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ABSTRACT

Diffusion and phase transformations in far-from-equilibrium alloys: The case of irradiated metals in nuclear reactors

The excess of lattice point defects in many driven systems—such as materials subjected to thermal quenching, corrosive environments, severe mechanical stress, or irradiation—acts as the primary driving force governing steady states and their deviation from equilibrium. For instance, the long-term evolution of Frenkel pairs (vacancies and self-interstitial atoms) formed during primary radiation damage can lead to non-equilibrium segregation at extended defects and unexpected phase transformations.

Using irradiation as an example, we will present an overview of the multiscale approaches currently employed to model the evolution of metallic alloy microstructures in systems far from equilibrium. These approaches span multiple length and time scales, starting with the atomic-scale processes of point defect creation, migration, and annihilation, and extending to long-range diffusion, which drives the formation of point defect clusters such as voids, dislocation loops, and the precipitation of stable or metastable secondary phases. Moreover, sustained fluxes of point defects toward extended microstructural defects can induce localized solute redistributions at these defect sinks, a phenomenon known as radiation-induced segregation. To model these phenomena, a detailed description of the kinetic flux couplings between atoms and point defects, along with the changes in thermodynamic driving forces induced by a-thermal events—such as the generation of lattice point defects—is essential.

We demonstrate how to use our diffusion code KineCluE to compute the kinetic flux couplings [1] an d our recent development of statistical physics methods to compute free energies and equilibrium c oncentrations of point defects [2] directly from *ab initio* studies of randomly sampled solid solutions. We then introduce the concept of semi-coherent phase diagram, incorporating point defect supersat uration as an additional axis [3]. The resulting simulations will be compared with nano-scale experim ental characterizations of Fe-based model alloys.

[1] T. Schuler, L. Messina and Maylise Nastar, Com. Mat. Sc., 172 (2020) 109191.
[2] K. Li, T. Schuler, C-C Fu and Maylise Nastar, Acta Mat., 281 (2024) 120355.
[3] M. Nastar, L. Belkacemi, E. Meslin and M. Loyer-Prost., Commun. Materials 2 (2021), 32.