The understanding of H/He irradiated in W by a multi-scale approach

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A sequential multi-scale approach combining Monte Carlo, Density functional theory/Molecular dynamics and Cluster dynamics (MC-DFT/MD-CD) has been developed to effectively couple atomic diffusion events with displacive and continuous processes at finite temperature, which enables us to investigate the large time and size scale behavior of the irradiated ions in nuclear device related materials. The evolution of different types of defects with time and depth is obtained. Specifically, the cases of H and He in tungsten are discussed in details, where the evolution of different types of defects with time and depth is investigated. The calculated results are comparable with experiments. The contribution to the ion concentration and the depth profile could provide the understanding on the dominated factors among the multi-micromechanisms such as trapping, diffusion, grain boundary and dislocation, etc., which is obviously important for estimating damages to the nuclear materials.

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