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Simulation of Impurity Diffusion in a Strained Nanowire Using Off-Lattice KMC

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Abstract. Kinetic Monte Carlo (KMC) is a stochastic model used to simulate crystal growth. However, most KMC models rely on a pre-defined lattice that neglects dislocations, lattice mismatch and strain effects. In this paper, we investigate the use of a 3D off-lattice KMC algorithm. We test this method by investigating impurity diffusion in a strained FCC nanowire. While faster than a molecular dynamics simulation, the most general implementation of off-lattice KMC is much slower than a lattice-based algorithm. An improved procedure is achieved for weakly strained systems by pre-computing approximate saddle point locations based on unstrained lattice structures. In this way, one gives up some of the flexibility of the general method to restore some of the computational speed of lattice-based KMC. In addition to providing an alternative approach to nano-materials simulation, this type of simulation will be useful for testing and calibrating methods that seek to parameterize the variation in the transition rates for lattice-based KMC using continuum modeling.

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1 Introduction

Kinetic Monte Carlo (KMC) is a stochastic model that simulates the atomic details of crystal growth and evolution using probabilistic rules to govern deposition, diffusion and other transition processes [1]. This technique was first adopted in the early 1970s [2, 3] and had found many uses in surface diffusion on adsorbed mono layers [4], growth of

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polymer crystals [5] and self-organized nanowires [6]. In contrast to the thermodynamic Monte Carlo methods, which aimed at predicting the equilibrium state of molecular systems, KMC seeks to provide information about a system's evolution. In KMC, transition rates between states depend on both the energy of the configuration before hopping, as it would be in other Monte Carlo techniques, and on the energy barrier between the states [7]. The aim of this method is to identify a significant set of possible events to describe the general behavior of evolution processes and to find the energy barrier between the saddle point and local minima for each of these. The principal KMC algorithm is based on the method of Bortz, Kalos and Lebowitz [8] (BKL), which will be introduced in Section 2.

In KMC, all lattice points, energy barriers and diffusion rates are normally defined before computation begins. As a consequence, dislocations, lattice mismatch and strain effects are neglected. A molecular dynamics (MD) simulation can be used for off-lattice simulation, however, it is limited to a time scale on the order of 10^{-6} seconds or less. An off-lattice KMC (OLKMC) simulation can be used for longer simulations while taking into account some elastic effects. Off-lattice KMC will also be useful for testing and calibrating other macroscopic tools, such as schemes that aim to combine continuum modeling with KMC.

Off-lattice simulations themselves can be implemented in a number of ways, with the usual tradeoff between faithful representation of the physical processes and computational speed. At one extreme, Jonsson *et al.* [9] have implemented a method that uses harmonic transition state theory (TST), described below, to estimate transition rates between local minima for the energy landscape in the full n-particle configuration space. Further, they make no assumptions about the approximate location of the saddle points separating two energy minima. This represents the most computationally intensive version of OLKMC, where random initial guesses must be used to locate transition points. In this method, locating the set of transition points is the most costly part of the algorithm. Even with parallel implementation this type of calculation is presently limited to a few hundred atoms or less.

An approach which is less computationally intensive, but less accurate, is found in the work of Much *et al.* [10, 11] in which an OLKMC algorithm has been developed to simulate the early stage of heteroepitaxial growth for adsorbate layers. A simple *Lennard-Jones* potential is employed in their simulation. The transition points are sought in a "frozen crystal" approximation where only a single atom is moved within the configuration space in order to locate approximate saddle points. This method has been used to simulate surface diffusion during "1+1"-dimensional epitaxial growth and submonolayer "2+1"-dimensional growth growth. The resulting simulation is considerably fast, but still does not approach the computational speed of latticed based simulation and the saddle point problem is again the most intensive part of the algorithm.

Still another approach to incorporating elastic effects into KMC can be found in the works [12–14]. These authors use a model where the transition rate is approximated by using only the binding site energy. The atoms interact through a nearest neighbor net-