§16. Multiscale Modeling of Radiation Damage Processes in Fusion Materials

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Continuous efforts are being made towards the development of new methodology that predicts 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. Therefore, to understand the processes well, a wide variety of researchers are needed and the NIFS collaboration programs have been playing an important role. This collaboration activity recently proceeds with the different collaboration program between Kyoto University and JAEA for the DEMO-BA projects.

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, which are reported in [1] and [2]. Participants whose major are the plasma-surface interaction study newly join this year.

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 β-SiC during irradiation, molecular dynamics and molecular static calculations have been performed to obtain the formation and binding energies of relaxed configuration of defect clusters in β-SiC, which are necessary when the nucleation and growth process of clusters is investigated.

The calculated lowest formation energies of isolated silicon- and carbon-interstitials are 3.17 eV and 3.24 eV, respectively. The most stable configuration of isolated silicon interstitial is the TC configuration where a silicon atom is located at the tetrahedral position surrounded by four regular carbon lattice atoms. On the other hand, the energetically favorable configuration for isolated carbon interstitial is the C-C dumbbell configuration in which two carbon atoms share a regular carbon lattice site along <100> direction. These stable configurations are consistent with those obtained by our previous ab-initio calculation.

The calculated lowest formation energy of SIA-clusters with the cluster size $n=n_I^{Si}+n_I^C$ are also calculated. The formation energy strongly depends on the size and chemical composition of clusters. As to the most stable configuration of the clusters, surprisingly, each silicon interstitial in the clusters also maintains the TC configuration, while each carbon interstitial in the clusters maintains the C-C dumbbell configuration, as well.

Also, preliminary calculations were conducted to obtain the formation energy of relatively large SIA-clusters. Fig. 1(a) shows the configuration of SIA(91, 91) which was relaxed at 300K. As shown in the figure, the SIA(91,91) is a disc-shaped defect containing stacking fault on the closed-packed (111) plane, with the estimated diameter of 2.1 nm. When the relaxation was done at a higher temperature, the stacking fault was eliminated and the SIA-cluster was unfaulted to be a perfect loop, as indicated in Fig. 2(b). In order to clarify the mechanism of the unfaulted process, further investigation is underway.

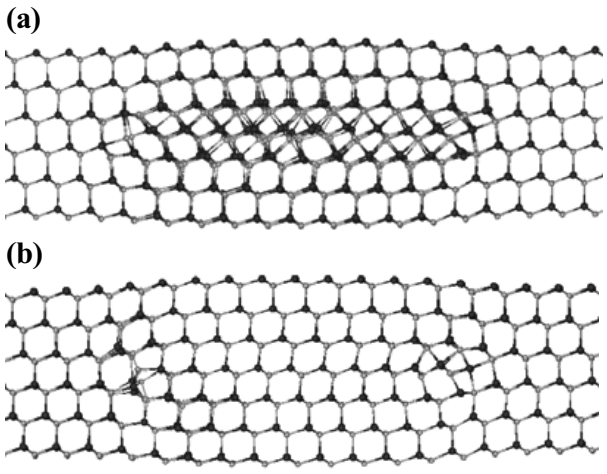

Figure 1 The configuration of SIA(91, 91) relaxed at (a) 300K and (b) 600K obtained by the MD and MS calculations. Some preliminary calculations show that a metastable SIA(91, 91) is a disc-shaped defect containing stacking fault on the closed-packed (111) plane, as shown in (a). When the relaxation is done at a higher temperature, the stacking fault is eliminated and the SIA-cluster is unfaulted to be a perfect loop, as indicated in (b).This work will be published in ref. [3].

1) Report of multiscale modelng of radiation damage in materials, Vol. 4, Febuary 2010, in Japanese.
2) Report of multiscale modelng of radiation damage in materials, Vol. 5, Febuary 2010, in Japanese.
3) Y. Watanabe, et al., MMM-4 conference proceedings, Tallahassee, Florida, USA.