§65. Rate Theory Modeling of Defect Evolution under Cascade Damage Conditions

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Production of cascade vacancy clusters has long been observed in experiments and demonstrated by computer simulation studies. Generally, vacancy clusters are medium thermally stable at low to temperatures. Vacancy clusters, which are randomly introduced at very high production rates and possess a long lifetime, should impose great influences on point defect processes, microstructural evolution resultant property and changes in irradiated materials.

There have been some models of microstructural evolution in irradiated materials which include a description of cascade cluster evolution. These models have been to some extent successful in assessing the effects of cascade vacancy cluster production qualitatively. However, recent molecular dynamics investigations of cascade defect production reveal that the initial size distribution of cascade vacancy clusters might be largely different from the assumption in those models. In this work, a model of defect evolution in irradiated materials was developed, taking account of cascade vacancy cluster production in various manners according to the latest molecular dynamics simulation results. Using the developed model, the influences of cascade vacancy cluster production, configuration, clustering fraction and initial size distribution on the effective point defect flux and microstructural evolution were investigated.

Microstructural and microchemical changes as consequences of defect migration and accumulation are generally understood to be responsible for the irradiation-induced property degradation in fusion reactor materials. Therefore, the defect production characteristics and the effective flux of freelv migrating point defects under cascade damage conditions are among the kev issues to assess the materials behavior under fusion environment by mechanistic modeling. Attempts to clarify the defect production efficiency have been made for years both by experiments and computation. Computer simulations of cascade events by means of molecular dynamics has shown 10 to 20 percent of surviving defect fractions (SDF) in typical fcc metals at elevated temperatures. Results from the maximum swelling rate measurements are generally consistent with the calculated SDF at high temperatures, however, effective free defect rates derived production from other experiments including loop growth radiation measurement and induced segregation or radiation induced diffusion analyses yielded to as low as several tenth percent. This discrepancy is most likely attributed to the effect of fine defect structures in part due to the complexity of defect production behavior particular to high energy cascade. Such microstructural effect should influence swelling rates as well but have never been assessed systematically.

Also in this work, issues related to characterization of cascade-induced defect production by microstructural analysis, including swelling rate analysis in reactorirradiated austenitic alloys and loop growth rate analysis in electron- and heavy ionirradiated austenitic model alloy, are discussed.

References

- Katoh,Y., Muroga,T. Kohyama,A., Stoller, R.E., Namba,C., and Motojima,O., Journal of Nuclear Materials (in printing).
- 2) Katoh,Y. and Muroga,T., Journal of Nuclear Materials (in printing).
- Katoh,Y., Muroga,T., Kohyama,A., Stoller, R.E., Namba,C. and Motojima,O., NIFS-386 (1995) National Institute for Fusion Science