Multiscale Modeling of Neutron Irradiated Materials

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The reliability, safety and economics of advanced nuclear energy system are strongly dependent on the performance of materials under neutron irradiation. Due to the long-term and high-cost features of neutron experiments and even the la ck of a fusion-relevant neutron source, computer simulation as an indispensable and legitimate physical tool is of great importance to understand microstructure evolution and property degradation of materials under neutron irradiation. Because of the multiscale nature of neutron irradiation damage (from cascade collision to defect evolution and eventually macroscopic property variation), multiscale modelling approaches provide a significant pathway to study irradiation with different temporal and spatial domains. Herein, taking tungsten as a prototypical example, the recent progress will be reported in developing multi-scale modelling platform of materials under neutron irradiation, which we name as NINUM^3. The developed platform contains two comprehensive databases (i.e., defect property database & displacement cascade database) and a set of computational tools in the multiscale framework (i.e., object kinetic Monte Carlo and cluster dynamics for defect evolution simulation, and dislocation dynamics and crystalline plasticity finite element method for mechanical property calculation). Based on the NINUM^3 platform, we have investigated the microstructure evolution and hardness increase of tungsten under irradiation at different conditions, which are quantitatively consistent with the experimental results from HFIR and BR2 irradiation samples as well as ion implantation with a specific helium-dpa ratio, thus verifying the accuracy and reliability of the present platform. By employing the NINUM^3 platform, we explicitly reproduce the self-assembly process of neutron irradiation defects from chaotic distribution into void lattice, and further predict the irradiated microstructure and corresponding hardness increase/thermal conductivity decrease of tungsten under fusion neutron irradiation based on the neutron spectrum of CFETR.