Glenn T. Seaborg Center Seminar

Understanding the Atomic-Scale Aspects of Radiation Damage and Aging in Pu and Pu/Ga Alloys through Computer Simulations

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The aging of plutonium and the subsequent possible implications to stockpile has been an area of intense interest and study in the past decade. In this talk, I will focus on very recent work aimed at understanding fundamental aspects of radiation damage production and annealing through the use of very large-scale classical molecular dynamics simulations. Because Pu and Pu/Ga alloys are complex materials with intricate phase diagrams, atomistic simulations require the computationally expensive interatomic potentials (Modified Embedded Atom Method) developed by Michael Baskes and Steven Valone at LANL, to capture many of the intricacies of the relative free energies of the different states of the material. With these simulations, performed in collaboration with LANL, on very large supercomputers including LLNL BlueGene/L and Sandia RedStorm, it has been possible to examine the structures and details of the damage and damage evolution from energetic recoils up to 85 keV in energy, associated with natural alpha-decay in Plutonium. Our studies indicate the initial generation of a glassy-state in the Pu and Pu/Ga alloys, followed by a very slow annealing, resulting in an "un-classical" structure of self-interstitial defects surrounding a vacancy defect cloud, which further surrounds a self-interstitial defect cluster. Much of these findings can be described in terms of phase stability and the relative free energy of the fcc phase versus a disordered amorphous phase.

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