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Combining DFT, Cluster Expansions, and KMC to Model Point Defects in Alloys[1] N. A. MODINE, A. F. WRIGHT, S. R. LEE, S. M. FOILES, C. C. BATTAILE, Sandia National Laboratories, J. C. THOMAS, A. VAN DER VEN, University of California, Santa Barbara — In an alloy, defect energies are sensitive to the occupations of nearby atomic sites, which leads to a distribution of defect properties. When radiation-induced defects diffuse from their initially non-equilibrium locations, this distribution becomes time-dependent. The defects can become trapped in energetically favorable regions of the alloy leading to a diffusion rate that slows dramatically with time. Density Functional Theory (DFT) allows the accurate determination of ground state and transition state energies for a defect in a particular alloy environment but requires thousands of processing hours for each such calculation. Kinetic Monte-Carlo (KMC) can be used to model defect diffusion and the changing distribution of defect properties but requires energy evaluations for millions of local environments. We have used the Cluster Expansion (CE) formalism to "glue" together these seemingly incompatible methods. The occupation of each alloy site is represented by an Ising-like variable, and products of these variables are used to expand quantities of interest. Once a CE is fit to a training set of DFT energies, it allows very rapid evaluation of the energy for an arbitrary configuration, while maintaining the accuracy of the underlying DFT calculations. These energy evaluations are then used to drive our KMC simulations. We will demonstrate the application of our DFT/MC/KMC approach to model thermal and carrier-induced diffusion of intrinsic point defects in III-V alloys.

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Normand Modine
Sandia National Laboratories

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