Modeling and simulations of irradiation induced void superlattices

Yipeng Gao, Yongfeng Zhang, Jian Gan

Idaho National Laboratory, 2525 Fremont Avenue, Idaho Falls, ID 83415

The formation and self-organization of voids and gas bubbles under irradiation is a unique dynamic phenomenon, which affects the swelling behavior and mechanical stability of nuclear materials. We develop a rate-theory based phase field model to investigate the formation mechanism of void superlattices, and associated material properties under different irradiation conditions. The superlattices are found to the result of thermodynamic instability and kinetic anisotropy, both of which determine the characteristic symmetry and wavelength of the superlattices. In particular, the symmetry of a superlattice is dictated by the anisotropic diffusion of interstitial atoms, affected by the short range reaction between voids and interstitials under irradiation. Systematic analyses on the symmetry selection of void superlattices are performed for different materials and under different irradiation conditions. Our study provides a new insight into the formation mechanism of superlattices, which can be utilized to guide experimental design for tailored microstructure under irradiation.