Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2018-0015

Vol. **25**, No. 4, pp. 1024-1044
April 2019

A Novel Second-Order Scheme for the Molecular Beam Epitaxy Model with Slope Selection

Lizhen Chen[1], Jia Zhao[2,*] and Yuezheng Gong[3]

[1] *Beijing Computational Science Research Center, Beijing, P.R. China.*
[2] *Department of Mathematics & Statistics, Utah State University, Logan, UT, USA.*
[3] *College of Science, Nanjing University of Aeronautics and Astronautics, Nanjing 210016, P.R. China.*

Received 16 January 2018; Accepted (in revised version) 16 May 2018

Abstract. Molecular beam epitaxy (MBE) is an important and challenging research topic in material science. In this paper, we propose a new fully discrete scheme for the well-celebrated continuum MBE model with slope selection. First of all, we use a multi-step strategy to discretize the MBE model in time. The obtained semi-discrete scheme is proved to possess properties of total mass conservation, unconditionally energy stability and uniquely solvability. The rigorous error estimate is then conducted to show its second-order convergence. The semi-discrete scheme is further discretized in space using the Fourier pseudo-spectral method. The fully discrete scheme is also shown to preserve mass-conservation and energy-dissipation properties. Afterward, several numerical examples are presented to validate the accuracy and efficiency of our proposed scheme. In particular, the scaling law for the roughness growing and effective energy decaying are captured during long-time coarsening dynamic simulations. The idea proposed in this paper could be readily utilized to design accurate and stable numerical approximations for many other energy-based phase field models.

AMS subject classifications: 65N22, 65M12, 65M70

Key words: Phase field, linear scheme, molecular beam epitaxy, energy stable.

1 Introduction

Molecular beam epitaxy (MBE) method is a broadly used approach of thin-film deposition of a single crystal. So this strategy is widely applied in semiconductor manufacture. In recent years, MBE becomes an important and challenging research topic in material science. In the meanwhile, many mathematical models have been developed to study

*Corresponding author. *Email addresses:* `lzchen@csrc.ac.cn` (L. Chen), `jia.zhao@usu.edu` (J. Zhao), `gongyuezheng@nuaa.edu.cn` (Y. Gong)

the epitaxy dynamics, ranging from molecular dynamics simulations to continuum models [1,6,11,16,18,20,23,24,29,32].

In this paper, we focus on one broadly-used continuum model for the MBE, which is derived via an energy variational approach and satisfies an energy dissipation law (i.e., thermodynamically consistent) [23, 24, 33, 35]. Consider a smooth domain Ω, and use $\phi(\mathbf{x},t):\Omega\to\mathbb{R}$ to denote the height function of MBE, and the effective free energy is given as

$$E(\phi)=\int_\Omega\Big[\frac{\varepsilon^2}{2}|\Delta\phi|^2+f(\nabla\phi)\Big]d\Omega. \tag{1.1}$$

Here the first term represents the isotropic surface diffusion effect, and the second term approximates the Enrlich-Schwoebel effect that the adatoms stick to the boundary from an upper terrace, contributing to the steepening of mounds in the film [3]. The evolution equation for ϕ could be derived via a L^2 gradient flow associated with the effective free energy functional $E(\phi)$, i.e., the equation reads as

$$\partial_t\phi=-M\frac{\delta E}{\delta\phi}, \tag{1.2}$$

where M is the mobility parameter (with $\frac{1}{M}$ proportional to the relaxation time). For simplicity of notations, we consider periodic boundary condition in this paper.

If we choose the second term of (1.1) as $f(\nabla\phi)=-\frac{1}{2}\ln(1+|\nabla\phi|^2)$, the corresponding equation would be

$$\partial_t\phi=-M\Big(\varepsilon^2\Delta^2\phi+\nabla\cdot\Big(\frac{\nabla\phi}{1+|\nabla\phi|^2}\Big)\Big), \tag{1.3}$$

and the energy dissipation rate of (1.2) could be calculated as

$$\frac{dE}{dt}=-\int_\Omega M\Big(\varepsilon^2\Delta^2\phi+\nabla\cdot\Big(\frac{\nabla\phi}{1+|\nabla\phi|^2}\Big)\Big)^2 d\Omega. \tag{1.4}$$

On the other hand, if we choose $f(\nabla\phi)=\frac{1}{4}(|\nabla\phi|^2-1)^2$, the corresponding equation would become

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

and the corresponding energy dissipation rate of (1.2) could be calculated as

$$\frac{dE}{dt}=-\int_\Omega M\Big(\varepsilon^2\Delta^2\phi+\nabla\cdot((1-|\nabla\phi|^2)\nabla\phi)\Big)^2 d\Omega. \tag{1.6}$$

In addition, both models (1.3) and (1.5) obey the total mass conservation law

$$\frac{d}{dt}\int_\Omega\phi(\mathbf{x},t)d\Omega=0. \tag{1.7}$$

When the surface gradient $|\nabla\phi|$ is small ($|\nabla\phi|\ll 1$), by the Taylor expansion, we can easily recognize $\frac{1}{1+|\nabla\phi|^2}\approx 1-|\nabla\phi|^2$. Then model (1.5) could be formally derived from model