§6. Modeling of Irradiation Performance and Fundamental Data for Fusion Materials

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The degradation of materials behavior under irradiation is one of the most critical factors which determine the lifetimes of the components of future fusion machines. It has been highly required to predict the property changes of the materials under irradiation quantitatively with basic understanding and established databases. Materials in future nuclear energy systems such as fusion reactors will be used in severe environment including high dose irradiation of high energy neutrons especially in first wall/blanket structures. As no intensive neutron sources are available to test the materials for first wall/blanket structures, it is essential to predict materials behavior under fusion irradiation environments. Modeling is not only the mechanistic understanding of macroscopic irradiation effects from short and fine scales of phenomena but also providing the critical methodology for its quantitative estimation by connecting fine scale estimations.

In this study, the importance of modeling and database systems to predict irradiation performance of fusion reactors is discussed based on the evaluation of current progress of computational materials research. There are many stages of radiation damage evolution between these femto second region to the lifetime of the expected fusion energy system. It is also the role of modeling to link these different stages of irradiation effects, each of which has its best way of evaluation.

(1) Modeling of Defect Production and Database of Molecular Dynamics Results

Molecular dynamic (MD) simulation is a best way to clarify the collisional phase of single cascade displacement damage formation. Displacement damage under high energy neutrons begins with the formation of a primary recoil atom (PKA) in irradiated materials.

Estimation of PKA energy spectrum in the irradiated materials requires extensive collaboration between materials researchers and nuclear data people. Based on the discussion in this research, a special committee in the Society of Atomic Energy Research initiated to develop a new dpa calculation code for irradiation experiments in fission reactors and expected fusion environments.

When the energy of PKA is high enough to displace other atoms sequentially, cascade damage is formed within 0.1 psec. The number of initial Frenkel pairs, N_F at the beginning of the calculation can be associated with the PKA (primary knock-on atom) energy E_p, using the following equation as derived by the MD simulation of Bacon et al [1], showing the number of Frenkel pairs after the quenching stage.

$$N_F = A(E_p)^m \qquad (1)$$

Database of these constants, e.g. A and m, is collected and evaluated for several materials. Morishita et al estimated these values for vanadium, niobium and tantalum as shown in Figure 1. When Nr is larger than 1, m is found to be nearly 0.75 for all the materials. However, m is found to be about 1.2, when the Nr is smaller than 1, because replacement collision sequences are major mechanisms of Frenkel pair production.

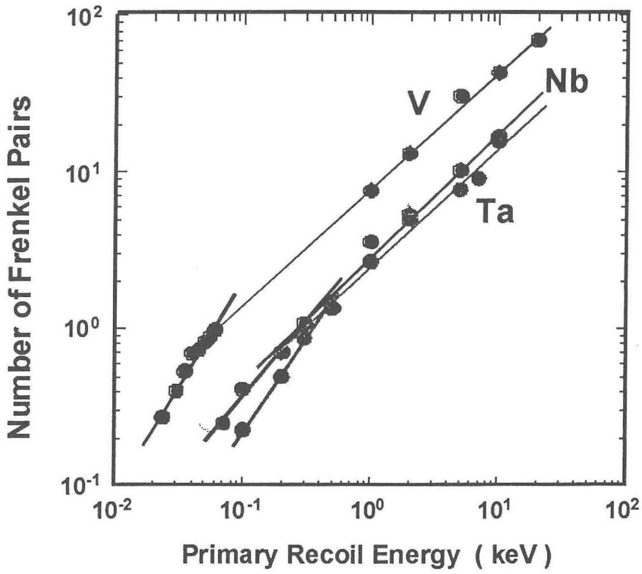

Fig. 1 Number of Frenkel Pairs by Displacement Damage Sequences in V, Nb and Ta.

(2) Modeling of Microstructural Evolution

It is still not easy to extend the MD calculation to the evaluation of microstructural evolution because of the limited computational capabilities. Mone-Carlo type simulation is a promising methodologies to describe complex defect clustering and microstructural changes in irradiated materials. Future efforts for modeling and database evaluation in this research should be directed to the estimation of bias for point-defects in addition to dislocation dynamics simulation under applied stress and deformation.

References
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