Applied Numerical Mathematics 128 (2018) 139–156

Contents lists available at ScienceDirect

Applied Numerical Mathematics

www.elsevier.com/locate/apnum

Regularized linear schemes for the molecular beam epitaxy model with slope selection

Lizhen Chen [a], Jia Zhao [b,*], Xiaofeng Yang [c,d]

[a] Beijing Computational Science Research Center, Beijing, China
[b] Department of Mathematics & Statistics, Utah State University, Logan, UT, USA
[c] Department of Mathematics, University of South Carolina, Columbia, SC 29208, USA
[d] School of Mathematical Sciences, University of Electronic Science and Technology of China, Chengdu, 610054, China

ARTICLE INFO

Article history:
Received 6 August 2017
Received in revised form 8 January 2018
Accepted 4 February 2018
Available online 8 February 2018

Keywords:
Phase field
Molecular beam epitaxy
Energy stable
Linear scheme

ABSTRACT

In this paper, we propose full discrete linear schemes for the molecular beam epitaxy (MBE) model with slope selection, which are shown to be unconditionally energy stable and unique solvable. In details, using the invariant energy quadratization (IEQ) approach, along with a regularized technique, the MBE model is first discretized in time using either Crank–Nicolson or Adam–Bashforth strategies. The semi-discrete schemes are shown to be energy stable and unique solvable. Then we further use Fourier-spectral methods to discretize the space, ending with full discrete schemes that are energy-stable and unique solvable. In particular, the full discrete schemes are linear such that only a linear algebra problem need to be solved at each time step. Through numerical tests, we have shown a proper choice of the regularization parameter provides better stability and accuracy, such that larger time step is feasible. Afterward, we present several numerical simulations to demonstrate the accuracy and efficiency of our newly proposed schemes. The linearizing and regularizing strategy used in this paper could be readily applied to solve a class of phase field models that are derived from energy variation.

1. Introduction

Molecular beam epitaxy (MBE) is an epitaxy method for thin-film deposition of single crystals. So far quite a few mathematical models as well as the accompanying numerical simulation tools have been developed to study dynamics of the MBE growth process [3,5,16,20,21,36,45]. For the continuum model, there are several approaches developed to model molecular beam epitaxy growth. One popular approach is the energy-variational based. In [12], Golubovic introduces the effective free energy formation of the MBE growth model (without slope selection); and in [30], Moldovan and Golubovic introduce the MBE growth model (with slope selection), where the anisotropic MBE models are also considered (affecting the coarsening dynamics). Notice that there are many other cases, where the surface motion could not be generated by an effective free energy functional [13,23–27].

Given the effective free energy, we present the MBE growth model and discuss its energy dissipation properties which serve as a guideline for us developing numerical schemes. Let $\phi(x,t)$ be the epitaxy surface height with $x \in \Omega$, where Ω is a

* Corresponding author.
E-mail addresses: lzchen@csrc.ac.cn (L. Chen), jia.zhao@usu.edu (J. Zhao), xfyang@math.sc.edu (X. Yang).

https://doi.org/10.1016/j.apnum.2018.02.004
0168-9274/

confined domain in R^2. Under typical conditions for MBE growth, the height (ϕ) evolution equation is given in a relaxation dynamical form of a L^2 gradient flow:

$$\phi_t = -M\frac{\delta E}{\delta \phi}, \tag{1.1}$$

where M is the mobility coefficient, E is the effective free energy (which represents the kinetic asymmetry in attachment and detachment of adatoms to and from terrace boundaries [28]) and $\frac{\delta E}{\delta \phi}$ denotes the variational derivative of E with respect to ϕ.

