Available at
www.ElsevierMathematics.com
POWERED BY SCIENCE DIRECT®
Applied Mathematics Letters 16 (2003) 1165–1170
Applied Mathematics Letters
www.elsevier.com/locate/aml

Multiple Domain Dynamics Simulated with Coupled Level Sets

C. RATSCH, C. ANDERSON AND R. E. CAFLISCH
Institute for Pure and Applied Mathematics, UCLA
Los Angeles, CA 90095, U.S.A.
and
Department of Mathematics, UCLA
Los Angeles, CA 90095, U.S.A.

L. FEIGENBAUM, D. SHAEVITZ, M. SHEFFLER AND C. TIEE
Institute for Pure and Applied Mathematics, UCLA
Los Angeles, CA 90095, U.S.A.

(Received and accepted March 2003)

Communicated by J. R. Ockendon

Abstract—We adapt the level-set method to simulate epitaxial growth of thin films on a surface that consists of different reconstruction domains. Both the island boundaries and the boundaries of the reconstruction domains are described by different level-set functions. A formalism of coupled level-set functions that describe entirely different physical properties is introduced, where the velocity of each level-set function is determined by the value of the other level-set functions.

Keywords—Level set, Island dynamics, Epitaxial growth, Surface reconstructions.

1. INTRODUCTION

Epitaxial growth is the growth of a thin film as a single crystal which is in registry with the underlying substrate. For many of the most demanding applications, molecular beam epitaxy (MBE) is the growth technique that allows the highest degree of control of the surface and interface morphology. In specific applications, such as quantum well devices, morphological features at the surface or at the interface between different layers can strongly influence system performance. It is therefore desirable to have theoretical models that can predict reliably the growth morphology of a growing film.

Because of the wide range of length and time scales, modeling and simulation of growth must be performed at several different levels. An atomic-level stochastic simulation technique often

This research was part of the NSF-sponsored program "Research in Industrial Projects for Students" at the Institute for Pure and Applied Mathematics at UCLA. We also acknowledge support from the NSF focused research group Grant DMS-0074152. We would like to thank M. Gyure and S. Osher for stimulating discussions.

0893-9659/03/$ - see front matter Typeset by AMS-TEX
doi: 10.1016/S0893-9659(03)00173-3

used to model epitaxial growth is kinetic Monte Carlo (KMC). However, realistic KMC models that include the relevant atomistic details are often prohibitively slow because of the wide range of rates of the microscopic processes. To go beyond the atomic level, we have developed an island dynamics model and a level-set method for its simulation [1–4]. This model allows us to include fast events without having to resolve each individual event explicitly [5]. It is the purpose of this letter to describe an extension of this model that allows us to include the surface chemistry without going explicitly to an atomistic resolution.

1.1. Level-Set Methods for Moving Interfaces

The level-set method is a numerical technique for computing interface motion in continuum models [6]. The essential idea of the method is to represent the interface as a level set of a *smooth* function, $\phi(\mathbf{x})$; for example, the set of points where $\phi = 0$. If the known interface velocity is not smoothly defined off the interface, we define a smooth extension, $\mathbf{v}(\mathbf{x})$, to all of the domain. Then, the interface motion is captured simply by convecting the values of the smooth function ϕ with the smooth velocity field $\mathbf{v}$. Numerically, this is accomplished on a fixed, regular spatial grid by solving the convection equation

$$\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = 0. \tag{1}$$

Note that since the boundary Γ consists of level sets of ϕ, and v is the normal velocity, then $\mathbf{v} \cdot \nabla \phi = v|\nabla \phi|$.

1.2. The Uniform Density Model for Island Dynamics

We implemented and applied an island dynamics model for MBE and a level-set method for its numerical simulation [2,3]. Here, the island boundaries Γ_k for islands of height k are described as

$$\Gamma_k = \{\mathbf{x} : \phi(\mathbf{x}) = k\}. \tag{2}$$

All the physical information enters into the normal velocity v. If we denote ρ as the (spatially constant) adatom density, N as the total number of islands, and if we assume irreversible attachment, the velocity of the island boundaries can be calculated as

$$v = Da\rho, \tag{3}$$

where ρ is the density which is obtained from

$$\frac{d\rho}{dt} = F - 2\sigma D\rho^2 - D\rho \int_\Gamma ds. \tag{4}$$

In (4), D is the adatom diffusion constant, F is the deposition rate, and σ describes the capture efficiency [7,8]. The second term on the right side is the nucleation rate which reflects the fact that two atoms are needed to form a new island. The last term describes the capture of adatoms by existing islands.

