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Thermodynamics of point defects in deformable lattices ROMAN GROGER, LIBOR SMEJKAL, Institute of Physics of Materials, Academy of Sciences of the Czech Republic, TURAB LOOKMAN, Theoretical Division, Los Alamos National Laboratory, USA — We develop a mean-field model that can be used to study the evolution of microstructure and the density of point defects in irradiated materials. Within this model, the lattice is viewed as an elastic template that is distorted by point defects. The stresses that each defect exerts on its immediate neighborhood in the lattice are represented by its elastic dipole tensor. The lattice responds to these stresses by developing long-range strains that mediate interactions between spatially separated defects. Nonlocal (gradient) elasticity is used to describe the elastic strain energy of the distorted lattice. This gives rise to the gradients of strain in the free energy and ensures an accurate representation of the phonon dispersion curves. In order to demonstrate this model, we consider a cubic lattice with a given density of randomly distributed vacancies and $\langle 100 \rangle$ split interstitials (dumbbells). The occupation of each cell is described by a "spin" with the states {ideal lattice, vacancy, and the three orientations of the $\langle 100 \rangle$ dumbbell}. The evolution of this spin field is obtained by the Monte Carlo (Metropolis) method, with the free energy calculated for each state of the system as described above. Double spin-flip mechanism is adopted to conserve the total mass of the system.

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