ratio of 3, but remains almost constant of about 1.5 for the subsequent cascade events. However, for the cluster with initial He/V ratio of 1, the ratio decreases continuously during the first several events of displacement cascades, in

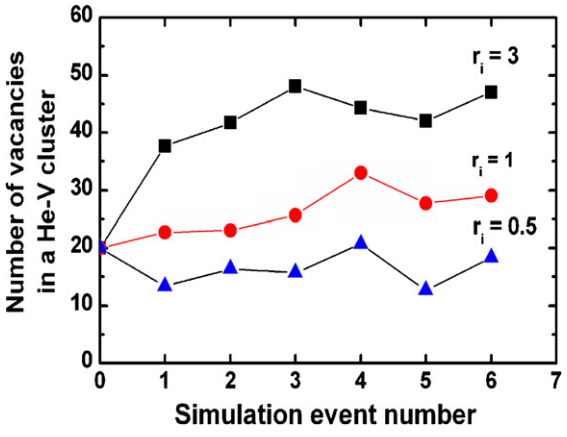

Fig. 8. The number of vacancies in He–V clusters versus the number of cascade events simulated during isotropic 5 keV displacement cascades.

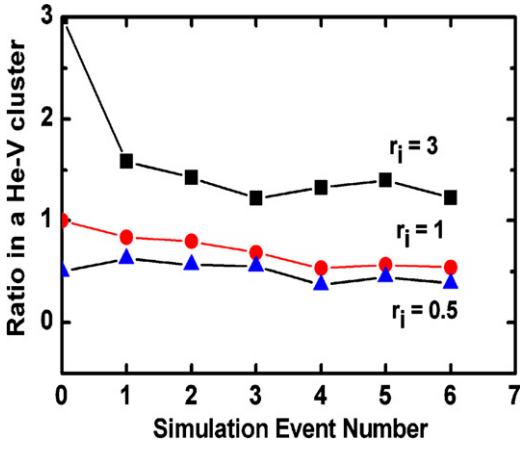

Fig. 9. The He/V ratio of clusters versus the number of cascade events simulated during isotropic 5 keV displacement cascades.

contrast to that of the cluster with the initial He/V ratio of 0.5, where the ratio shows an increase after the first three events of cascades, but remains almost the same for the subsequent cascade interactions. As described above, the He–V clusters with the He/V ratios of 1 and 0.5 can be partially dissolved due to the direct impacting of displacement cascades because of the small internal pressure within the clusters. This leads to the emission of He atoms from the clusters, and thus, decreases the ratio. After four cascade events, the He/V ratio is about 0.5.

4. Conclusions

The effects of displacement cascade and cascade overlap on He–V clusters are investigated by MD simulations. It has been found that the growth or dissociation of He–V clusters strongly depends on the He/V ratio and the recoil energy under mono-energetic cascade events. For the initial He/V ratio larger than 1, the size of He–V clusters increases and the He/V ratio decreases with increasing the PKA energy, but the size of He–V clusters with the initial He/V ratio less than 1 decreases after the displacement cascade, and the He/V ratio increases. We also found that large He–Vacancy clusters are more stable than small clusters for the same helium-to-vacancy ratios under mono-irradiation condition. During isotropic 5 keV cascade overlaps ('isotropic cascade' means that cascade events are initiated in a random location at the same radius from the cluster, but with the same high index direction), the size of He–V clusters with the He/V ratio of 3 is found to change significantly after the first three cascade events, and the number of vacancies in He–V clusters increases, leading to a rapid decrease in their ratio. However, during subsequent cascade bombardments, only a few He atoms close to their boundary are affected by cascade impacts, and most of the resolved He atoms return to their mother clusters. For the He/V ratio of 1, during the first three events, the He–V clusters are almost stable with a small increase in the number of vacancies. During subsequent cascade events, the number of vacancies in clusters increases significantly, and the clusters are partially dissolved to form a few small He–V clusters, while the ratio remains almost constant during cascade overlap for the clusters with the initial He/V ratio of 0.5. It has been found that the number of vacancies produced by the cascade, the initial He/V ratio, the PKA energy and the phenomena occurring in the thermal spike phase all play significant roles in the observed phenomena.