We have also implemented a more sophisticated model where the spatially varying adatom density is obtained from solving a diffusion equation [3,4]. However, in this letter, we will use the uniform density model as described by equations (3),(4) and will focus on the consequences of surface reconstructions. Mathematically, this implies that for the level-set function (that represents island boundaries) the velocity is discontinuous across the boundary between reconstruction domains.

2. THE COUPLED LEVEL-SET FORMALISM

2.1. Surface Reconstructions

Atoms on a surface "reconstruct" (rearrange structurally, lowering the symmetry of the surface relative to its bulk termination) to lower the surface energy. For example, under typical As-rich growth conditions, the surface of InAs(001) or GaAs(001) exhibits the so-called $\alpha_2(2 \times 4)$ and $\beta_2(2 \times 4)$ structures, as can be seen for example in recent scanning tunnelling microscopy (STM) experiments [9]. Different surfaces have different reconstructions, and there might be more than just two reconstructions. The energetics of the stability of the surface reconstructions on InAs(001) and GaAs(001) is well understood [10–14]. One effect of the different reconstructions is that the mobility of adatoms, and thus, the entire growth dynamics on the surface will be different for different reconstructions. Thus, it is desirable to include the effect of surface reconstructions in any growth model. We propose the following model to account for such changes in the surface mobility.

2.2. Modifications to the Island Dynamics Model

In addition to the level-set function ϕ that describes the island boundaries, we introduce a second level-set function ψ, such that the the set of points $\psi(\mathbf{x}) = 0$ denotes the boundary between two reconstruction domains. In case there are more than two domains, we introduce n level-set functions denoted ψ_i such that reconstruction i is represented by $\psi_i > 0$ (and all other $\psi_j < 0$). The level-set function ψ evolves according to

$$\frac{\partial \psi}{\partial t} + u|\nabla \psi| = 0, \tag{5}$$

where the normal velocity u describes the velocity of the boundary of the reconstruction domains. For the example of the α_2 and β_2 reconstructions, this velocity is intimately connected to the adsorption and desorption of As-dimers, which depend on the external physical conditions such as temperature and pressure [15].

The adatom diffusion constant D takes on different values on the different reconstruction domains, which will be denoted as D_i. Then the model equations (3),(4) need to be modified accordingly, and read

$$v_i = D_i a \rho_i, \tag{6}$$

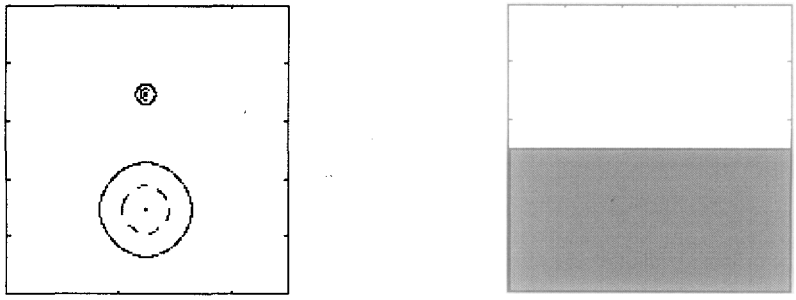
$$\frac{d\rho_i}{dt} = F - 2\sigma D_i \rho_i^2 - D\rho_i \int_{\Gamma_i} ds, \tag{7}$$

where the subscript i denotes that the equations are solved only on the corresponding reconstruction domain.

For all the results shown below, we have implemented a simple first-order directional upwind scheme (that is separate in each direction) to solve equations (1),(5). The scheme is not guaranteed to be conservative, but accuracy is sufficient for the current purpose. Equations (7) are solved using a backward Euler scheme. The main purpose of this letter is to demonstrate the feasibility of the proposed model of coupled level-set functions rather than high accuracy for certain physical results. If accuracy becomes more important, higher-order schemes could easily be used.

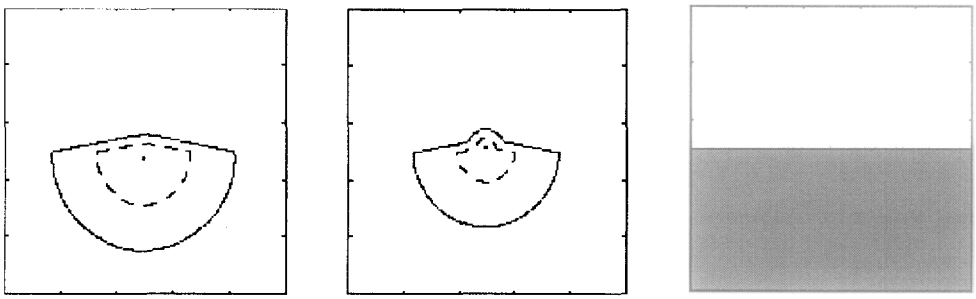
3. RESULTS

Different diffusion constants imply that islands on different reconstruction domains will grow with a different velocities. This is shown in Figure 1, where two islands are placed in two different domains. For simplicity, we assume $u = 0$ (i.e., the boundary between reconstruction domains



(a) (b)

Figure 1. Two islands growing in two separate reconstruction domains where the velocity in Domain 1 is five times larger than the velocity in Domain 2. Panel (a) shows ϕ (which represents the island boundaries) at different times $t_1 = 1$ (dashed line) and $t_2 = 2$ (solid line). Panel (b) shows ψ (the domain boundary).



