

Long-term evolution of cascades in bcc tungsten: effects of size distribution of interstitial clusters

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Molecular dynamics (MD) cascade simulations of single crystal tungsten are carried out for two empirical potentials with cascade energies ranging from 0.1 keV to 100 keV at 300 K. The simulation results show that even though the defect production varies slightly for all cascade energies studied, these two empirical potentials produce very different results of interstitial clusters (ICs) size distribution and space distribution of defects with cascade energies larger than 30 keV. Meanwhile, object kinetic Monte Carlo (OKMC) is used to model a single cascade annealing process based on the primary damage database from the MD simulation. Our results demonstrate that due to the difference of ICs size distribution and space distribution of defects between these two potentials, the annealing efficiency of a single cascade varies greatly with cascade energies larger than 30 keV.