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Errors of an Implicit Variable-Step BDF2 Method for a Molecular Beam Epitaxial Model with Slope Selection

Xuan Zhao[1,*], Haifeng Zhang[1] and Hong Sun[1,2]

[1]*School of Mathematics, Southeast University, Nanjing 210096, P.R. China.*
[2]*Department of Mathematics and Physics, Nanjing Institute of Technology, Nanjing 211167, P.R. China.*

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Abstract. Unconditionally stable and convergent variable-step BDF2 scheme for solving the MBE model with slope selection is derived. Discrete orthogonal convolution kernels of the variable-step BDF2 method are commonly utilized for solving the phase field models. We present new inequalities, concerning the vector forms, for the kernels especially dealing with nonlinear terms in the slope selection model. The convergence rate of the fully discrete scheme is proved to be two both in time and space in L^2 norm under the setting of the variable time steps. Energy dissipation law is proved rigorously with a modified energy by adding a small term to the discrete version of the original free energy functional. Two numerical examples including an adaptive time-stepping strategy are given to verify the convergence rate and the energy dissipation law.

AMS subject classifications: 35Q92, 65M06, 65M12, 74A50

Key words: Molecular beam epitaxial growth, slope selection, variable-step BDF2 scheme, energy stability, convergence.

1. Introduction

Over the past decades, the dynamics of molecular beam epitaxy (MBE) model attracted broad interest from the fields of chemistry, material science, mathematics, etc. The epitaxial growth process offers a controllable method to obtain lateral heterojunction with an atomically sharp interface, for attractive materials in making smaller transistors [26, 43]. Atomistic, continuum, and hybrid models from various scales are applied to study the evolution of the surface morphology during epitaxial growth. MBE is the most widely used technique for growing thin epitaxial layers of semiconductor crystals and metallic materials [17]. In addition, Nair *et al.* [34] introduced the growth of superconducting Sr_2RuO_4 thin films by MBE on (110)$NdGaO_3$ substrates with transition temperatures of up to 1.8 K.

*Corresponding author. *Email addresses:* xuanzhao11@seu.edu.cn (X. Zhao), 220211744@seu.edu.cn (H.F. Zhang), sunhongzhal@126.com (H. Sun)

In this paper, we consider an MBE model with slope selection in the two-dimensional domain $\Omega = (0,L)^2 \subset \mathbb{R}^2$. Let $u(\mathbf{x},t)$ be the epitaxy surface height with space variable $\mathbf{x} \in \Omega$ and time variable $t \geq 0$. The height evolution equation [33] has the form

$$u_t + \delta\Delta^2 u - \nabla \cdot f(\nabla u) = 0, \quad \mathbf{x} \in \Omega, \quad 0 < t \leq T, \tag{1.1}$$

and is supplemented by periodic boundary conditions and the initial data $u(\mathbf{x},0) = \varphi_0(\mathbf{x})$. Here, $\delta > 0$ is the constant that represents the width of the rounded corners on the otherwise faceted crystalline thin films. The vector f defined by

$$f(\mathbf{v}) = \left(|\mathbf{v}|^2 - 1\right)\mathbf{v}$$

is the nonlinear bulk force. When $t \to \infty$, one obtains $|\nabla\phi| \to 1$, that is why it is called the model with slope selection. There is also a counterpart model, where $f(\mathbf{v}) = -\mathbf{v}/(1+|\mathbf{v}|^2)$, called MBE model without slope selection due to that during the coarsening process $|\nabla\phi|$ does not converge to a constant. For any $u \in H^1(\Omega)$, we define the energy function

$$E(t) = \int_0^t \|u_t(\cdot,\cdot,s)\|^2 ds + \frac{\delta}{2}\|\Delta u(\cdot,\cdot,t)\|^2 + \frac{1}{4}\iint_\Omega \left(|\nabla u(x,y,t)|^2 - 1\right)^2 dxdy.$$

The following energy dissipation law holds:

$$\frac{dE(t)}{dt} = 0, \quad t > 0.$$

The model (1.1) has been used to study interfacial coarsening dynamics in epitaxial growth with slope selection, where the fourth-order term models surface diffusion, and the nonlinear second-order term models the well-known Ehrlich-Schowoebel effect, which consequently leads to the formation of mounds and pyramids on the growing surface. Gyure *et al.* [15] conducted an experiment to show the unstable growth of thin films on rough surfaces. The MBE of InAs buffer layers is performed on InAs(001) substrates, in the experiment, which exhibit large-small-large wavelength oscillations as the thickness of buffer layers increasing. This morphological instability in the rough-smooth-rough pattern is fundamentally due to the Ehrlich-Schwoebel effect.

The well-posedness for the growth equation with slope selection for different boundary conditions was studied in King *et al.* [20]. Li and Liu [22] proved the well-posedness and the solution regularity for the initial-boundary-value thin film epitaxy model. The Galerkin spectral method was applied to solve the numerical solution of the model with or without slope selection. In addition, numerical results showed the decay of energy and roughness at different time stages. Li *et al.* [25] analyzed the gradient flow modeling the epitaxial growth of thin films with slope selection in physical dimensions. The improved local and global well-posedness for solutions with critical regularity were established. Several lower and upper bounds for the gradient were obtained.

Due to the high order derivatives and the nonlinear term, it takes a long time to reach the steady state in the dynamics of the MBE model. As is well known that the linearized