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Characterization of the relation between energy landscape and the time evolution of complex materials using kinetic ART KOKOU GAWONOU N'TSOUAGLO, JEAN-FRANCOIS JOLY, LAURENT KARIM BELAND, Departement de Physique, Universite de Montreal, PETER BROMMER, Department of Physics and Centre for Scientific Computing, University of Warwick, NORMAND MOUSSEAU, Departement de Physique, Universite de Montreal —
In the last two decades, there has been a considerable interest in the development of accelerated numerical methods for sampling the energy landscape of complex materials. Many of these methods are based on the kinetic Monte Carlo (KMC) algorithm introduced 40 years ago. This is the case of kinetic ART, for example, which uses a very efficient transition-state searching method, ART nouveau, coupled with a topological tool, NAUTY, to offer an off-lattice KMC method with on-the-fly catalog building to study complex systems, such as ion-bombarded and amorphous materials, on timescales of a second or more. Looking at two systems, vacancy aggregation in Fe and energy relaxation in ion-bombarded c-Si, we characterize the changes in the energy landscape and the relation to its time evolution with kinetic ART and its correspondence with the well-known Bell-Evans-Polanyi principle used in chemistry.

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