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

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Materials in fusion reactors will be used in severe environment including high dpa irradiation by high energy neutrons especially in first wall/blanket structures. Materials behavior under irradiation is one of the most critical factors which determine the lifetime of the component of future fusion systems. Modeling of materials behavior is not only the mechanistic understanding of macroscopic irradiation effects from short and fine scales of phenomena but also providing the critical methodology for the quantitative estimation of the reliability of the irradiated materials for long term operation.

In this study, the importance of modeling and quantitative evaluation of radiation environments to predict irradiation performance of fusion reactors is discussed based on the evaluation of current progress of computational study.

(1) Modeling of Dose Rate Effects and Microstructural Evolution in Model Alloys under Cascade Damage

There have been a number of studies showing that there exist strong dependences of microstructural evolution and resultant property changes on the atomic displacement rate. For example, the effect of dose rate on void swelling seems to exist in both pure metals and alloys, and in both BCC and FCC crystal systems with the primary influence concentrated in the transient regime. The transient shift leads to a decrease in the transient regime as the dpa rate decreases, and the strength of the transient shift increases with increasing temperature.

It was shown that the net vacancy flux to voids is proportional to $(\mathrm{dpa/sec})^{1/2}$ over a large range of dpa levels and dpa rates, indicating that recombination dominates point defect annihilation in this experiment [1]. It appears that this is the essential mechanism of the effect of dose rate on microstructural evolution. At high dose rates, point defects are generated at higher concentrations, resulting in a higher fraction of point defects annihilated by recombination. On the contrary, at lower dose rates, the fraction of point defect absorbed by sinks is higher relative to that at higher dose rates. The recombination fraction increases both with increasing dpa rate but also with decreasing temperatures, accounting for the apparently opposing effects of these two variables. In the post-transient regime, however, there is very little effect of these two variables. A model has been developed to explain this behavior and to extrapolate to other irradiation conditions for which insufficient data are available.

The recombination rate of point-defects observed at very low dose rates is too large to be caused by random-diffusion recombination, but may be caused by 1-D motion of I-clusters formed under cascade damage. It also appears that there seems to exist bias factors of cavities that depend on their size. This may be caused by segregation to cavity surfaces. This can also alter the cavity growth rate at different dose rate.

(2) Development of a dpa code, NPRIM, for neutron irradiation environments

A computer code, NPRIM, has been developed to be free from a tedious computational effort, which has been devoted to the calculation of derived quantities such as displacement per atom (dpa) and helium production rate [2].

The NPRIM code works with graphical user interface on PC platforms of the Windows and Macintosh. Several neutron spectra are prepared as typical neutron fields, such as the JMTR, HTTR, YAYOI, JOYO, HFIR, ATR and ITER. Neutron cross sections concerning to damage reactions based on JENDL3.2 and/or ENDF/B-VI are given with a fine group as the SAND IIA 640-group-structure. The dpa cross sections based on ENDF/B-IV of the ASTM Standard E693-79 and ENDF/B-V of the SPECTER code are also installed. Damage calculations are used the Robinson's numerical approximation to the Lindhard partition. For the automatical transformation of energy group structure, the input neutron spectrum and output damage index are allowed in free energy grids in the range from 10^{-10} to 20 MeV. The results include reaction-dependent variation and uncertainties.

Using the NPRIM code, the calculation has been performed for typical neutron fields. For example, the results of dpa for iron in two kinds of neutron fields of JMTR, YAYOI show relatively small quantity of deference within 2% with those by ASTM Standard E693 practice and SPECTER code. This code enables us to study a damage correlation in materials irradiated under deferent neutron environments.

The free download site of the NPRIM code is http://marie.q.t.u-tokyo.ac.jp/nprim/indexj.html.

References

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