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Modeling of cascade damage interactions by Monte-Carlo method

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Abstract

The effect of interactions of cascade damage on clustering and point-defect behavior in α-iron at 563 K is simulated by the Monte-Carlo (MC) method. Cascade damage near the existing cluster increases recombination of point-defects, but freely migrating defects formation is not strongly modified by the overlapping. Growth and shrinkage of vacancy clusters depends on the distance between cascades. Small interstitial clusters tend to grow by the interaction of nearby cascades. Clustering, recombination and the production of freely migrating defects are quantitatively estimated for two 10 keV cascade interactions.

1. Introduction

Changes in macroscopic properties of irradiated materials with energetic particles are generally resulted from irradiation-induced microstructural changes, such as production of point-defects, formation of clustered defects and microchemical evolution. Mechanical properties and microstructural evolution under irradiation are usually complicated and non-linear functions of irradiation parameters, such as energy, mass, flux, fluence of incident particles and irradiation temperature. A lot of efforts have been made to clarify irradiation performance of materials based on physical mechanisms, and to establish a framework for extrapolative prediction of material behavior in fusion reactors.

Mechanistic modeling of radiation damage processes involves multiple time and spatial scales of phenomena [1–5]. Recent progress in computing power provides detailed information on cascade damage evolution. We have come to know, for example, subcascade formation during the collisional stage, formation of molten-like structure at the center of cascade, significant recombination of interstitials and vacancies during the quenching stage, and the intracascade clustering of both types of defects by the highly localized and segregated production of the interstitials and vacancies [6–10]. All of these phenomena are strongly dependent on the material, temperature and primary knock-on atom (PKA) energy [11]. A certain fraction of point-defects produced in the cascade eventually escapes from the cascade to interact with each other outside the cascade region, and the others annihilate or form clusters near the cascade region [12,13].

Kinetic Monte-Carlo (MC) simulation is a useful method to deal with migration and interaction of defects in the larger spatial and temporal scales than molecular dynamics (MD) simulations. Soneda and Diaz de la Rubia [14] successfully estimated production and annealing kinetics of cascade damage in BCC Fe using a combination of MD and kinetic MC simulations.

In this study, the effect of cascade damage overlapping on defect behavior is discussed by using MC method. Defect clustering, freely migrating defects and recombination by the interaction of new cascade with pre-existing defect clusters are estimated. These interactions are dependent on time interval and distance of the two cascades, which are also determined by the irradiation flux. The short term interactions of subcascades from a single high energy primary knock-on atom before the annealing stage of cascade evolution have

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been studied by molecular dynamics simulations [15,16]. When we are going to evaluate long term behavior of the irradiated materials, formation of defect clusters and freely migrating defects from a single cascade damage may be strongly modified by the formation of nearby cascade, even if the cascade volume is very limited.

2. MC simulation of defect behavior

In the MC simulation, mobile defects can jump to the nearest lattice site with a probability of $P = v \exp(-E_m/k_B T)$, where v is the jump frequency of defects, 10^{13} s^{-1}, and E_m is the migration energy. A conventional 'metropolis method' is applied for a scheme of the kinetics of defect migration, where one of the defects in computational volume is randomly chosen and moved at the nearest neighbour position. Whether the migration is accepted or not depends on a difference in total energies between, before and after the migration:

$$\Delta E = \sum_i E_i \text{ (after)} - \sum_i E_i \text{ (before)}. \quad (1)$$

In order to calculate ΔE, we used the many-body EAM-type potential for α-iron that was derived by Finnis and Sinclair [17].

The spatial distribution of point-defects in the cascade at the beginning of the simulation is assumed to have core of vacancies surrounded by interstitials, which is typical of 10 keV or lower energy cascades without subcascade structure. The high dense region (HDR) of vacancies is a spherical area at the center of the calculation cell, and vacancies are covered by an interstitial region at the periphery of the HDR. The number of initial Frenkel pairs, N_F, at the beginning of the calculation can be associated with the PKA energy E_p, using the following equation as derived by the MD simulation of Bacon et al. [9], showing the number of Frenkel pairs after the quenching stage:

$$N_F = A(E_p)^m. \quad (2)$$

The HDR size is also determined from N_F and the vacant lattice site density in the HDR, which is fixed at 2% as estimated by binary collision and annealing calculations [18].

