Accumulation behavior of radiation defects in tungsten by molecular dynamics calculation

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The increase in the tritium retention due to the trapping effect of radiation defects in tungsten used as a plasma facing material raises engineering concerns about the sustainability of the fuel cycle and radiation safety in fusion reactors. The retention increase is determined by the type and number of surviving defects and the trapping strength of each defect. Trapping characteristics, such as the tritium trapping energy of each defect and the maximum number of tritium atoms that each defect can trap, have been extensively studied by experiments and computational simulations. On the other hand, the accumulation behavior of radiation defects is yet to be sufficiently understood. In this study, the type and number of surviving radiation defects formed in tungsten were investigated using molecular dynamics (MD) calculations.

The LAMMPS code was used for MD simulations. To investigate the accumulation behavior of radiation defects as a function of radiation dose in units of displacements per atom (dpa), recoil simulations were iteratively conducted. The recoil energy was fixed at 3.2 keV, which is the average recoil energy of primary knock-on atoms in the helium-cooled pebble-bed DEMO reactor [1]. The recoil atom and direction were chosen randomly for each recoil event. To estimate the potential model dependence, the MD simulations were performed with three potential models and the results were compared.

The MD simulation results showed that the saturation of the defect number is achieved when the ratio of the number of vacancies to the number of W atoms in the system is about 1%. The saturation was achieved at around 0.5 dpa. The majority of the formed SIAs were clustered, while the vacancies were less clustered. These observations were similarly obtained for all three potential models, and are consistent with the results reported in a previous MD study in which Frenkel pairs were randomly introduced into a simulation cell to surrogate radiation defect formation [2].

To confirm the validity of the present simulation results, the equilibrium concentration of deuterium in a system containing 1% vacancy was calculated under conditions of 673 K and 1 atm D_2 gas. To simplify the problem, all vacancies were assumed to be monovacancies. Subsequently, the calculated equilibrium concentration was compared with an experimental result of similar conditions [3], which showed reasonable agreement. The influence of radiation defects on the tritium retention will be discussed in the presentation, considering the large gap in the conditions between experiments and the present simulations (e.g., much higher defect formation rate, much shorter time in the phase of thermal defect evolution, etc, in MD, and ignoring the effect of defect clustering in the equilibrium concentration calculation).

[1] M.R. Gilbert et al., J. Nucl. Mater. 467 (2015) 121-134.
[2] P.M. Derlet and S.L. Dudarev, Phys. Rev. Mater. 4 (2020) 023605.
[3] Y. Hatano et al., Nucl. Fusion 53 (2013) 073006.