THE FORMATION AND STABILITY OF HE-VACANCY CLUSTERS WITHIN DISPLACEMENT CASCADES IN α-Fe—F. Gao, H. L. Heinisch, and R. J. Kurtz (Pacific Northwest National Laboratory)*

This extended abstract highlights results in a series of published papers [1-5] on recent work partially funded by the Office of Fusion Energy Science.

EXTENDED ABSTRACT

Molecular dynamics (MD) methods have been utilized to study the formation of vacancy clusters created by displacement cascades in α-Fe containing concentrations of substitutional He atoms varying from 1-5%. These He concentrations are not necessarily intended to represent specific conditions within a fusion reactor (average end-of-life He concentrations in the first wall are expected to be on the order of 0.15%), but they provide an opportunity to investigate the effects of substantial amounts of He on cascade processes and microstructure development under damage producing conditions.

Results of cascade simulations show that

- There are distinct differences in the number and size of vacancy clusters within displacement cascades in α-Fe with and without substitutional He atoms.
- Many large vacancy clusters are formed within cascade cores in α-Fe containing helium atoms, in contrast to a few small vacancy clusters observed in pure α-Fe.
- The number of Frenkel pairs at 600K is slightly lower than that at 100K, but the number of He–vacancy clusters increases with increasing temperature for the same He concentration and energy recoils.

The stability of He-vacancy clusters during single cascade and multiple cascade overlap has also been investigated for helium-to-vacancy ratios ranging from 0.2 to 3. Results indicate that

- The effect of displacement cascades on a helium-vacancy cluster strongly depends on the helium-to-vacancy ratio and PKA energy.
- He-vacancy clusters (He-V) can be dissolved when the He/V ratio is less than 1, but for He/V ratios equal to and larger than 1, the He-V clusters are very stable for the energies considered.

Most of the details pertaining to the methodology used in the simulations of the cascade induced He-vacancy (He-V) cluster formation and their stability within single or multiple cascades are described in detail in references [1-3]. For the present studies, the Finnis–Sinclair [6], Wilson–Johnson [7], and Beck [8] potentials were used to describe the interactions of Fe–Fe, Fe–He and He–He, respectively. All simulations were carried out using MD methods with periodic boundary conditions and constant volume. To study formation of He-V clusters, several He concentrations have been considered, ranging from 1 at% to 5 at%, where Fe atoms in the test cells are randomly replaced by He atoms. For each concentration, primary knock-on atom (PKA) energies, *Ep*, ranged from 500 eV to 20 keV at temperatures of 100 and 600 K. A total of 200 cascades were simulated for each condition. In order to study He-V cluster stability within displacement cascades, initial clusters with 10 and 20 vacancies were chosen, having He/V ratios varying from 0.2 to 3. Individual cascades from single primary knock-on atoms (PKA) with recoil energies of 2, 5, and 10 keV were initiated.

To investigate the influence of He atoms on defect production, displacement cascades were also generated in α-Fe without helium, and these simulations are in general agreement with the previous studies, where large vacancy clusters are not observed, and most of the vacancies are single vacancies. Figure 1 shows the defects remaining in 10 keV cascades with 5 at% He concentration at a temperature of 100 K. It is somewhat surprising to see that a large number of vacancies are formed within the cascade

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core, together with He interstitials removed from their substitutional positions. These helium atoms are retrapped by vacancies, forming He-vacancy (He_nV_m ,$n<m$) clusters. The total defect density within the cascade core in this case is much higher than that for cascades in pure a-Fe, and the clustering of He is significant. Another interesting result in the He-doped Fe is that only a few self-interstitial atoms (SIAs) are generated, which is much less than that in pure α-Fe, as shown in Fig. 1. Also, the size and number of interstitial clusters are found to be much smaller than those in pure α-Fe. Moreover, the fraction of surviving SIAs that are in clusters of size two or larger decreases with increasing He concentration [1,4].