The migration energies employed here are taken as 0.26 and 0.41 eV for single- and di-interstitials, and 0.52 and 0.47 eV for single- and di-vacancies, respectively, all of which were obtained by experiments [19]. It is assumed that larger clusters which consisted of three or more point-defects grow without releasing any point-defects at this temperature. It has already been recognized that relatively large interstitial clusters have very low-activation energy for one-dimensional motion along the ⟨1 1 1⟩ directions [14]. In the present study, both interstitial and vacancy clusters which contain two or more point-defects are assumed to be immobile for simplicity to investigate interaction of cascades. The temperature is fixed at 563 K. No lattice relaxation is included in the energy calculation.

3. Results and discussion

In the previous paper [20], we found that the defect density is more responsible for vacancy clustering and recombination in the cascade region than the size of cascade, and that the fraction of self-interstitial atoms escaping from a single cascade is larger than that of escaping vacancies at 563 K. Vacancies tend to form clusters at the center of a cascade, which lead to spatial unbalance in the production between the freely migrating vacancies and self-interstitials. It was also found that, for the cascade with larger size of vacancy-rich regions, escaping vacancies strongly decrease, whereas the fraction of recombined point-defects is almost constant.

Fig. 1 shows an example of cascade interaction with existing defect clusters by a former cascade. Here the second cascade up to 10 keV is assumed to have interstitials around a vacancy core. For the typical displacement rate in the blanket structural materials of expected magnetic fusion reactors, cascade overlapping usually happens after the annealing stage of the first cascade damage. To estimate these interactions, there are many kinds of parameters, such as PKA energies, time and distance. MC simulations can provide statistical information for these non-linear phenomena.

Figs. 2 and 3 show the calculated size distributions of interstitial clusters and vacancy clusters by the interactions of two 10 keV cascades at 563 K in BCC Fe. Distributions of defect clusters are found to be dependent on the distance between two cascades [20]. These distributions are obtained from 60 cases of the combinations of two 10 keV cascades whose centers are defined as the distance between the two cascades. The infinity means two independent cascades without any direct interaction. It should be noted that freely migrating defects from any other cascades may change the clustering behavior, however, it can be ignored within the present time range of the interaction of new cascade with the existing clusters by a former cascade.

Interstitial clusters tend to grow larger at any overlapping distance of cascade interaction, and the fraction of smaller clusters decreases. Growth of vacancy clusters are clearly observed by the direct overlapping of vacancy rich region of the second cascade with existing vacancy clusters, as vacancy clusters tend to be produced near the center of cascades. Some of the existing vacancy clusters are annihilated by the interstitial-rich region of the second cascade. Larger vacancy clusters are found to

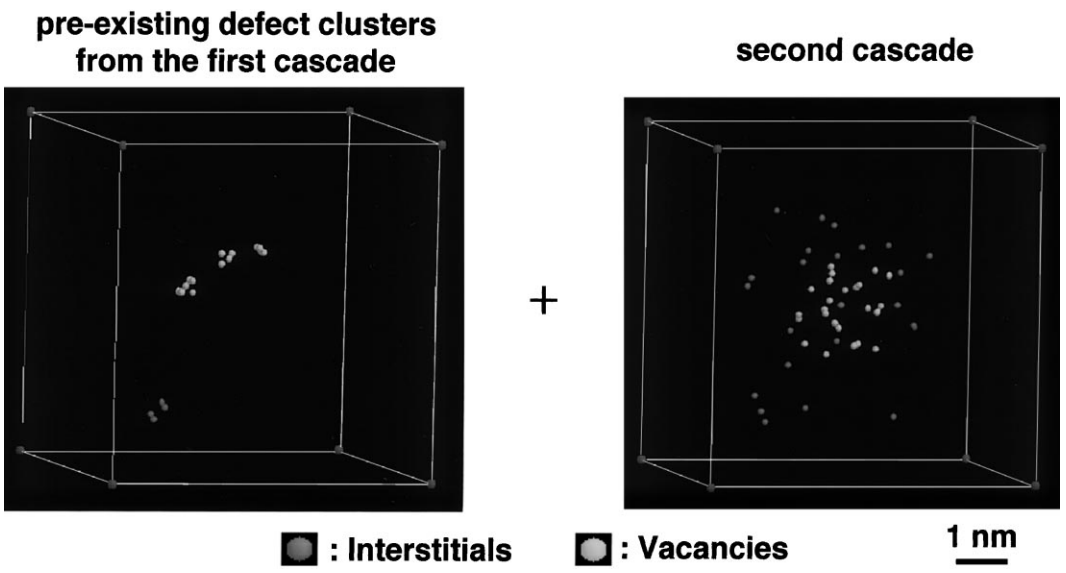

Fig. 1. An example of interaction of existing defect clusters from the first cascade with the second cascade damage.