(a) (b) (c)

Figure 2. Growth of an island that has been nucleated just below (a) and just above (b) the domain boundary. Panels (a) and (b) show ϕ (which represents the island boundaries) at different times $t_1 = 1$ (dashed lines) and $t_2 = 2$ (solid lines). Panel (c) shows ψ (the domain boundary).

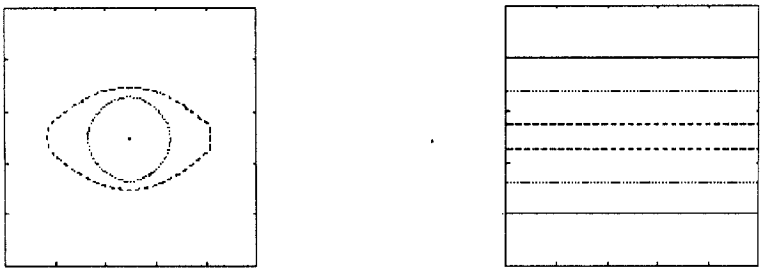
does not move). The velocity v_1 in the upper domain is assumed to be five times larger than in the lower domain, and as expected the island in Domain 1 grew five times faster.

Interesting effects happen when an island grows across the domain boundary. This is shown in Figure 2, where again we assume $u = 0$. The velocities are chosen as $v_2/v_1 = 5$. In Figure 2a, the island was initially placed just below the domain boundary. As the island grows across the domain boundary, growth in Domain 1 is significantly slower, leading to the deformation that can be seen in Figure 2a. The shape in Domain 1 is almost triangular, with a slope of 5. It can easily be verified that this slope corresponds exactly to the ratio v_2/v_1.

In Figure 2b, the island was initially placed just above the domain boundary. As the island crosses into Domain 2, it grows much quicker in Domain 2, leading to the half-circular shape in Domain 2. Moreover, as the island grows faster in Domain 2 to the side, it also moves back into Domain 1, leading to the triangular side-facets in Domain 1. These triangles again have a slope that corresponds to the ratio $v_2/v_1 = 5$.

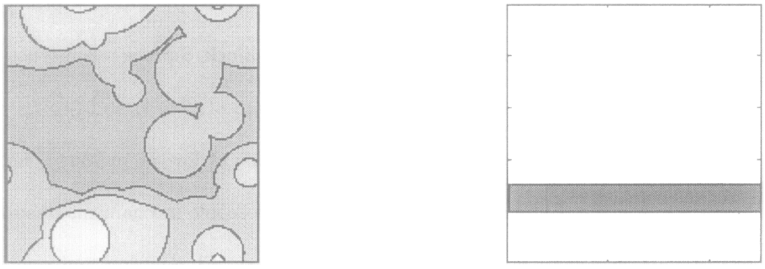
In the previous figures, we have always assumed that $u = 0$. In Figure 3, we show a typical result of an island that has been seeded in Domain 2, where Domain 2 is shrinking at a velocity $u = 1$, and where $v_2 = 5$ and $v_1 = 1$. The island grows faster as long as the boundary is still within Domain 2, and we observe similar deformations of the island shape as in the static case. There are no instabilities or discontinuities of the island boundary across the reconstruction domain boundary. Clearly, the exact evolution of the deformation of the island shape depends on the interplay of the different velocities and the initial geometry.

Finally, in Figure 4, we show typical simulation results of the entire island dynamics model. In this result, we chose $u = 1$, $D_2 = 5 \times 10^6$, $D_1 = 10^6$, and $F = 1.0$. All the features



(a) (b)

Figure 3. Coupled level-set formalism for one island. Panel (a) shows ϕ (which represents the island boundaries) at different times $t_1 = 1$ (dotted line) and $t_2 = 2$ (dashed line). Panel (b) shows ψ (the domain boundary), where the dotted (dashed) lines correspond to $t_1 = 1$ ($t_2 = 2$), and the solid lines represent the initial configuration ($t_0 = 0$).