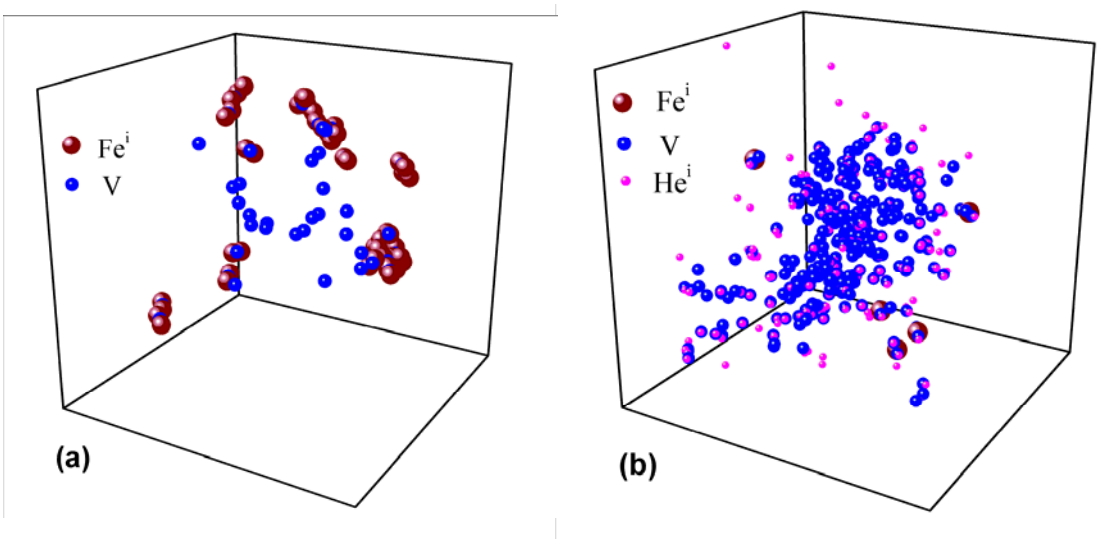

Fig. 1. Typical point defect distributions within 10 keV displacement cascade simulations at 100 K after 20 ps in (a) pure α-Fe and (b) α-Fe with 5 at% substitutional He, where the defect type is identified by the different size of spheres, as indicated in the plots.

The probability of He/vacancy clustering and the size of the largest clusters tend to increase with increasing He concentration and PKA energy. Also, a higher proportion of vacancies than SIAs form clusters, in contrast to those found in pure α-Fe. Data for the final numbers and size distributions of helium-vacancy (He_nV_m) clusters for all the cascades in Fe with 1 at% He and 5 at% He, respectively, are plotted in the form of histograms as a function of PKA energy in Fig. 2. The figure demonstrates quantitatively that the number and size of clusters both increase with increasing He concentration. Furthermore, a striking result of the present series of damage cascade simulations is that the majority of He_nV_m clusters contain more vacancies than helium interstitials, with helium-to-vacancy (He/V) ratios in the range from 0.5 to 0.8.

The temperature dependence of He–V clusters within displacement cascades, as discussed in Ref. [5], demonstrates that the total number of Frenkel pairs (counting both He and Fe point defects) increases with increasing PKA energy and He concentration, but decreases slightly with increasing irradiation temperature for the same He concentration and PKA energy. The number density of He–V clusters slightly increases with increasing temperature, while the mean size of He–V clusters remains almost constant for the same He concentration and PKA energy. Such clusters might act as the smallest nucleation sites for the formation of large He bubbles observed experimentally.

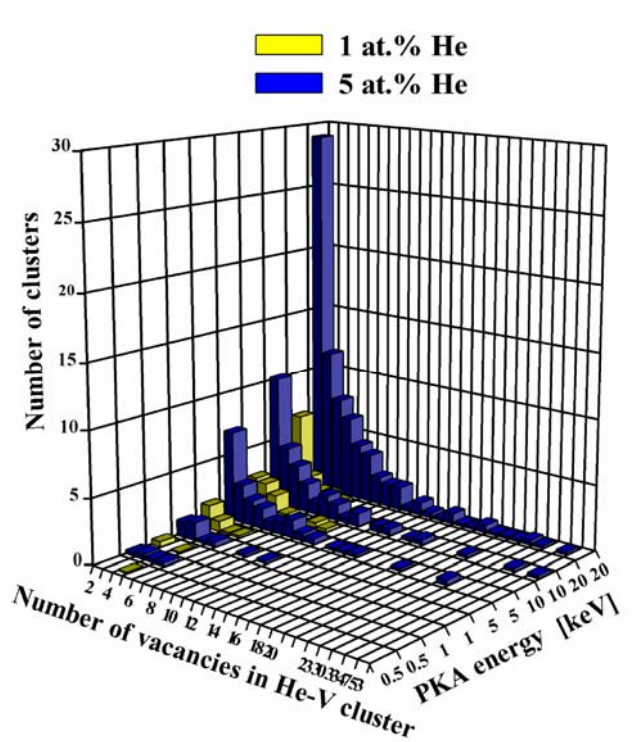

Fig. 2. Size distribution of He_nV_m *(n<m)* clusters with concentrations of 1 at% and 5 at% substitutional He at 100 K. Note that the horizontal axis for number of vacancies is nonlinear.

