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A kinetic Monte Carlo approach for the analysis of trapping effect on the defect accumulation in neutron-irradiated Fe

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ABSTRACT

The trapping effect of self-interstitial atom (SIA) clusters in neuron-irradiated Fe was analyzed in terms of generic traps. The effect of the cut-off size between sessile and glissile SIA clusters was investigated. The accumulation of SIA clusters decreased drastically as the cut-off size increased, which originated from the elimination of the SIA clusters at a grain boundary through its one-dimensional motion. When the immobile generic traps were introduced to the kinetic Monte Carlo simulation model, the effect of trap parameters was assessed. An increase in the binding energy between the trap and SIA-species resulted in a decrease in the number of mono-SIAs that were dissociated from the trap and a corresponding delay in visible SIA clusters. The size-dependent prefactor for the dissociation rate of trapped SIA clusters was necessary for a realistic accumulation behavior of SIA clusters. The trap density affects the density and size of the accumulated SIA cluster density during irradiation. This parameterization of generic traps provided insight into the mechanism of accumulation of SIA and SIA cluster.

1. Introduction

Low-alloy steel, which is used for constructing pressure vessels in nuclear reactors, suffers from long-term degradation of its mechanical properties, owing to defects in its crystal structure caused by neutron irradiation [1–4]. Experimental analysis of the behavior of irradiation defects is considered to be difficult, and multiscale computer simulation has been adopted as an alternative method for the evaluation of performance degradation of neutron-irradiated low-alloy steel.

A kinetic Monte Carlo (KMC) method is utilized to extend the results of molecular dynamics (MD) to a realistic time scale, and to enable the study of the growth behavior of defect clusters formed in materials over a long period of time [5,6]. The reliability of the KMC simulation depends on the model parameters of a given system, including migration energies of the defects, binding energies and various reaction events [7]. Therefore, a thorough understanding of the model parameters is essential to obtain accurate results in the simulation.

When the KMC simulation is applied to elucidate defect accumulation in Fe, there are difficulties in describing the accumulation behavior of self-interstitial atom (SIA) loops and clusters, which are known to cause matrix damage in Fe. It is reported that the SIA clusters have high mobility in MD simulations [8], but these mobile SIA clusters could not induce the large irradiation defects in Fe alloys under irradiation. Thus, the concept of generic traps for SIAs must be introduced in order to have good agreement with the experiments though the mechanism of generic traps is not clearly understood. The implementation of generic traps could include the introduction of immobile or mobile object to hold SIAs defects with various parameters, such as the binding energy. It is necessary to determine the effect of trapping parameters on the accumulation behavior of SIA clusters.

In this study, the trapping effect is investigated in terms of the cut-off size, binding energy, size-dependent prefactor of the dissociation rate, and trap density. In addition, the overall tendency of parameterization is discussed.

2. Simulation method

From among the various available forms of KMC, the object KMC simulation was chosen for this system. The detailed salient features of the object KMC are described in [7]. The KMC code, BIGMAC [5], has been used for simulating the accumulation of cascades. The model parameters in Fe used by Domain and Soneda [7,8] were suitably customized to the present system. Only single vacancies were considered to be mobile. All sizes of mono-size SIAs and SIA clusters were assumed to be mobile. The diffusivities of

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vacancies and SIAs were taken from the values of Soneda's works [6,8]. The reaction radii for each defect and dissociation rates were taken from the model of Domain el al. [7].

In order to study the trapping effect, generic traps for SIA and SIA cluster were introduced to the model. The authors postulated that generic traps were immobile and had a large reaction radius (2 nm). Generic traps are considered to react with only SIAs and SIA clusters (SIA-species) are thought to form immobile trapped SIA-species. This assumption is rather basic and requires further research.

The operation conditions of the high-flux isotope reactor (HFIR) at Oak Ridge National Laboratory were used for the simulation system [9]. The dose rate and maximum simulation time were fixed at 1×10^{-6} dpa/s and 2.3×10^5 s, respectively, [7]. A 20 keV cascade was used, which was obtained from MD (MOLDY) as input in KMC. The dimensions of the simulation box were $53 \times 59 \times 61$ nm with periodic boundary conditions (PBC). These noncubic boxes are beneficial for larger exploration of the simulation box under PBC conditions [10]. 1D migrating SIA clusters that jumped over a distance of approximately 1 μm without reacting were removed from the simulation box in order to consider an elimination of the defect at a grain boundary.

3. Results and discussion

3.1. Effect of cut-off size

Fig. 1 shows the size distribution of SIA clusters with different cut-off sizes between sessile and glissile SIA clusters at 0.2 dpa. The SIA clusters larger than the cut-off size were immobile during the simulation. Because of the small simulation box size, it should be noted that the lowest limit of the density is $\sim 5.0 \times 10^{21}$, and this is a tradeoff for saving simulation time. The diffusion of mono- and di-SIA clusters in the simulation box causes an increase in the average size and number density of visible SIA clusters (>~2 nm). This result is considered from the high mobility of the di-SIA clusters, which shows 3D motion. The introduction of tri-SIA clusters into the simulation box results in a simultaneous decrease in the size and number density of the SIA clusters. At a temperature of 343 K, tri-SIAs are known to exhibit 1D motion [8]. Owing to this 1D motion, the defect covers a very small reaction area during its diffusion, and hence, the SIAs can be removed without interaction with other species. The decrease in the size and density of SIAs become pronounced as the cut-off size of the mobile species increases. There is a slight aggregation of SIA clusters over a cut-off size of seven. Therefore, in order to obtain realistic results, it is necessary to introduce generic traps into the system.

