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Effect of Irradiation Condition on the Isochronal Annealing of Fe: Kinetic Monte Carlo Simulation Approach

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1. Introduction

Isochronal annealing is a simple and useful method for analyzing the defects kinetics and irradiation effects on materials. Irradiation on a material at a very low temperature results in immobile defects. Annealing through the same time with a constant rate of heating can yield the defect recovery phenomena in various stages and useful information about defects. However, these experiments need a very sophisticated apparatus and careful experimental conditions. As an alternative way to perform the experiments, a multiscale computer simulation is used to analyze the irradiation damage in materials with low a cost [1]. The Kinetic Monte Carlo (KMC) method is part of the multiscale modeling method, and it especially deals with the growth of the defects during irradiation. KMC is able to extend the results of displacement cascade data from molecular dynamics (MD) to a realistic time scale, and it can be used as an alternative tool to analyze an isochronal annealing result [2].

In this study, the isochronal annealing of Fe was investigated using the Kinetic Monte Carlo simulation method. The irradiation condition was varied from random distribution to neutron irradiation. The accumulation behavior of defects was analyzed, and their tendency was also discussed.

2. Methods and Results

2.1 New OKMC code

The newly developed object Kinetic Monte Carlo code was implemented by the C++ computer language. It has many new features to increase the accuracy of the simulation. The new functions can obtain jump rates and dissociation rates of various defects in KMC without a huge memory allocation. Many cascades with various energies can be inserted simultaneously in a simulation. The infinite periodic boundary condition was introduced for the large-scale simulation and reduction of the calculation time. The change in temperature during simulation was also implemented, and this feature was used for the isochronal annealing method in this simulation study.

2.1 Simulation method and condition

All basic data about the mobility and stability of defects were utilized from the result of various researchers [3-6]. In the newly developed KMC code, defects are considered as spherical objects with a center position and a reaction radius. The objects are characterized by their species, mobility, and dissociation rate. The size and concentration distributions of defects produced by various irradiation methods were simulated in this study. Isochronal annealing simulations were carried out with a holding time of 300 s. The temperature intervals were 0.03, and the range was 77 K to 800 K, respectively.

2.3 Comparison with other code

Figure 1 shows the annealing results of one 20 keV cascade from neutron irradiation using another KMC code BIGMAC, and the newly developed KMC code. The simulation temperature was 343 K. The x-axis shows the simulation time, and the y-axis shows the number of vacancies, interstitials, vacancy clusters, and interstitials clusters in the simulation box. All model parameters and running parameters for the annealing simulation were identical between the two codes. For statistical reasons, the simulations were conducted repeatedly over 100 times with various random numbers. The differences in defects numbers between the two codes were very small. Though there were some long-term scatters, it is clear that the newly developed KMC code can replace the BIGMAC code

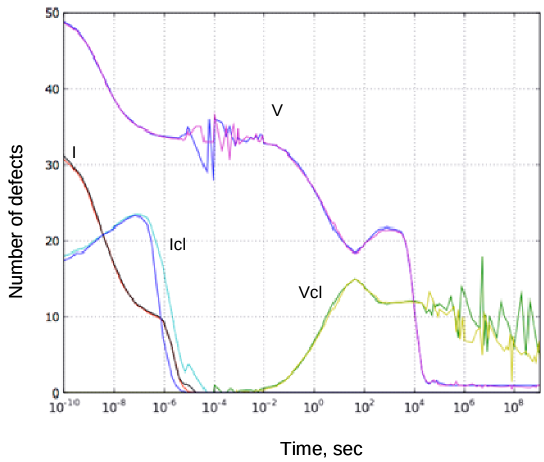

Fig. 1. The annealing simulation of a 20 keV cascade

for simulating cascade annealing.

2.4. Effect of the irradiation method during isochronal annealing

In Fig. 2, we report the evolution of the total number of defects from the 20 keV cascade calculated by KMC simulations as a function of temperature. For comparison, the result of an electron irradiation which caused only Frenkel pairs is reported, too. As expected, the difference between the two initial conditions resulted in very different behavior qualitatively as well as quantitatively. In the electron irradiation condition, the defects recombined at a low temperature because of the high mobility of single vacancies and SIAs. In contrast, in the case of neutron cascade irradiation, the total number of defects slowly decreases with temperature. It is suggested that most point defects are composed of clusters after irradiation. So, only a small amount of point defects can migrate and recombine at a low temperature in 20 keV cascade annealing. Without a doubt, the cascade caused a higher accumulation of defects and additional irradiation degradation.

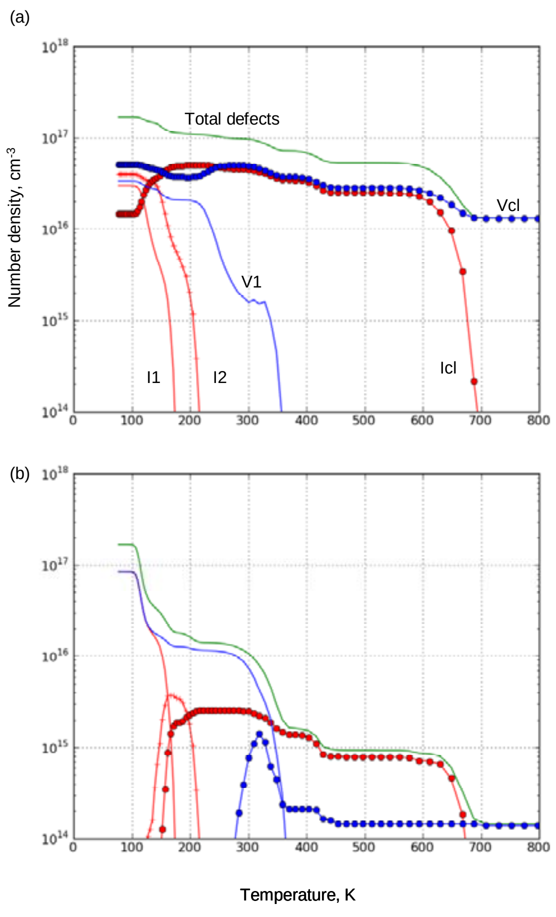

Fig. 2. Effect of the irradiation method on the isochronal annealing method: (a) 20 keV neutron cascade irradiation, (b) electron irradiation.

3. Conclusions

The effect of the irradiation condition on the evolution of defects in the isochronal annealing simulation is elucidated. The electron irradiation on the materials led to an increase in the mobile defects with a single size and resulted in a high recombination rate at the low temperature. In contrast, the neutron cascade led to an increase in the cluster density of the defects. The immobile clusters could not recombine and survive at high temperature. This KMC simulation on isochronal annealing provided insight into the effect of the irradiation condition of the accumulation of the defect and defect cluster.

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