# Effect of a Model Parameter on Kinetic Monte Carlo Simulations for Microstructural Evolution in Fe

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## 1. Introduction

Low-alloy steel, which is used for constructing pressure vessels for nuclear reactors, suffers from long-term degradation of its mechanical properties owing to defects in its crystals structure caused by neutron irradiation.

However, since the experimental analysis of the behavior of irradiation defects is difficult, multiscale computer simulation is used as an alternative method for the same.

A kinetic Monte Carlo (KMC) method is used to extend the results of molecular dynamics (MD) to a realistic time scale, thus enabling 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 highly accurate results using the KMC simulation.

In this study, the effect of various parameters on the accumulation behavior in Fe system was assessed. First, the change in the jump rate of the species was analyzed. Then, the effect of the maximum size of mobile self interstitial atom (SIA) was analyzed in terms of defect accumulation. These results were compared with those reported in the literature.

## 2. Methods and Results

### *2.1 KMC Simulation*

From among the various available forms of KMC, the object KMC simulation was chosen for our system. The detailed salient features of the object KMC are described elsewhere [7]. The model parameters used by Domain and Soneda [7,8] were suitable modified so that they could be used in our system. The operation conditions of the high-flux isotope reactor (HFIR) at Oak Ridge National Laboratory were used for our simulation system. The dose rate and maximum simulation time were fixed at 0.23 dpa and $2.3 \times 10^5$ s, respectively. The dimensions of the simulation box were 53 × 59 × 61 nm with periodic boundary conditions.

### *2.2 Effect of Vacancy and SIA Jump Rate*

Figure 1 shows the size distribution of defects in the simulation box at various jump activation energies of the vacancies. Only single vacancies and were allowed to move freely within the box.

The number density of small vacancies was found to be high when the migration energy of a single vacancy (Em) was 1.3 eV. In that case, the mobility of a single vacancy was very low and the diffusion distance was restricted during the simulation. Consequently, numerous small vacancies were formed in the system, and the number density of vacancy clusters decreased with an increase in their size. When the migration energy was 0.69–0.87 eV, single vacancies interacted with one another during the simulation time, leading to

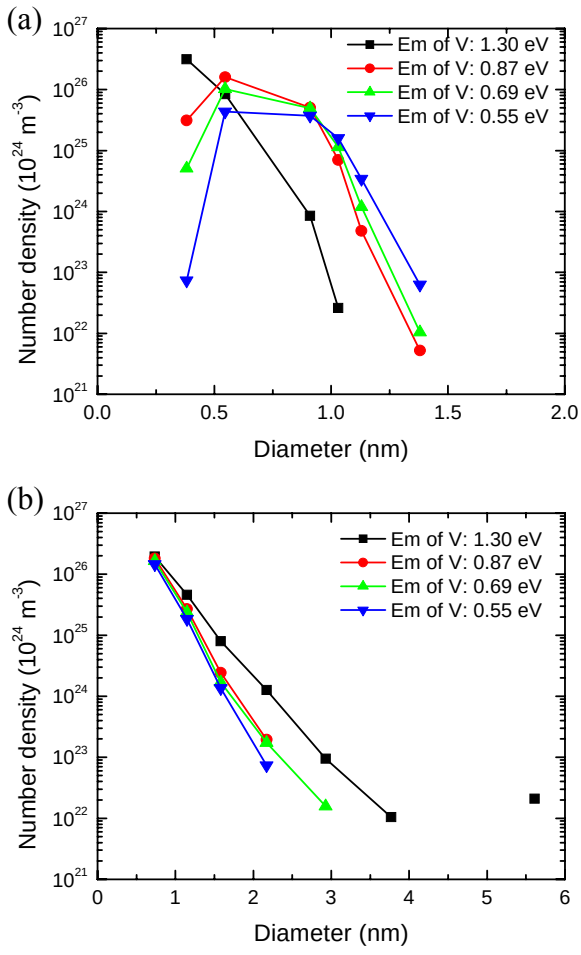


Fig 1. Size distribution of (a) vacancy clusters and (b) SIA clusters at different jump activation energies of a vacancy. The size is calculated from the number of defects.

an increase in the number density of large-sized vacancy clusters. This increase became pronounced when Em decreased to 0.55 eV, which is the experimentally calculated value for ultra-high-purity Fe [8].

Since the migration energy of a single SIA is very low, the SIAs have a very long diffusion distance. Prior to the migration of the vacancies, all the SIAs interacted with other defects. The remaining clusters were immobile, and their size decreased owing to their interaction with the vacancies. The sizes of the SIA clusters decreased as the mobility of a vacancy increased.

### *2.3 Effect of Change in Mobile Species*

Figure 2 shows the effect of the cut-off size between sessile and glissile SIA clusters on the number density of SIA clusters. The SIA clusters larger than the cut-off size is immobile during the simulation.

The diffusion of mono- and di-SIA clusters (red line) in a crystal causes a decrease in the number density of small SIA clusters. The probable reason for this is the high mobility of the di-SIA clusters. The introduction of tri-SIA clusters into the crystal results in a simultaneous decrease in the size and number density of the SIA clusters At the temperature of 343 K, tri-SIAs is known to show 1-D motion [7]. Owing to this 1-D motion, the defect covered a very small area during its diffusion, and hence, the SIAs could be removed without any interaction with other species. The decrease in the size and density of SIAs became pronounced as the cut-off size of the mobile species increased. There was a very slight aggregation of the SIA clusters at a cut-off size of 20. Therefore, in order to obtain realistic results, it is very important to decide the cut-off size of mobile SIA clusters, and to further modify the existing model parameters.

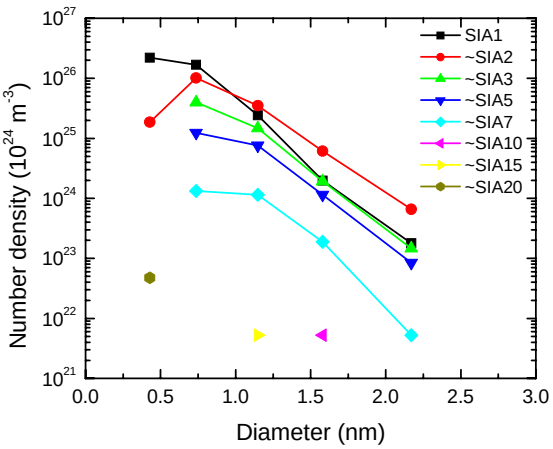


Fig 2. The number density of SIA clusters as a function of size for different cut-off values between sessile and glissile interstitial clusters.

## 3. Conclusion

An increase in the Em of a vacancy resulted in a corresponding decrease in the number density of small vacancies and a shift in the mode value of the cluster size. The size and number density of SIA clusters decreased with an increase in the mobility of a vacancy.

The cut-off size of mobile SIA clusters is a very crucial factor that decides their aggregation. This is because of the 1-D motion of the SIA clusters and their removal without allowing them to react with other species. For a more accurate modeling, more in-depth studies on the trapping mechanism are required.

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