

MD AND KMC MODELING OF THE GROWTH AND SHRINKAGE MECHANISMS OF HELIUM-VACANCY COMPLEXES IN FE—K. Morishita, R. Sugano (Institute for Advanced Energy, Kyoto University), and B. D. Wirth (Department of Nuclear Engineering, University of California Berkeley)

EXTENDED ABSTRACT

A multiscale modeling approach, which is based on atomistic simulations, was applied to investigate the growth and shrinkage mechanisms of helium–vacancy (He–V) clusters in Fe. Molecular dynamics (MD) simulations with empirical interatomic potentials were used to determine energies for the formation and dissociation of clusters as a function of their size and He density. Both the number of He atoms and vacancies in a cluster ranged from 0 to 20. The dissociation energy of clusters showed a strong dependence on the He density, rather than the cluster size, indicating that the growth and shrinkage of clusters strongly depend on the He density.

A kinetic Monte Carlo (KMC) model has been developed to simulate the long-time cluster behavior, using the binding and dissociation energies obtained from MD. The KMC simulations indicated that He stabilizes He–V clusters by suppressing thermal vacancy emission and by promoting thermal self-interstitial Fe atom emission. A preliminary KMC simulation to investigate the migration behavior of He–V clusters is also presented. The diffusion of a He–V cluster depends on the size and lifetime of the cluster, and therefore depends on the He density and cluster size.

Reference

K. Morishita, R. Sugano, and B. D. Wirth, *Journal of Nuclear Materials* 323 (2003) 243.