MD STUDY OF SELF-IRRADIATION EFFECTS ON DISLOCATION DYNAMICS IN δ-Pu

A.V. Karavaev, V.V. Dremov, G.V. Ionov
Russian Federal Nuclear Center – Zababakhin Institute of Technical Physics (RFNC-VNIITF)
Snezhinsk, Russia (a.v.karavayev@vniitf.ru, a.v.karavaev@gmail.com)

Self-irradiation of fissile materials such as plutonium and its alloys continuously produces primary radiation defects and decay products, for example, radiogenic helium, which tend to accumulate, migrate through the lattice, form clusters, and so on. The microstructure of the point defects greatly influences the material mechanical properties. Within Molecular Dynamics we investigate equilibrium thermodynamics of radiation defect clusters using Thermodynamic Integration Method. We study how radiogenic helium behaves in fcc Pu-Ga alloys and determine the equilibrium parameters of helium bubbles which agree well with experimental data. We also study the behavior of clustered primary radiation defects in Pu-Ga alloys and obtained their equilibrium parameters. Using stress relaxation method, we investigate dislocation dynamics under shear stresses down to strain rates close to zero. We evaluate Peierls stress and quasi-static elastic-plastic material properties. Simulations are performed both in the absence of other defects, and in the presence of radiation defects of different morphology. Nanometer helium bubbles are shown to cause dislocation pinning which causes the increase of the yield stress. Our quantitative estimates for the effect of aging on the static yield stress agree well with experiment. The developed techniques may be extended to other materials for predicting their behavior under irradiation.