# §20. Multiscale Modeling of Radiation Damage Processes in Fusion Materials

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Continuous efforts have been made towards the development of a new methodology predicting the behavior of fusion materials during irradiation, which is one of the important technologies for development of new radiation-resistant materials and for reliable assessment of reactor lifetime. Radiation damage processes leading to the degradation of materials due to irradiation are essentially multiscale phenomena that have a wide variety of time-, length- and energy-scales.

One of our research actions in this year is to have several meetings to exchange information to each other about multiscale modeling of radiation damage processes. [1] Another action in this year is to carry out the research of theoretical modeling on defect interactions in SiC, where SiC/SiC composites are one of promising candidates for the blanket structural material, because of high stability at high temperature. As a first step towards constructing a model for simulating microstructural evolution in $\beta$-SiC during irradiation, molecular dynamics and molecular static calculations have been performed to obtain the formation and binding energies of relaxed configuration of vacancy clusters in $\beta$-SiC as a function of the size, vacancy composition, and vacancy configuration of clusters, which are necessary when the nucleation and growth process of clusters is investigated.

The formation energy of vacancy clusters is defined as energy required to introduce a vacancy cluster into an otherwise perfect $\beta$-SiC crystal, which is given by $E_F(n_V^{Si}, n_V^C)=E^{tot}-N_{Si}\varepsilon_{Si}-N_C\varepsilon_C$, where $N_{Si}$ and $N_C$ are the numbers of silicon atoms and carbon atoms in the system, respectively. $E^{tot}$ is the total potential energy of a relaxed system containing the cluster. $\varepsilon_{Si}$=−6.21 eV and $\varepsilon_C$=−6.61 eV are the calculated cohesive energies of a silicon atom and a carbon atom in a perfect $\beta$-SiC crystal, respectively. Using the formation energy thus evaluated, the binding energies of vacancies to a cluster are also evaluated.

The formation energies of an isolated silicon-vacancy and an isolated carbon-vacancy in β-SiC were calculated to be $E_F(1,0)$=3.49 eV and $E_F(0,1)$=2.56 eV, respectively. A carbon vacancy has the dilatational displacement field, where 1st nearest neighbor (1NN) silicon atoms are displaced by $0.09a_0$ away from the vacancy and 2nd nearest neighbor (2NN) carbon atoms are displaced by $0.01a_0$ away from 1NN atoms. A silicon vacancy has also the dilatational displacement field with the same amount of atomic displacements as above.

The formation energy of vacancy clusters in β-SiC depends, not only on the numbers ($n_V^{Si}$, $n_V^C$), but also on the vacancy configuration of clusters, which is, *as a first approximation*, represented by the number of dangling bonds in the cluster. It was, in many cases, observed that a vacancy cluster with the fixed numbers ($n_V^{Si}$, $n_V^C$) takes the lowest formation energy when the number of dangling bonds in the cluster is the smallest. Besides, vacancy absorption process by a vacancy cluster is considered to occur so as to reduce the *total* number of dangling bonds in the cluster.

Fig. 1 shows the size dependence of the lowest formation energy of clusters, where cluster size is defined by $n=n_V^{Si}+n_V^C$. As shown in the figure, the lowest formation energy is an increasing function of $n$. Consider an empirical relationship for void formation energy as described by $E_F=4\pi R^2\gamma(1-\delta/R)$, where $\gamma$ is the surface energy for *flat* surface, $\delta$ is a constant, and $R$ is void radius having a relationship with $n$ as $4\pi R^3/3=n\Omega$. Here, $\Omega$ is the atomic volume, and the second term in this equation represents a correction term due to the curvature of void surface. When the calculated formation energies of vacancy clusters with $n_V^{Si}/n_V^C=1$ were used to fit to the empirical expression, $\gamma$=11.98 eV/nm$^2$ was obtained. Surprisingly, this value is in good agreement with the calculated surface energies of $\gamma$=10.25, 13.50, 17.25, 21.88 and 25.60 eV/nm$^2$ for (111), (110), (211), (100)Si and (100)C flat surfaces, respectively. It indicates that the classical expression of spherical void energy agrees well with the formation energy of nanovoids as small as one vacancy.

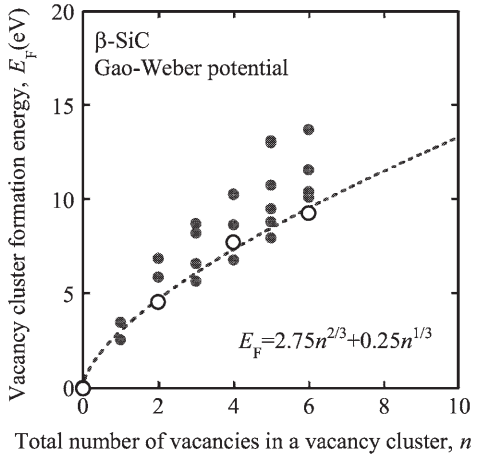


Fig. 1 The lowest formation energy of vacancy clusters in SiC as a function of cluster size, $n=n_V^{Si}+n_V^C$, where $n_V^{Si}$ and $n_V^C$ are the numbers of silicon- and carbon-vacancies in a cluster.

1) Report of multiscale modelng of radiation damage in materials, Vol. 3, November 2008, in Japanese.