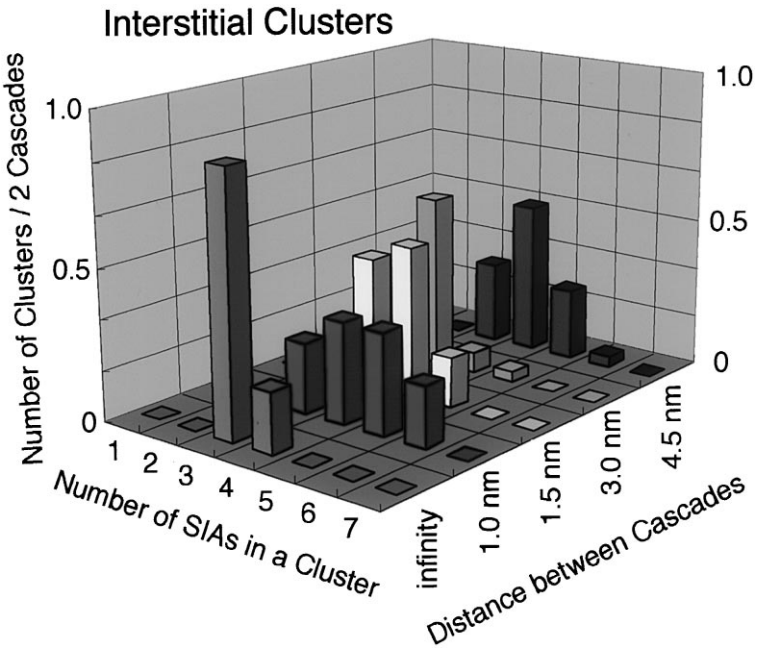

Fig. 2. Size distributions of interstitial clusters in BCC Fe at 563 K produced by two 10 keV cascades as a function of distance between cascades.

shrink efficiently by the second cascade when the distance between the two cascades is larger than 3.0 nm.

Fig. 4 shows the recombination and escaping fractions of defects from the second cascade as a function of distance between the centers of two cascades comparing with those in the single isolated cascade cases. The escaping vacancies and interstitials are defined by the defects migrating out of a volume of $L\times L\times L$ ($L=30a_0$) at this temperature as in the previous paper [20]. It is clearly shown that the pre-existing defect clusters increase the recombination rate of vacancies and interstitials from nearby cascades. It is also found that the

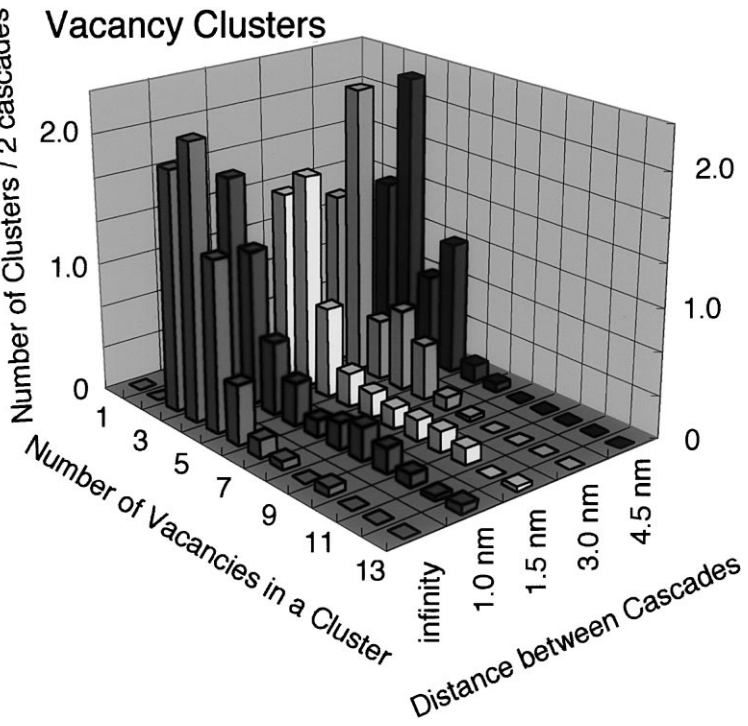

Fig. 3. Size distributions of vacancy clusters in BCC Fe at 563 K produced by two 10 keV cascades as a function of distance between cascades.

