

Abstract Submitted
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Large scale application of kinetic ART, a near order-1 topologically- based off-lattice kinetic Monte-Carlo algorithm with on-the-fly calculation of events LAURENT KARIM BELAND, FEDWA ELMELLOUHI, NORMAND MOUSSEAU, Dept de physique, Universite de Montreal — Using a topological classification of events¹ combined with the Activation-Relaxation Technique (ART nouveau) for the generation of diffusion pathways, the kinetic ART (k-ART)² lifts many restrictions generally associated with standard kinetic Monte Carlo algorithms. In particular, it can treat on and off-lattice atomic positions and handles exactly long-range elastic deformation. Here we introduce a set of modifications to k-ART that reduce the computational cost of the algorithm to near order 1 and show applications of the algorithm to the diffusion of vacancy and interstitial complexes in large models of crystalline Si (100 000 atoms).

¹B. D. McKay, Congressus Numerantium 30, 45 (1981).

²F. El-Mellouhi, N. Mousseau and L. J. Lewis, Phys Rev B, 78,15 (2008).

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