Development of the simulation code for the migration of irradiation defects in tungsten for tritium inventory evaluation

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In a fusion reactor, tungsten will be exposed to high heat flux, neutrons, helium ash and fuel plasma including tritium. The neutron irradiation will generate defects in tungsten, and the migration of those defects under irradiation will result in clustering and annihilation of defects. These irradiation defects would be a strong trapping site for deuterium. Therefore, the prediction of the accumulation of irradiation defects during reactor operation is necessary for tritium inventory evaluation in the vacuum vessel to estimate the hazard of loss of vacuum accident. In this study, the migration of irradiation defects and subsequent accumulation and annihilation of them were evaluated by newly developed code where all reactions of defects with different sizes and kinds were simultaneously calculated using rate equations under various damaging conditions and temperatures. Then, the consequent defect density in tungsten was compared to the experimental data of deuterium retention in damaged tungsten.

The brief content of the code is as follows. The dimension of tungsten crystal grain was simplified as cylindrical shape. The vacancy and interstitial atoms are pair defects, and the clusters of these defects were considered. The diffusion coefficients and thermal stabilities of these defects were referred from the ab-initio calculation [1], and these parameters with increasing the size of defects were estimated by the capillary extrapolation. The diffusion, recombination, accumulation and thermal decomposition of defects clusters with different cluster sizes were simultaneously calculated. Using this code, as the preliminary calculation the densities of vacancy clusters were estimated for tungsten under heavy ion (6.4 MeV Fe^{2+}) irradiation. The literature data [2,3], where the deuterium trap density in tungsten irradiated by heavy ion irradiation was evaluated, is used for the validation check of the code.

The density of vacancy clusters in tungsten with the increase of 6.4 MeV Fe^{2+} irradiation fluence was estimated by the simulation code, and compared to the deuterium trap density in tungsten irradiated by the same heavy ion with similar damage levels. Here, the vacancy density was evaluated by the number of mono-vacancy corresponding to all vacancy clusters although the size-population of vacancy clusters became larger with increasing irradiation temperature due to the enhancement thermal diffusion of vacancy. Time-evolution of vacancy density estimated in this simulation code was almost consistent with deuterium trap density. In the presentation, the estimation of vacancy density in tungsten irradiated by 6.4 MeV Fe^{2+} under various temperatures, and the comparison with the trapped deuterium density in the irradiation defects will also be discussed. Thereafter, the validity and capability of the simulation code developed in this study will be evaluated.

[1] C.S.Becquat et al., J. Nucl. Mater., 403 (2010) 75-83.
[2] Y. Hatano et al., Nucl. Mater. Energy. 9 (2016) 93-97.
[3] B. Tyburska et al., J. Nucl. Mater., 395 (2009) 150-155.