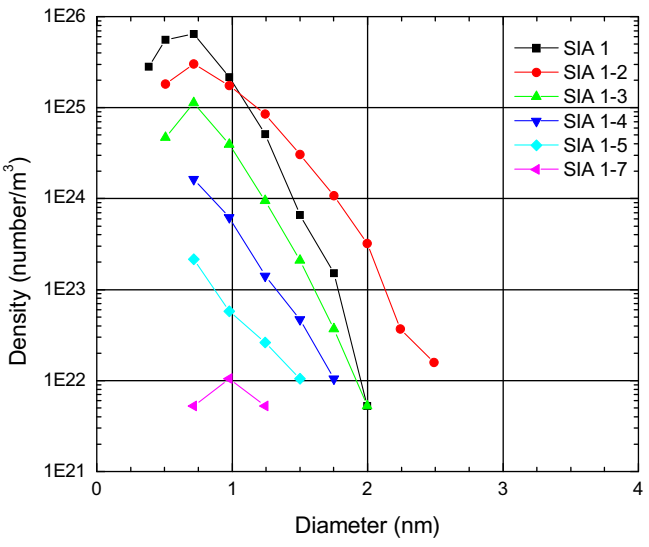

Fig. 1. The number density of SIA clusters as a function of size for different cut-off sizes between sessile and glissile SIA clusters.

3.2. Effect of binding energy of a generic trap

A generic trap is a useful substitute to analyze the accumulation behavior of the irradiation effect until the application of ab initio or MD for the mechanism of SIA clustering. The sink strength between a generic trap and a SIA-species can be expressed in terms of the thermally activated process, dissociation rate. The dissociation rate is determined by an binding energy and prefactor in KMC. In this study, the effect of the binding energy of the generic trap on the accumulation behavior of SIA clusters was analyzed.

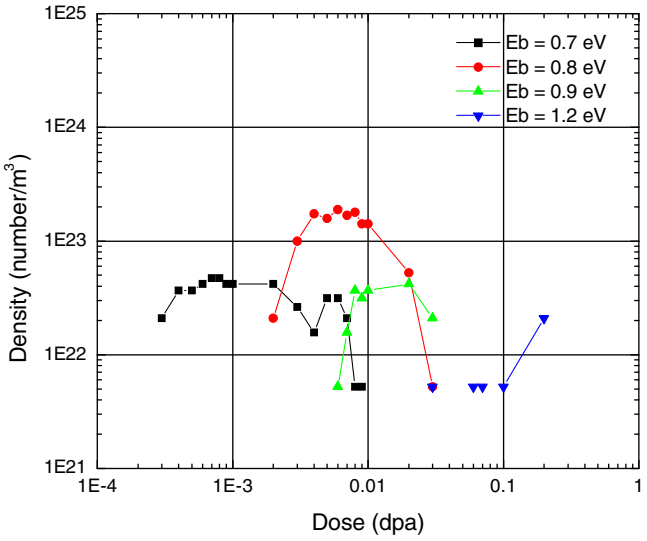

Fig. 2. The number density of visible SIA clusters containing more than 50 SIAs versus dose with different binding energies between a generic trap and SIA clusters. The dissociation rate was the same in all sizes of the trapped SIA clusters.

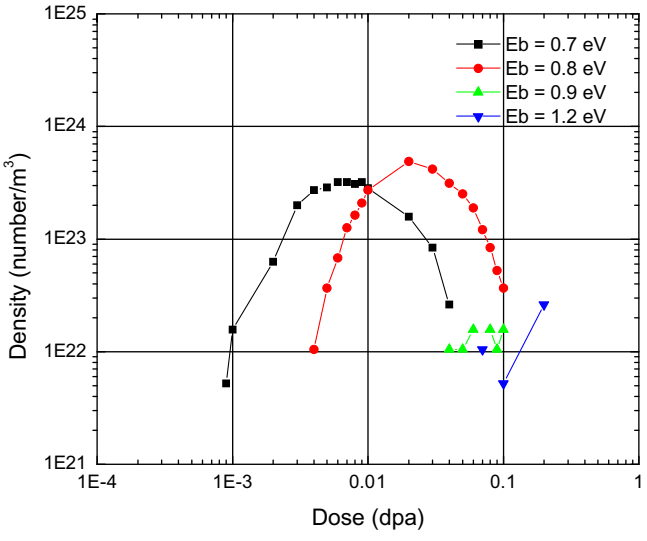

Fig. 3. The number density of visible SIA clusters versus dose with different binding energies between the generic trap and SIA clusters. The exponent n for the prefactor was 1. The dissociation rate was decreased as a function of 1/size.