Acknowledgements

Some of authors (F. Gao, R. Kurtz and H. Heinisch) are grateful to the support by the US Department of Fusion Energy Science under Contract DE-AC06-76RLO 1830. Other authors (L. Yang, X.T. Zu and Z.G. Wang) are grateful for the Program for Innovative Research Team in UESTC and the Program for New Century Excellent Talents in University (NCET-04-0899).

References

[1] Steven J. Zinkle, Phys. Plasmas 12 (2005) 058101.
[2] A. Van Veen, R.J.M. Konings, A.V. Fedorov, J. Nucl. Mater. 320 (2003) 77.
[3] E.H. Lee, J.D. Hunn, T.S. Byun, L.K. Mansur, J. Nucl. Mater. 280 (2000) 18.
[4] R. Vassen, H. Trinkaus, P. Jung, Phys. Rev. B 44 (1991) 4206.
[5] J.D. Hunn, E.H. Lee, T.S. Byun, L.K. Mansur, J. Nucl. Mater. 282 (2000) 131.
[6] J. Henry, M.H. Mathon, P. Jung, J. Nucl. Mater. 318 (2003) 249.
[7] F. Gao, D.J. Bacon, P.E.J. Flewitt, T.A. Lewis, J. Nucl. Mater. 249 (1997) 77.
[8] Yu.N. Osetsky, D.J. Bacon, B.N. Singh, J. Nucl. Mater. 307–311 (2002) 866.
[9] D.J. Bacon, Yu.N. Osetsky, Mater. Sci. Eng. A 365 (2004) 46.
[10] K. Morishita, R. Sugano, B.D. Wirth, T. Diaz de la Rubia, Nucl. Instrum. and Meth. B 202 (2003) 76.
[11] B.D. Wirth, E.M. Bringa, Phys. Scr. T 108 (2004) 80.
[12] R.J. Kurtz, H.L. Heinisch, J. Nucl. Mater. 329–333 (2004) 1199.
[13] M.I. Baskes, MRS Bull. (1986) 14.
[14] M.I. Baskes, V. Vitek, Metall. Trans. A 16 (1985) 1625.
[15] L. Yang, X.T. Zu, H.Y. Xiao, F. Gao, H.L. Heinisch, R.J. Kurtz, K.Z. Liu, Appl. Phys. Lett. 88 (2006) 091915.
[16] P. Dauben, R.P. Wahi, H. Wollenberger, J. Nucl. Mater. 141–143 (1986) 723.
[17] H. Trinkaus, J. Nucl. Mater. 318 (2003) 234.
[18] L. Yang, X.T. Zu, H.Y. Xiao, F. Gao, H.L. Heinisch, R.J. Kurtz, Z.G. Wang, K.Z. Liu, Nucl. Instrum. and Meth. B 255 (2007) 63.
[19] G.J. Ackland, D.J. Bacon, A.F. Calder, T. Harry, Philos. Mag. A 75 (1997) 713.
[20] W.D. Wilson, R.D. Johnson, in: P.C. Gehlen, J.R. BeelerJr., R.I. Jaffee (Eds.), Interatomic Potentials and Simulation of Lattice Defects, Plenum, 1972, p. 375.
[21] D.E. Beck, Mol. Phys. 14 (1968) 311.
[22] T. Seletskaia, Yu.N. Osetskiy, R.E. Stoller, G.M. Stocks, J. Nucl. Mater. 367–370 (2007) 355.
[23] L. Yang, X.T. Zu, Z.G. Wang, F. Gao, H.L. Heinisch, R.J. Kurtz, J. Appl. Phys. submitted for publication.
[24] F. Gao, D.J. Bacon, A.F. Calder, P.E.J. Flewitt, T.A. Lewis, J. Nucl. Mater. 230 (1996) 47.