Abstract Submitted
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The dynamical activation-relaxation technique (DART): an on-the-fly kinetic Monte-Carlo algorithm[1] FADWA EL-MELLOUHI, MICHEL COTE, LAURENT J. LEWIS, NORMAND MOUSSEAU, Dep. de physique and RQMP, Univ. de Montreal, Quebec, Canada — We present DART, the dynamical activation-relaxation technique, that combines the activation-relaxation technique (ART nouveau) with a non-lattice KMC method that allows the on-the-fly identification of barriers and the full treatment of lattice deformations. Most KMC schemes rely on the use of a fixed list of events and barriers, which are drawn with the proper weight during the simulation. While this works well for a number of problems (such as metal-on-metal growth), it cannot be used for processes where the events may change with time. DART overcomes this limitation. ART nouveau has been used extensively for the study of activated mechanisms in different materials within both an empirical and an ab-initio description of the systems. In the DART implementation, KMC moves are based on a catalog of events constructed on-the-fly using ART. After each KMC move, this catalog is updated so as to take into account new environments that may appear. A topological description of the structure of the system at each moment allows the method to identify rapidly these new environments and to move forward efficiently. In this talk, we will describe the method and present the case of interstitial diffusion in Si. Our results are compared with previous molecular-dynamics and on-lattice KMC simulations.

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