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Statistical models for the microstructural evolution in irradiated metals and alloys DAVID J. SROLOVITZ, JOERG ROTTLER, ROBERTO CAR, Princeton Inst. for the Science and Tech. of Materials, Princeton University, Princeton NJ 08544 — The macroscopic mechanical properties of metals are intimately related to their microstructural features and their spatiotemporal evolution. We discuss a simplified statistical model for the dynamics of point defects in bcc metals that is solved through kinetic Monte Carlo (kMC) and rate equations. Self-interstitial atoms and vacancies can be produced in abundance upon irradiation with energetic particles, but they subsequently anneal due to recombination and absorption at sinks such as dislocations and grain boundaries. The model reveals a sequence of kinetic regimes that lead to a final steady state and allows us to study the size distribution of voids that form when vacancies aggregate into cluster. Here we focus on random alloys, where the point defect diffusivities are modified due to the presence of multiple exchange frenquencies. In addition, complex dealloying processes occur at sinks if the alloy components diffuse preferentially through one diffusion mechanism (self-interstitial or vacany exchange) only. We illuminate these effects with a generic kMC/rate equation model for binary alloys.

Joerg Rottler
Princeton University

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