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

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Continuous efforts for modeling the microstructural evolution in materials during irradiation are being made for development of the advanced method of predicting the behavior of materials in fusion reactors, which will provide a basis of the development of new materials used in reactors and also a basis of the development of evaluation methods of material's lifetime. Radiation damage processes leading to microstructural changes in materials 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 hold a meeting to exchange opinions about the methodology of multiscale modeling of radiation damage processes. [1)]

Other action in this year is that the research of theoretical modeling on defect interactions in SiC materials is carried out. SiC/SiC composites are expected as one of blanket candidate materials in future fusion reactors. It is generally known that point defects and defect clusters such as interstitial loops and voids are produced and accumulated in materials during irradiation, and that the creation of these defects will influence their material properties such as mechanical properties, dimensional stabilities and thermal mechanical properties. Therefore, of course, many irradiation experiments on SiC material have also been widely conducted so far to obtain quantified relationships between irradiation conditions and the changes of material's property and performance due to irradiation. Unfortunately, however, defect accumulation process in this material has not yet been well understood, because SiC material has an ionic nature in addition to a covalent one, and therefore, point defects and defect clusters in the material can have effective electric charges which will lead to the complicated diffusion and growth behavior of defects. The ambiguities of this knowledge will lead the difficulty in modeling the behavior of SiC material during irradiation.

Ryazanov et al. have already proposed a model for formation of interstitial loops taking into account the charge state of defects in SiC under irradiation, where interstitial loops grow and maintain its neutral charge. However, interstitial loops in their model were limited within the category of relatively large perfect loops, and therefore, their model cannot be applied to small loops (including embryos) which are very important as an entity of loops at the first stage of loop nucleation and growth process.

In the present study, an advanced model of the formation of interstitial loops taking into account the charge state of defects in SiC under irradiation is here developed, which is appropriate for small loops. First, the capture efficiency of mobile defects by a defect cluster is theoretically derived, where electric interaction between an interstitial loop and an isolated interstitial atom is considered. And then, the numerical simulation of accumulation process of small interstitial loops during high-energy electron irradiation is conducted using the kinetic rate theory based model with the capture efficiency derived above. And finally, the results are compared with experiments, where SiC is irradiated by high-energy electrons in high voltage electron microscopy (HVEM).

Fig. 1 shows the time dependence of the concentration of clustered interstitials (CLIs) as a function of cluster charge states. The concentration of CLIs greatly depends on charge states and decreases with increasing the magnitude of charges. This figure also shows the result of HVEM experiments. As shown in the figure, when the charge state increases, the calculated concentration of CLIs approaches to the experimental data, implying that the capture efficiency derived here is important; namely, electric interaction between a loop and an isolated interstitial atom may play an important role on loop nucleation process.

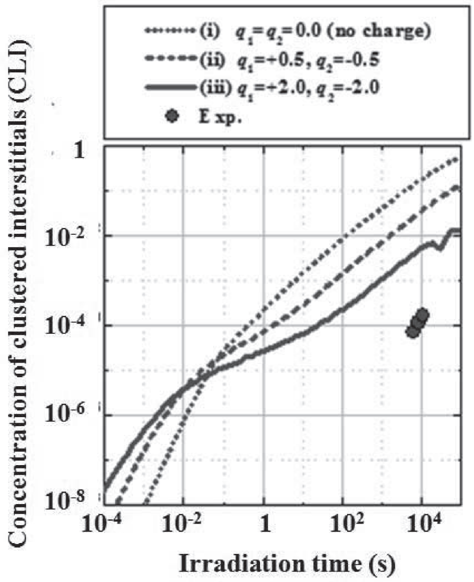

Fig. 1 Time dependence of the concentration of CLIs in SiC evaluated by kinetic rate theory calculation using the derived capture efficiency.

1) Report of multiscale modelng of radiation damage in materials, Vol. 2, Febuary 2008, in Japanese.