

§46. Dose-rate Dependence of Microstructural Evolution in Fusion Materials during Irradiation

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Cubic silicon carbide (β -SiC) is a component of SiC/SiC composites that are candidates for blanket structural materials of nuclear fusion reactors. In the present study, in order to clarify formation kinetics of self-interstitial atoms (SIA) clusters in β -SiC during irradiation, the nucleation and growth process of SIA-clusters were investigated by a kinetic Monte-Carlo (KMC) simulation technique.

Growth or shrinkage of a defect cluster is determined by a balance between influx (absorption rate) and outflux (thermal dissociation rate) of point defects into and from the defect cluster. The influx of point defects into a disc-shaped SIA-cluster was obtained here as the following equation in the unit of s^{-1} :

$$v_k^{\text{influx}} = \frac{2\pi^2 R}{\Omega \ln(r_m/r_0)} D_k C_k, \quad (1)$$

where D_k and C_k are the diffusion coefficient and concentration of type k point defect in the matrix, respectively, in which k denotes silicon vacancy, carbon vacancy, silicon interstitial (I^{Si}) and carbon interstitial (I^{C}). Ω is the mean atomic volume and R is the cluster radius. Here, the cluster volume is given by $V=n\Omega=\pi R^2 d$. The cluster size is defined as $n=n_1^{\text{Si}}+n_1^{\text{C}}$ that is the total number of interstitials contained in an SIA-cluster, in which n_1^{Si} and n_1^{C} are the numbers of silicon- and carbon interstitials in the cluster, respectively. The outflux of point defects from a disc-shaped SIA-cluster was obtained here as the following equation in the unit of s^{-1} :

$$v_k^{\text{outflux}} = \frac{2\pi^2 R}{\Omega \ln(r_m/r_0)} D_k \exp\left(-\frac{E_B^{\text{cluster}-k}}{k_B T}\right), \quad (2)$$

where $E_B^{\text{cluster}-k}$ is the binding energy of a point defect to an SIA-cluster. The binding energy is defined as energy required to remove a point defect from an SIA-cluster. Notice that defect energies required in Eqn. (1) and (2) were already obtained by molecular dynamics calculations in our previous work [1,2]. Events considered in the KMC simulations are the absorption and the emission of interstitials into and from an SIA-cluster characterized by size and composition, in which the occurrence probability of each event was assumed to be proportional to v_k^{influx} and v_k^{outflux} , respectively.

Fig. 1 shows the KMC simulation results of the time evolution of size of SIA-clusters in β -SiC at 973 K [3]. The nucleation and growth process of the clusters are successfully demonstrated. At first, significant absorption and emission events occur, and then the absorption event becomes more dominant. From the figure, the incubation period for the cluster nucleation can be clearly identified. The incubation period for the cluster nucleation strongly

depends on the diffusion fluxes ratio ($D_1^{\text{Si}}C_1^{\text{Si}}:D_1^{\text{C}}C_1^{\text{C}}$). As the ratio is far from 1:1, the incubation period becomes longer; namely, more time is needed for the cluster nucleation. Fig. 2 is the nucleation and growth path of the clusters at 973 K, showing that each path almost goes along the diagonal line of the figure. This means that each cluster grows while keeping its composition near stoichiometric. This composition is energetically favorable. It may indicate that, at this relatively high temperature, the thermal stability of an SIA-cluster is the most crucial for the nucleation and growth process of the cluster. This kind of information is important for modeling the formation of defect clusters in compound materials during irradiation.

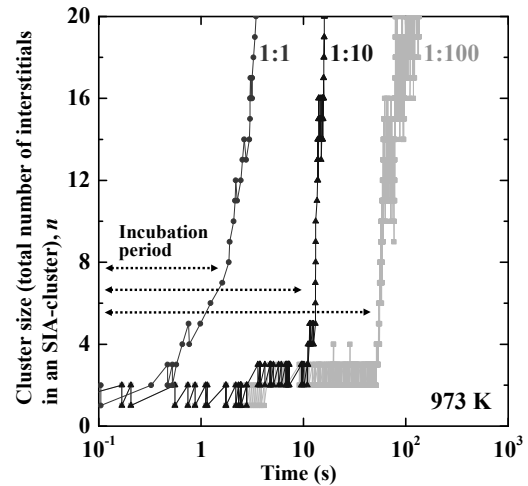


Fig. 1. Time evolution of size of SIA-clusters in β -SiC at 973 K obtained from the KMC simulations.

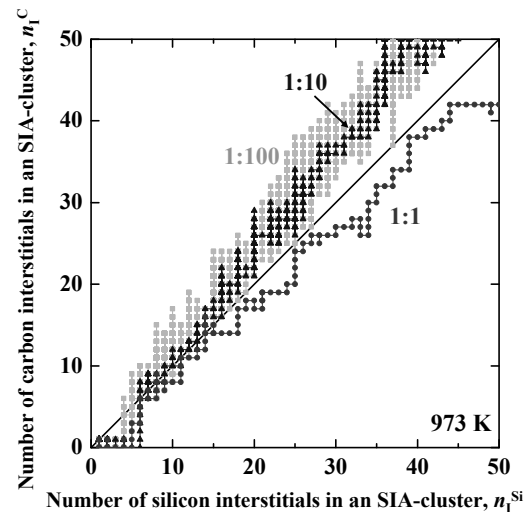


Fig. 2. Nucleation and growth path of SIA-clusters in β -SiC at 973 K obtained from the KMC simulations.

- 1) Watanabe, Y. et al.: Nucl. Instrum. Meth. B 267 (2009) 3223.
- 2) Watanabe, Y., Morishita, K., Kohyama, A.: J. Nucl. Mater. (in press)
- 3) Watanabe, Y., Morishita, K., Yamamoto, Y.: Nucl. Instrum. Meth. B 269 (2011) 1698.