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An efficient method to treat low barriers in kinetic ART simulations PETER BROMMER, NORMAND MOUSSEAU, Département de physique, Université de Montréal, Québec, Canada — In kinetic Monte Carlo (KMC) the time scale of the simulation is dominated by the height of the lowest energy barrier separating two states. Rapid back-and-forth movements across very low barriers called flickers are a major limitation of the technique, as they can cost considerable CPU time without advancing the simulation. To accelerate KMC simulations, an energy basin finding algorithm has been presented [1]. In the kinetic Activation-Relaxation technique (kART) [2], KMC events are constructed during the simulation, taking full care of elastic deformations while avoiding the need for complete event search at every step. To account for low energy barriers located in this package, we implement a basin identification scheme that works on the fly as well. We apply this method to interstitial diffusion in bcc iron. There, rapid diffusion paths with low barriers for properly aligned interstitial clusters limit the simulated time. With our method, we can prevent unproductive oscillations in this diffusive basin while maintaining an appropriate distribution of exit states. This considerably extends the time scales accessible to simulation.
[1] Puchala *et al.*, *J. Chem. Phys.* **132**, 134104 (2010)
[2] El-Mellouhi *et al.*, *Phys. Rev. B*, **78**, 153202 (2008).

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

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