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K-ART study of defect evolution on experimental time scales in bcc iron and Cu–Zr interfaces PETER BROMMER, NORMAND MOUSSEAU, Département de physique, Université de Montréal, Québec, Canada — Defects in metals are challenging to study in linear simulation schemes like molecular dynamics (MD), as diffusive activation barriers are typically high compared to k_BT, and most ressources are devoted to integrating out thermal vibration. Simultaneously, low-energy non-diffusive rearrangements (so-called basins) are serious obstacles for methods that use state-to-state trajectories like kinetic Monte Carlo (KMC). We combined the kinetic Activation-Relaxation technique (k-ART, [1]), an off-lattice, self-learning KMC method which correctly reproduces long-range interactions, with an autonomous basin identification scheme that averages over all in-basin transitions. This allows us to study defect evolution on much longer time scales than MD. In this talk, we present results on the vacancy cluster formation in bcc iron and interface diffusion in the Cu–Zr system.

[1] Béland, Brommer, *et al.*, *Phys. Rev. E*, **84**, 046704 (2011).

Peter Brommer
Département de physique, Université de Montréal, Québec, Canada

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