The stability of pre-existing He-V clusters within cascades was studied for clusters of different He/V ratio, and the results were analyzed using graphical depictions of the cascade damage. Figure 3(a) shows the peak displacements of the cascade, from which it can be seen that the thermal spike phase completely involves the He/V cluster. The final damage state is shown in Fig. 3(b), and it is surprising to note that 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 the original cluster, which decreases the He/V ratio to 1.44. However, the simulations with the He/V ratio less than 1 demonstrate that the initial cluster has been partially dissolved after cascade impacting and two small clusters are re-nucleated in the center of the cascade. Besides two small He-V clusters, there were some single vacancies and small vacancy clusters formed in the cascade core. In contrast, the He-V clusters with initial He/V ratios of about 1.0 are very stable even when impacted by a high energy cascade. It is clear from these simulations that the effect of a cascade of a given PKA energy on a He-V cluster depends on the He/V ratio. A high He/V ratio leads to the increase in the number of vacancies in the clusters, whereas the lower ratio may provide a possibility for the cluster to be dissolved.

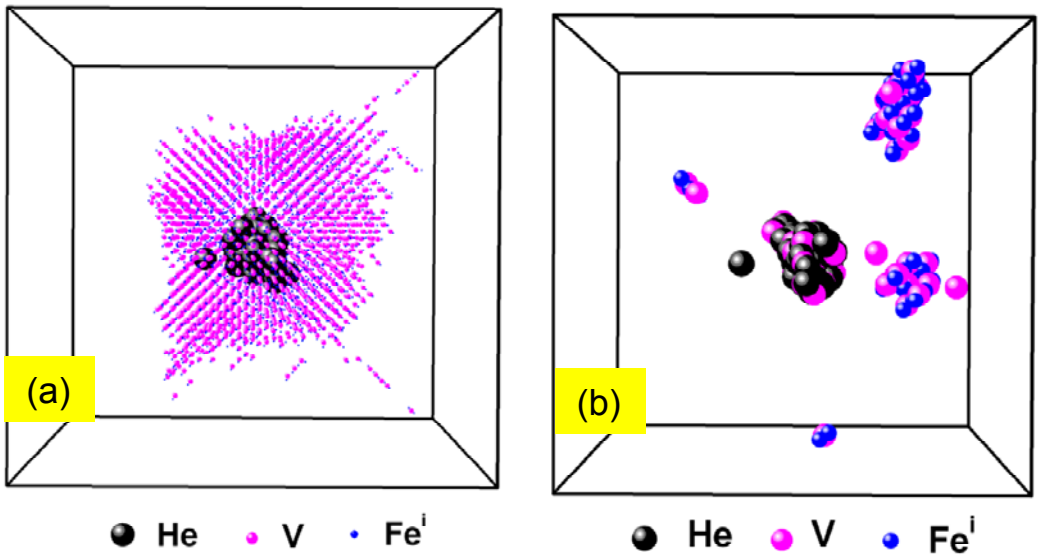

Fig. 3. Atomic structures of a cluster with a He/V ratio of 3: (a) the peak displacements of the cascade with PKA energy of 5 keV and (b) the final damage state.

Conclusions

Formation of He-V clusters within cascades and the stability of these clusters under cascade-producing irradiation, as well as temperature effects, have been studied using molecular dynamics methods. The number and size of vacancy clusters within displacement cascades are distinctly different in the cases with and without substitutional helium atoms examined in these simulations. Large numbers of helium/vacancy clusters are generated directly in displacement cascades, and the sizes of these clusters are much larger than those observed for clusters in pure α-Fe. The effect of temperature on the total number of Frenkel pairs produced is small, but the number density of He–V clusters increases with increasing temperature. The displacement cascades have significant effects on the stability of He-V clusters. The growth or dissociation of He-V clusters strongly depends on the He-V ratio and recoil energy. For an initial He/V ratio larger than 1, the cascades dramatically change the vacancy concentration in the clusters, resulting in an increase in the He-V cluster size and a decrease in the He/V ratio. The He-V clusters with initial He/V ratios less than 1 can be completely or partially dissolved by a cascade, and one or a few small He/V clusters can be renucleated. In contrast, the He-V clusters with initial He/V ratios of about 1.0 are very stable even when impacted by a high energy cascade.

References

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