For the effective free energy, two widely used phenomenological expressions are as follows: (1) with slope selection expression [30]

$$E(\phi) = \int_\Omega \Big(\frac{\varepsilon^2}{2}(\Delta\phi)^2 + \frac{1}{4}(|\nabla\phi|^2 - 1)^2\Big)d\Omega, \tag{1.2}$$

and without slope selection expression [12]

$$E(\phi) = \int_\Omega \Big(\frac{\varepsilon^2}{2}(\Delta\phi)^2 - \frac{1}{2}\ln(1 + |\nabla\phi|^2)\Big)d\Omega, \tag{1.3}$$

where ε is a constant (inversely proportional to the size of the system). A detailed discussion of differences between these two free energies could be found in [28]. In short, the first term in the free energy represents the surface diffusion effect and the second term represents a continuum description of the effect that the adatoms (absorbed atoms) must overcome a higher energy barrier to stick to a step from an upper rather than from a lower terrace. After substituting the expression of free energy (1.2) and (1.3) into the model (1.1), we obtain the two nonlinear MBE models: (1) MBE model with slope selection

$$\partial_t\phi = -M\Big(\varepsilon^2\Delta^2\phi - \nabla\cdot((|\nabla\phi|^2 - 1)\nabla\phi)\Big), \tag{1.4}$$

and (2) MBE model without slope selection

$$\partial_t\phi = -M\Big(\varepsilon^2\Delta^2\phi - \nabla\cdot(\frac{\nabla\phi}{1 + |\nabla\phi|^2})\Big). \tag{1.5}$$

A feature of the continuum MBE models considered in this paper, i.e. (1.4) and (1.5), is that it is derived from an energy variational approach and thereby satisfies an energy dissipation law (or thermodynamically consistent). The energy dissipation law, in fact, serves as a guide for the design of thermodynamically consistent (energy stable) numerical schemes. In practice, it is especially desirable in the design of numerical schemes that preserve the energy dissipation property at the discrete level. On the one hand, the preservation of the energy law is critical for the numerical schemes to capture correct long-time dynamics of the system. On the other hand, the unconditional stability of the energy dissipation preserving schemes provides flexibility for dealing with the stiffness issue in the model.

In this paper, we consider numerical approximations to the continuum MBE growth model (1.1) with free energy (1.2), which is obtained by minimizing the given free energy where the nonlinear potential is a fourth order Ginzburg–Landau double-well potential in terms of the gradient of a height function. Here we give a brief review of available papers in the literature on proposing efficient numerical schemes for solving the MBE model. In [46], Wang et al. used convex splitting strategy to propose unconditionally energy stable schemes for MBE model. Qiao et al. proposed an adaptive time-stepping strategy for the MBE model with slope selection [33], and Qiao et al. proposed energy stable schemes for the MBE model without slope selection and its convergence analysis [31]. Chen et al. proposed a linear energy stable scheme for MBE model without slope selection using convex splitting strategy [4]. In [28], Li et al. developed a spectral method for solving the MBE models. In [52], Xia proposed a full discrete stable scheme for MBE model without slope selection using discontinuous Galerkin method. Recently, Feng et al. developed a linearly preconditioned nonlinear conjugate gradient solver [8] and a second-order energy-stable BDF scheme for MBE model with slope selection [9]. Some other related papers include [19,22, 29,32,37].

Mainly, the strategies for developing energy stable schemes can be generally categorized into two parts. The first part named stabilized approach, where the nonlinear terms are treated explicitly, but some linear stabilizing terms are added to provide better stability of the scheme. This so-called stabilized approach have been broadly used in phase-field models, see [40,42–44,53,62,63,66,67]. Another approach is named “convex splitting”, which was originally proposed in [7] and has been exploited by the numerical analysis society [17,46,47,49,50]. The idea of convex splitting is to split the free energy as a convex potential minus another convex potential. Then the chemical potential from the first convex part is solved implicitly, and the rest is solved explicitly. The advantage of the stabilized approach is its simplicity to implement, as it is linear, but it is only first order in time (due to the first-order error introduced in the stabilizing term), and it has to assume/truncate the free energy (which should not be ignored in the continuum PDE level). For the convex splitting approach, its existence