MAR12-2011-002320

Abstract for an Invited Paper
for the MAR12 Meeting of
the American Physical Society

The kinetic activation-relaxation technique: an off-lattice, self-learning kinetic Monte Carlo algorithm with on-the-fly event search[1]

NOMAND MOUSSEAU, Université de Montréal

While kinetic Monte Carlo algorithm has been proposed almost 40 years ago, its application in materials science has been mostly limited to lattice-based motion due to the difficulties associated with identifying new events and building usable catalogs when atoms moved into off-lattice position. Here, I present the kinetic activation-relaxation technique (kinetic ART) is an off-lattice, self-learning kinetic Monte Carlo algorithm with on-the-fly event search [1]. It combines ART nouveau [2], a very efficient unbiased open-ended activated method for finding transition states, with a topological classification [3] that allows a discrete cataloguing of local environments in complex systems, including disordered materials. In kinetic ART, local topologies are first identified for all atoms in a system. ART nouveau event searches are then launched for new topologies, building an extensive catalog of barriers and events. Next, all low energy events are fully reconstructed and relaxed, allowing to take complete account of elastic effects in the system's kinetics. Using standard kinetic Monte Carlo, the clock is brought forward and an event is then selected and applied before a new search for topologies is launched. In addition to presenting the various elements of the algorithm, I will discuss three recent applications to ion-bombarded silicon, defect diffusion in Fe and structural relaxation in amorphous silicon.

This work was done in collaboration with Laurent Karim Béland, Peter Brommer, Fedwa El-Mellouhi, Jean-François Joly and Laurent Lewis.

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[1]This work was supported by the FQRNT (Quebec), NSERC (Canada) and the Canada Research Chair Foundation.