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Object Kinetic Monte Carlo Simulations of Annealing of Cascade Damage in Tungsten GIRIDHAR NANDIPATI, WAHYU SETYAWAN, HOWARD HEINISCH, RICHARD KURTZ, KENNETH ROCHE, Pacific Northwest National Lab, BRIAN ROCHE, University of Tennessee — Results are presented for a series of annealing simulations of displacement cascades in tungsten (W) using the kinetic Monte Carlo (KMC) code kSOME (kinetic simulation of microstructure evolution), which is our newly developed lattice-based Object KMC simulation code. In principle, kSOME can deal with migration, emission, transformation and recombination of all types of intrinsic point defects and their complexes. In addition, the interaction of these point defects with sinks such as dislocations, grain boundaries and free surfaces is also treated. We have studied the long-time annealing of displacement cascades in W obtained from molecular dynamics (MD) simulations. A database of displacement cascades in W was obtained using MD simulations for temperatures of 800-1300K and primary knock-on atom (PKA) energies in the range of 2 to 40 keV. The input data for the KMC simulations, such as activation energies for migration and dissociation of defects, and their capture radii were obtained from atomic-level calculations. The evolution of radiation damage was investigated as a function of time, temperature, dose and dose-rate. The results for W are compared with those for similar simulations of cascades in α -Fe.

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