

Abstract Submitted  
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**Long-time atomistic evolution of grain boundary in nickel using the kinetic activation-relaxation technique** SAMI MAHMOUD, MICKAL TROCHET, OSCAR RESTREPO, NORMAND MOUSSEAU, University of Montreal — The microscopic mechanisms associated with the evolution of metallic materials are still a matter of debate as both experimental and numerical approaches fail to provide a detailed atomic picture of their time evolution. Here, we use the kinetic activation-relaxation technique (k-ART) [1], an unbiased off-lattice kinetic Monte Carlo method with on-the-fly catalog building to overcome these limitations and follow the atomistic evolution of a 10.000-atom grain boundary Ni system over macroscopic time scales. We first characterize the kinetic properties of four different empirical potentials, the embedded atom method (EAM), the first and second modified embedded atom method (MEAM1NN and MEAM2NN respectively) and the Reax force field (ReaxFF) potentials. Comparing the energetics, the elastic effects and the diffusion mechanisms for systems with one to three vacancies and one to three self-interstitials in nickel simulated over second time scale, we conclude that ReaxFF and EAM potentials are closest to experimental values. We then proceed to study the long-time evolution of a grain boundary with the Reax forcefield and to offer a detailed description of its energy landscape, including the exact description of short and long-range effects on self-diffusion along the interface. [1] N. Mousseau *et al*, *Comput. Mater. Sci.*, vol. 100, pp. 111–123, 2015.

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