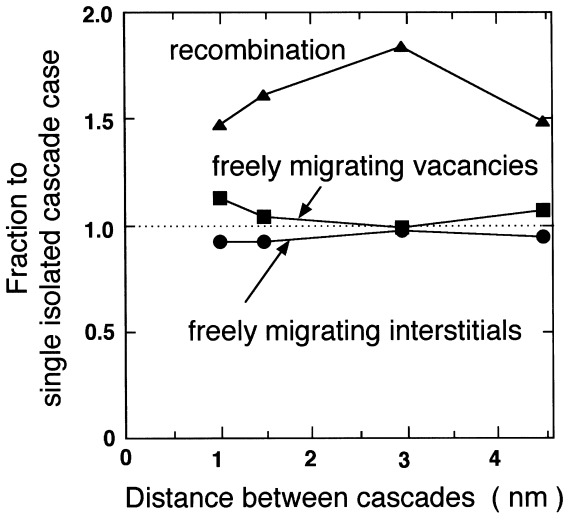

Fig. 4. The effect of 10 keV cascade formation near the existing defect clusters from a 10 keV cascade in BCC Fe at 563 K on the recombination and freely migrating defect formation as a function of distance between two cascades compared with those in the single isolated cascade case.

recombination rate shows the maximum value at 3.0 nm. Even if the second cascade strongly changes size distributions of defect clusters, the fraction of escaping vacancies and interstitials out of the cascade volume are not strongly modified by the overlapping.

Table 1 summarizes fractions of defect clusters, escaping defects, recombination of vacancies and interstitials by the overlapping of two 10 keV cascades comparing those from single isolated cascade cases. Here we calculate 360 different cases of interactions of cascades with pre-existing defect clusters. The separation distance between the center of mass of defect distribution after the quenching stage of both cascades is fixed at 4.5 nm. Average sizes of interstitial and vacancy clusters are also estimated.

These show one of the typical results of cascade interactions with nearby clusters at 563 K. Cascade overlapping increases the recombination of interstitials and vacancies and decreases residual defects in the clusters. Size of vacancy clusters decreases at the separation distance of 4.5 nm, because interstitials at the periphery of the second cascade annihilate the vacancy clusters. However, average size of interstitial clusters slightly increases. It is also found that fraction of escaping vacancies increases at this interaction distance and temperature.

These results come from a limited interaction condition. We should also consider PKA energy spectrum and effects of FMD to estimate detailed evaluation of defect behaviors. But future statistical estimation of many in-

Table 1
The effect of cascade overlap on residual defect clusters, freely migrating defects and recombination of vacancies and interstitials for the case of 4.5 nm separation two 10 keV cascades in BCC Fe at 563 K[a]

		Defect			
		Interstitial		Vacancy	
	Cascade event (s):	Single cascade (%)	Overlap of two cascades (%)	Single cascade (%)	Overlap of two cascades (%)
Residual defects		1.70	1.35	12.9	10.1
FMD		17.7	16.7	6.25	7.23
Recombination		80.7	82.5	80.7	82.5
Average size of clusters (nm)		3.18	3.29	4.24	4.06

[a] Both first and second cascades are initiated from 10 keV PKA. Distance between cascades is fixed at 4.5 nm.

teraction cases including the effect of highly mobile interstitial clusters will give us quantitative information on microstructural evolution in irradiated materials.

4. Conclusion

The effect of interactions of energetic cascades after the cooling phase on defect clustering and formation of FMD in Fe at 563 K is estimated by the MC method. Cascade damage near the existing clusters increases recombination of point-defects, but FMD formation is not strongly modified by the overlapping. Growth and shrinkage of vacancy clusters depends on the distance between cascades. Small interstitial clusters tend to grow by the interaction of nearby cascades at 563 K. Clustering, recombination and the production of FMD are quantitatively for two 10 keV cascade interactions.

Acknowledgements

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