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The island dynamics model on parallel quadtree grids

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ABSTRACT

We introduce an approach for simulating epitaxial growth by use of an island dynamics model on a forest of quadtree grids, and in a parallel environment. To this end, we use a parallel framework introduced in the context of the level-set method. This framework utilizes: discretizations that achieve a second-order accurate level-set method on non-graded adaptive Cartesian grids for solving the associated free boundary value problem for surface diffusion; and an established library for the partitioning of the grid. We consider the cases with: irreversible aggregation, which amounts to applying Dirichlet boundary conditions at the island boundary; and an asymmetric (Ehrlich–Schwoebel) energy barrier for attachment/detachment of atoms at the island boundary, which entails the use of a Robin boundary condition. We provide the scaling analyses performed on the Stampede supercomputer and numerical examples that illustrate the capability of our methodology to efficiently simulate different aspects of epitaxial growth. The combination of adaptivity and parallelism in our approach enables simulations that are several orders of magnitude faster than those reported in the recent literature and, thus, provides a viable framework for the systematic study of mound formation on crystal surfaces.

1. Introduction

Epitaxial growth is a complex, multiscale process in which a material is deposited on top of another one and takes on the crystalline orientation of the substrate. The growth process results in the formation and evolution of islands and steps [23,38], which accompany the fabrication of many modern opto-electronic devices below the roughening transition. Hence, epitaxial growth is of fundamental technological importance. Notable examples of related devices include transistors in microelectronics, quantum dots for photonic-crystal lasers, quantum dot-based enhancements in the energy sector, and devices for nonvolatile storage which is sought to replace hard drives, flash and RAM memories. Other applications of epitaxial growth include catalysts, which are used, e.g., in the energy sector, food processing, and environmental science.

In this paper, we introduce a computational approach for the simulation of island evolution in large epitaxial systems. Our main motivation is the need to make accurate predictions for the formation of crystal surface features, e.g. mounds, at large scales. We start with the island dynamics model (IDM) by Caflisch et al. [8,40]. This description relies on the for-

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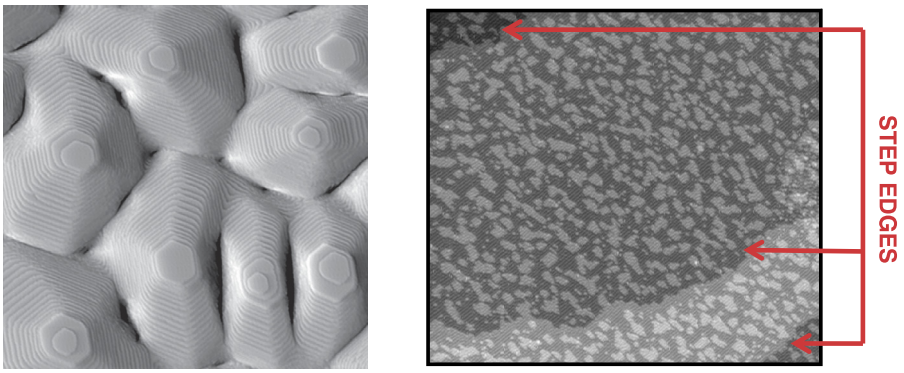

Fig. 1. Single-Tunneling-Microscope (STM) images of epitaxially grown thin films where macroscopic or mesoscale features may develop, e.g., mounds (left image from [24]) and step edges (right image from [4]).

mulation of a free boundary value problem, in the spirit of the Burton–Cabrera–Frank (BCF) theory [7]. The model has the following main elements: (i) a diffusion-type equation for the density of adsorbed atoms (adatoms) in the region (terrace) between successive steps, which includes nucleation in a mean-field sense; (ii) Dirichlet or Robin boundary conditions for the adatom density at the island boundaries; and (iii) a kinetic law for the normal velocity of each boundary by mass conservation. We numerically solve this system on a forest of quadtree grids, and in a parallel environment by using the framework introduced in the context of the level-set method by Mirzadeh et al. [32]. This framework utilizes the discretizations of Min and Gibou [30] for the associated free boundary value problem, and the `p4est` library of Burstedde et al. [6] for the partitioning of the grid. We apply our approach to the growth of mounds in *homoepitaxy*, where the deposited material is the same as the substrate.

From a physical viewpoint, basic processes that occur during epitaxial growth include the nucleation, growth, and coalescence of two-dimensional islands. Close to thermodynamic equilibrium, homoepitaxial growth proceeds atomic layer by atomic layer. However, growth is far from equilibrium for many homoepitaxial systems, and, therefore, the observed surface morphology is a result of kinetic limitations. In particular, multilayer growth may become unstable and, hence, mounds may form. This phenomenon has been observed experimentally for many epitaxial systems such as surfaces of Cu [17,55], Fe [47], Ag [53] or Pt [5].

The microscopic process that usually underlies mound formation is an additional (Ehrlich–Schwoebel, ES) energy barrier characterizing the attachment/detachment of atoms at island boundaries or edges of steps [16,44]. For some applications, these mounds can seriously degrade the performance of the device being grown; for example, in the case of metallic films the electric connections between layers can be hampered [49]. In contrast, in some other cases these mounds can be regarded as almost zero-dimensional defects with novel properties that can be exploited in the laboratory setting [54]. An example of such mounds which form for growth of Pt on Pt(111) is shown in Fig. 1 [left panel]. In the suitable kinetic regime of these systems, step edges with interesting dynamics are evident (see Fig. 1 [right panel]).

Hence, the understanding and control of crystal surface instabilities that lead to mound formation are significant goals in materials science. Accordingly, the development of computational methods that accurately and efficiently describe the growth of thin films has been the focus of intensive research [25,1,28,9]. Computational challenges in this direction are primarily due to the multiscale nature of epitaxial growth: On the one hand, growth of islands and the flow of steps is determined by the diffusion (and attachment) of individual adatoms, which sets time and length scales of the order of 10^{-6} sec and Ångstroms. On the other hand, typical devices can be microns in lateral size (and hundreds of layers thick), and are grown at timescales that are seconds or minutes.

To develop a computational approach faithful to the multiscale character of epitaxial growth, we use the IDM and a level-set method for its simulation [8,14,39,33,20,52,40]. The model has the mesoscale features of the BCF theory for steps [7], namely, coarse-graining of the atomistic dynamics in the lateral (parallel to a fixed reference plane) directions and retainment of atomistic detail in the growth direction; thus, the model is particularly well-suited for simulating epitaxial growth. Yet, this model has so far only used uniform grids on sequential machines.

In the present paper, we overcome this limitation via an approach that uses adaptive mesh refinement techniques and parallel strategies to significantly increase the size of systems that can be considered, as well as to offer a significant simulation speedup. To validate our computational approach, we carry out a series of numerical experiments associated with mound formation. In these examples, we invoke irreversible aggregation, which corresponds to a Dirichlet condition in the IDM; and an ES barrier which is modeled through a Robin condition at the step edge.

Section 2 provides an overview of the IDM (Section 2.1), and describes the multi-level-set representation for the motion of island boundaries (Section 2.2). Section 3 details the parallel strategy and the discretization algorithms for the simulation of multi-layer growth and dynamics of step edges. In Section 4 we present numerical examples that serve the validation of our computational approach. Section 5 concludes our paper with a summary of our framework and an outline of related, open problems.