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Simulation of Three-Dimensional Strained Heteroepitaxial Growth Using Kinetic Monte Carlo

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Abstract. Efficient algorithms for the simulation of strained heteroepitaxial growth with intermixing in 2+1 dimensions are presented. The first of these algorithms is an extension of the energy localization method [T. P. Schulze and P. Smereka, An energy localization principle and its application to fast kinetic Monte Carlo simulation of heteroepitaxial growth, J. Mech. Phys. Sol., 3 (2009), 521–538] from 1+1 to 2+1 dimensions. Two approximations of this basic algorithm are then introduced, one of which treats adatoms in a more efficient manner, while the other makes use of an approximation of the change in elastic energy in terms of local elastic energy density. In both cases, it is demonstrated that a reasonable level of fidelity is achieved. Results are presented showing how the film morphology is affected by misfit and deposition rate. In addition, simulations of stacked quantum dots are also presented.

AMS subject classifications: 82B80, 82B21, 82D25, 65C05

Key words: Heteroepitaxy, strained thin film, kinetic Monte Carlo.

1 Introduction

The computational cost of simulating heteroepitaxial growth with misfit strain using kinetic Monte Carlo (KMC) is orders of magnitude greater than that for strain-free growth due to the need to update the long-range elastic deformation of the film as the simulation proceeds. Until recently, this has prevented the widespread use of KMC for such simulations, especially in 2+1 dimensions. In this paper, we extend, from 1+1 to 2+1 dimensions, methods introduced in earlier work [1, 22], refine somewhat a key result upon which those methods are based, and introduce new approximations to further enhance computational performance.

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The rationale for KMC simulations aimed at understanding the growth and relaxation of crystals is based on molecular dynamics (MD) simulations and transition state theory. The essence of this model is that the system spends most of its time randomly oscillating within the N-particle configuration space about a local minimizer $x_m \in \mathbb{R}^{3N}$ of the system potential energy, $U(x)$, with rare transitions between these basins of attraction. The harmonic approximation to transition state theory estimates the rate $r_{a\to b}$ at which the transition occurs as

$$r_{a\to b} = K\exp\Big(-\frac{\Delta U}{k_B T}\Big), \tag{1.1}$$

where ΔU is the minimum energy barrier that must be overcome in moving from the initial, locally minimizing configuration, x_a, to a neighboring one, x_b, in configuration space, K is a weakly temperature-dependent oscillation "frequency" and $k_B T$ is an energy scale defined by the temperature of the film.

These observations suggest an alternative model where the Newtonian dynamics is replaced by a continuous time Markov-chain, with the system making relatively rare, random transitions between states that represent local minimizers, x_a, in the system's configuration space at rates $r_{a\to b}$ calculated from (1.1). More specifically, the energy barrier

$$\Delta U = U(x_s) - U(x_a), \tag{1.2}$$

requires locating both the initial local minimum, x_a, and the saddle point, x_s (where $\nabla U = 0$ and all but one of the principal curvatures are positive), separating the basins of attraction. Note that these local minima and saddle points are, in principle, determined by the motion of all of the particles simultaneously within the configuration space. When this sort of scheme is carried out in detail, it is referred to as off-lattice KMC or on-the-fly KMC [2, 6, 7]. While this is much faster than the corresponding MD simulation, or even accelerated MD simulations based on similar considerations [21, 24], it is still prohibitively expensive in that one could not hope to simulate the growth of a crystal on physically relevant space and time scales.

For single-crystal, homoepitaxial systems, an often-used and greatly simplified model immediately suggests itself. In the simplified approach, the states are approximated using occupation arrays structured in the form of a perfect lattice-most often simple cubic, but face centered cubic and other lattices are also used; the allowed transitions are restricted to a limited catalog of characteristic events (e.g., single particle moves to neighboring sites); and the transition rates are parameterized based on the local lattice configuration. Indeed, it is this type of model that people generally refer to when they speak of KMC.

A well known example is nearest-neighbor, bond-counting KMC. In this model, atoms are restricted to positions on a simple cubic lattice, and the surface of the film, $h_{ij} \in \mathbb{Z}$, is often assumed single valued (the solid-on-solid assumption). Only surface atoms can move, and they move by hopping to a randomly chosen neighboring site in one of the four orthogonal directions. The hopping rate for the surface atom at site (i,j) is taken to