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Kinetic Monte Carlo Simulation for Microstructural Evolution in Fe during Neutron Irradiation

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1. Introduction

The pressure vessels for light water reactors are composed of low alloy ferritic steels, which are known to experience severe embrittlement by neutron irradiation during the operation [1-4]. This phenomenon is explained as a matrix damage accumulation and radiation-induced copper precipitation [1]. However, these irradiation-induced defects are mostly below the resolution of TEM, and other advanced techniques such as 3D atom probe FIB or PAS are needed to confirm the mechanism, while many uncertainties still remain.

For a clear explanation of irradiation embrittlement, computer simulations are applied as a tool for analyzing an atomic scale defect behavior. These simulations are important to provide an insight in materials behavior, and can be applied to imitate high dose experiments which are very difficult to accomplish in practice. The mechanism for the formation of displacement cascades by neutron irradiation is now clearly established and can be described by molecular dynamics (MD). However, because of the short time span and small simulation volume covered by MD, other simulation methods must be used to extend the time and cell size of a simulation. Among the simulation techniques, a kinetic Monte Carlo (KMC) method is a very useful technique to simulate the defect behavior and the microstructure evolution in materials under irradiation [5-6].

In this study, we summarized the model that we used in our KMC simulations. The effect of the temperature on the defects distribution in Fe was provided. The interaction of the point defects with traps is also investigated.

2. Methods and Results

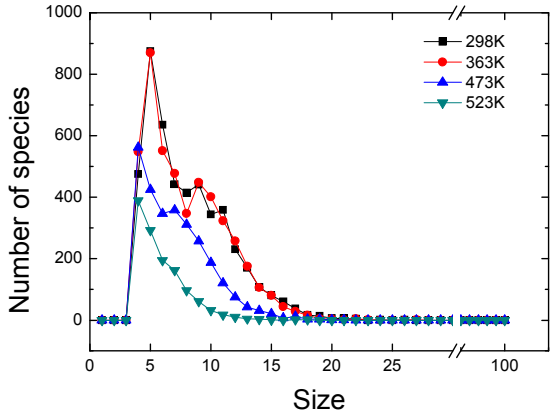
2.1 Kinetic Monte Carlo

Among the variations of KMC, we applied the object KMC simulation to our system. In Object KMC, all defects with different size and species are treated as objects. The objects have a center of mass positions and reaction radii in a simulation cell and migrate according to a lattice distance without any real atomic lattices. The objects can experience several events: jump, recombination, dissociation, trapping etc. The time to accomplish the events elapses according to a residence time algorithm [7].

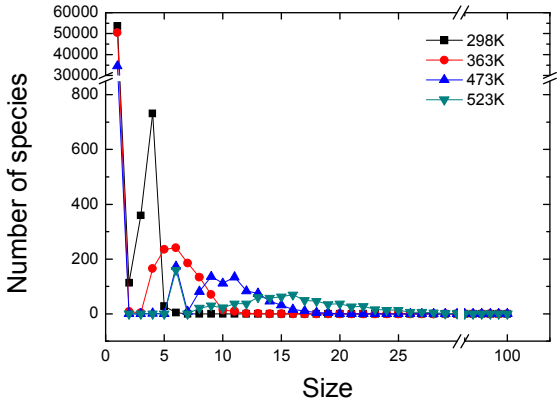
In this study, model parameter was based on the Soneda's work [8], and there are some variations in detail.

2.1 Effect of Temperature

Fig. 1 shows the effect of the irradiation temperature on the size and numbers of defects. The 20 keV cascade data from MD results were introduced in the simulation cell at a rate of 5.6×10^{-5} dpa/s, and total elapsed time was 1 s. The number of self interstitial atom (SIA) clusters decreased with an increasing temperature (Fig. 1(a)). In the case of vacancies, there are very large amounts of small vacancy clusters but larger vacancy clusters are scarce at 298 K. As the temperature increases, small vacancies disappear and the modal size of clusters is increased.



(a) Interstitial Atoms



(b) Vacancies

Fig. 1. Temperature effect on the distribution of Defects.

At a low temperature of 298 K, most of the vacancy clusters are thermally stable, and the SIAs with low diffusion activation energies move quickly. In the cases of a high temperature, vacancy clusters are thermally unstable, and small vacancy clusters are dissociated shortly after their formation. Thus the number of free vacancies is increased, and the growth of the large vacancy clusters is enhanced. Therefore, the growth of SIA clusters is suppressed by recombination with vacancies.

2.2 Effect of Dose

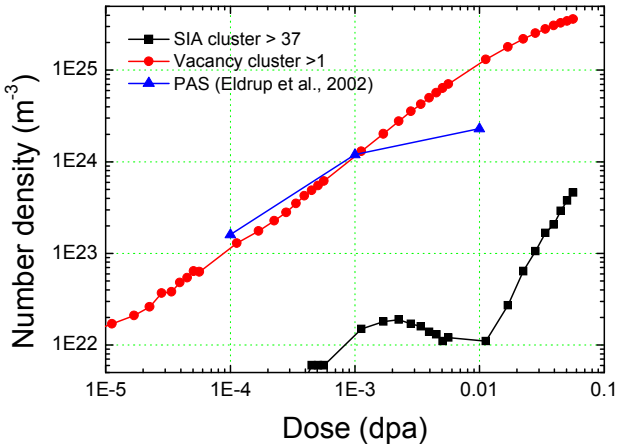


Fig. 2. Number densities of defects with increasing dose.

Fig. 2 shows the number density variation with a dose increase. The temperature of the system was 363K, dose rate was 5.6×10^{-5} dpa/s, and the total simulation time was 1000 s.

Vacancy cluster number density showed a linear relationship with the dose. The absolute value of the vacancy cluster density is similar to the PAS results from Eldrup [9]. In SIA clusters, the diameter of 37 member SIA clusters is ~1.5 nm, which is visible in TEM. The number density of SIA clusters showed a plateau between 10^{-4}~10^{-3} dpa, and increased drastically from 10^{-3} dpa. It is supposed that these SIAs can be observed by TEM only at a higher dose, and this result is similar to the results of other researchers [6].

3. Conclusion

In the present investigation, a kinetic Monte Carlo simulation for an irradiation experiment was provided. The increase in temperature affected the mobility and dissociation rate of the vacancies, and therefore the total defect distributions of the SIAs and vacancies were changed. As the dose increased, the number densities of the vacancy clusters and SIA clusters were increased. However, the SIA showed a stagnant period at a lower dose.

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