

# Kinetic Monte Carlo Simulation of a Trapping Effect on the Accumulation Behavior of Defect Clusters in Neutron-irradiated Fe

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## 1. Introduction

The multiscale computer simulation is used as an alternative way to analyze the irradiation damage in low-alloy steel recently [1]. A kinetic Monte Carlo (KMC) method is a part of the multiscale modeling method, and deals the growth of the defects during irradiation. The KMC is able to extend the results of displacement cascade data from molecular dynamics (MD) to a realistic time scale, and it needs appropriate modeling to obtain highly accurate results [2].

When the KMC simulation is applied to clarify defect accumulation in Fe, there are difficulties in describing the accumulation behavior of self-interstitial atom (SIA) loops causing matrix damage in Fe. It is because highly mobile SIA clusters could not accumulated to the large irradiation defects under irradiation. In order to have good agreement with the experiments, the concept of generic traps for SIAs should be introduced, though the mechanism of generic traps is not clearly understood till now. Indeed, 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 binding energy, trap density and other features of generic traps. In addition, the overall tendency of parameterization is also discussed.

## 2. Methods and Results

### 2.1 Simulation method

The object KMC simulation code has been used for simulating the accumulation of cascades, and detailed description of the object KMC are described elsewhere [2]. The model parameters of KMC from Domain and Soneda [2-4] were suitably applied to the present system. Only single vacancies were considered to be mobile and all sizes of mono-size SIAs and SIA clusters were assumed to be mobile.

In order to study the trapping effect, generic traps for SIA and SIA cluster were introduced to the model. We 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 are thought to form immobile trapped SIA clusters.

The operation conditions of the high-flux isotope reactor (HFIR) at Oak Ridge National Laboratory were used for the simulation system [5]. The dose rate and maximum simulation time were fixed at  $1 \times 10^{-6}$  dpa/s and  $2.3 \times 10^5$  s, respectively. A 20 keV cascade

obtained from MD was used as input in KMC. The dimensions of the simulation box were  $53 \times 59 \times 61$  nm with periodic boundary conditions (PBC). When SIA clusters jumped over a distance of approximately  $1 \mu\text{m}$  without reacting, they were removed from the simulation box as an elimination of the defect at a grain boundary.

### 2.2 Effect of binding energy of a generic trap

The sink strength between a generic trap and a SIA species can be expressed as a dissociation rate. The dissociation rate is determined by a binding energy and prefactor in KMC. In this section, the effect of the binding energy of the generic trap on the accumulation behavior of SIA clusters was analyzed.

Figure 1 shows the visible cluster density versus dose in Fe with different binding energies. In the simulation, the generic trap density was 100 atomic parts per million (appm) in all cases. The prefactor of the dissociation rate was constant regardless of SIA cluster size. When the binding energy was 0.7 eV, the visible trapped SIA clusters (size > 50 SIAs) were found at the dose of 0.0003 dpa. As the binding energy increases from 0.7 eV to 1.2 eV, the advent of visible trapped SIA clusters is delayed to a higher dose. This is because of dissociation rate of a mono-size trapped SIA. When the binding energy is high, the dissociation rate is slow, and the supply of mobile SIAs in the simulation

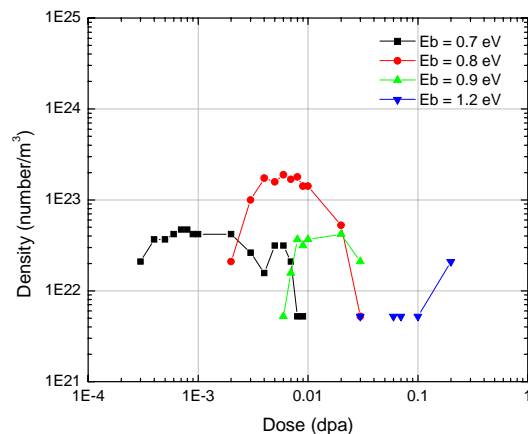


Fig. 1. The number density of visible SIA clusters containing more than 50 SIAs versus dose with different binding energies between a generic trap and SIA clusters. The dissociation rate was the same in all sizes of the trapped SIA clusters.

box decreases. The depletion of mobile SIAs lowers the growth rate of SIA clusters, thus visible SIA clusters could be found at an increased dose.

The visible SIA cluster densities were eventually decreased, except for the binding energy of 1.2 eV,  $t$ . It is considered that the 1D motion of the SIA clusters causes the decrease. When a large SIA cluster is separated from a trap, the cluster could be removed without reaction due to the 1D motion. The number of removed SIAs via 1D migration seems to be larger than that of trapping SIAs, and the total visible density of trapped SIA clusters decreased.

### 2.3 Effect of generic trap density

Figure 2 (a) shows the effect of the generic trap density on the accumulation behaviors of the visible SIA clusters. The binding energy and the prefactor of the size exponent were 0.8 eV and 2, respectively. As the density of the traps increased, the density of visible SIA clusters increased. When the trap density was 50 appm, there was a decrease in the visible SIA density at a high dose. It is thought that the low trap densities could not promote the accumulation of trapped SIA clusters. Figure 2 (b) shows the increase in the size and the density of trapped SIA clusters with the increase in trap density. Because a generic trap acts as a seed for the trapped SIA clusters, the density of traps is important for the corresponding SIA density.

### 3. Conclusions

The effect of various parameters of generic traps on the accumulation behavior in neutron-irradiated Fe is elucidated. An increase in the binding energy between the trap and SIA clusters leads to the decrease in the number of mono-SIAs dissociated from the trap and a corresponding delay in the advent of visible 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.

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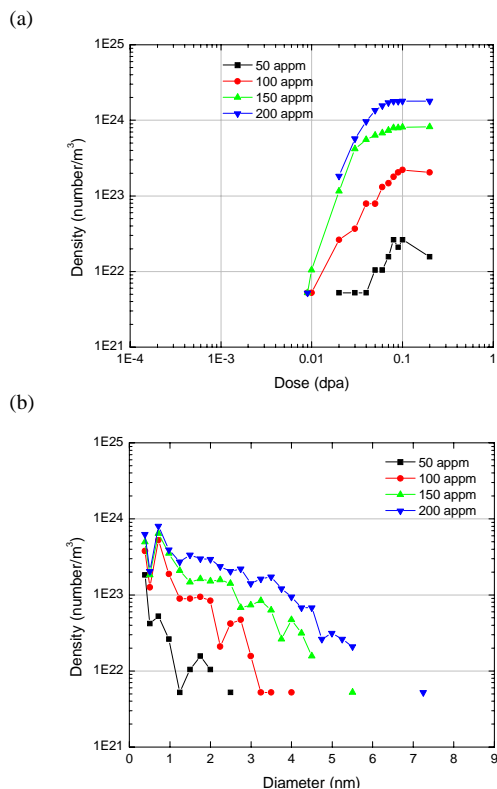


Fig. 2. The effect of trap density on (a) the number density versus dose, and (b) the size distribution of SIA clusters.