(a) (b)

Figure 4. A typical simulation of the full island dynamics simulation as explained in Section 2. Level-set functions ϕ and ψ are shown at $t = 2$ on the left and right, respectively. The initial geometry of the domains is that the upper and lower halves are Domain 1 and 2, respectively.

discussed above for special test geometries can be observed here as well. The main purpose of this figure is to demonstrate that our model and its numerical implementation are stable, and that no discontinuities occur. More detailed physical processes on the terraces and especially along the island and step edges need to be considered and included in the model to make a more direct comparison to reconstruction changes as they have been observed [9] or predicted [15] for InAs(001). It will be the aim of future work to look at physically more realistic systems where we will solve (coupled) diffusion equations for the separate species.

4. DISCUSSION AND CONCLUSION

We have developed a simple model for epitaxial growth where island boundaries are represented by a level-set function ϕ, and where the velocity for the island boundaries depends on the value of a second level-set function ψ. This leads to discontinuities in the velocity v. However, the level-set formalism is stable enough that this causes no numerical problems. The proposed formalism is easily applicable to a number of other multiphase problems, for example, growth and time evolution of magnetic domains (where the magnetization is represented by ψ), or growth with facets.

REFERENCES

1. M.F. Gyure, C. Ratsch, B. Merriman, R.E. Caflisch, S. Osher, J.J. Zinck and D.D. Vvedensky, Level set methods for the simulation of epitaxial phenomena, *Phys. Rev. E* **58**, R6927, (1998).
2. R.E. Caflisch, M.F. Gyure, B. Merriman, S.J. Osher, C. Ratsch, D.D. Vvedensky and J.J. Zinck, Island dynamics and the level set method for epitaxial growth, *Appl. Math. Lett.* **12** (4), 13–22, (1999).

3. S. Chen, M. Kang, B. Merriman, R. Caflisch, C. Ratsch, R. Fedkiw, M. Gyure and S. Osher, Level set method for thin film epitaxial growth, *Journ. Comp. Phys.* **167**, 475, (2001).
4. C. Ratsch, M.F. Gyure, R.E. Caflisch, F. Gibou, M. Petersen, M. Kang, J. Garcia and D.D. Vvedensky, Level set method for island dynamics in epitaxial growth, *Phys. Rev. B* **65**, 19503, (2002).
5. M. Petersen, C. Ratsch, R.E. Caflisch and A. Zangwill, Level set approach to reversible epitaxial growth, *Phys. Rev. E* **64**, 061602, (2001).
6. S. Osher and J.A. Sethian, Front propagation with curvature dependent speed: Algorithms based on Hamilton-Jacobi formulations, *J. Comp. Phys.* **79**, 12–49, (1988).
7. G.S. Bales and D.C. Chrzan, Dynamics of irreversible island growth during submonolayer epitaxy, *Phys. Rev. B* **50**, 6057, (1994).
8. F. Gibou, C. Ratsch, S. Chen, M.F. Gyure and R.E. Caflisch, Rate equations and capture numbers with implicit island correlation, *Phys. Rev. B* **63**, 115401, (2001).
9. W. Barvosa-Carter, R.S. Ross, C. Ratsch, F. Grosse, J.H.G. Owen and J.J. Zinck, Atomic scale structure of InAs(001) - (2×4) steady-state surfaces determined by scanning tunneling microscopy and density-functional theory, *Surf. Sci.* **499**, L129, (2002).
10. J.E. Northrup and S. Froyen, Energetics of GaAs(100) - (2×4) and (4×2) reconstructions, *Phys. Rev. B* **50**, 2015, (1994).
11. V.P. LaBella, H. Yang, D.W. Bullock, P.M. Thibedo, P. Kratzer and M. Scheffler, Atomic structure of the GaAs(001) (2×4) surface resolved using scanning tunneling microscopy and first-principes theory, *Phys. Rev. Lett.* **83**, 2989, (2000).
12. C. Ratsch, W. Barvosa-Carter, F. Grosse, J.H.G. Owen and J.J. Zinck, Surface reconstructions for InAs(001) studied with DFT and STM, *Phys. Rev. B* **62**, R7719, (2000).
13. W.G. Schmidt, S. Mirbt and F. Bechstedt, Surface phase diagram of (2×4) and (4×2) reconstructions of GaAs(001), *Phys. Rev. B* **62**, 8087, (2000).
14. S.-H. Lee, W. Moritz and M. Scheffler, Surface under conditions of low as pressure: Evidence of a novel surface geometry, *Phys. Rev. Lett.* **85**, 3890, (2000).
15. F. Grosse, W. Barvosa-Carter, J.J. Zinck and M.F. Gyure, Microscopic mechanisms of surface phase transitions on InAs(001), *Phys. Rev. B* **66**, 075321, (2002).
16. C. Ratsch, M.F. Gyure, S. Chen, M. Kang and D.D. Vvedensky, Fluctuation and scaling in aggregation phenomena, *Phys. Rev. B* **61**, R10598, (2000).