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ERROR ANALYSIS OF STABILIZED CONVEX SPLITTING BDFk METHOD FOR THE MOLECULAR BEAM EPITAXIAL MODEL WITH SLOPE SELECTION*

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Abstract

The k-th ($k = 3, 4, 5$) order backward differential formula (BDFk) is applied to develop the high order energy stable schemes for the molecular beam epitaxial model with slope selection. The numerical schemes are established by combining the convex splitting technique with the k-th order accurate Douglas-Dupont stabilization term in the form of $S\tau^{k-1}\Delta_h(\phi^n - \phi^{n-1})$. With the help of the new constructed discrete gradient structure of the k-th order explicit extrapolation formula, the stabilized BDFk scheme is proved to preserve energy dissipation law at the discrete levels and unconditionally stable in the energy norm. By using the discrete orthogonal convolution kernels and the associated convolution embedding inequalities, the L^2 norm error estimate is established under a weak constraint of time-step size. Numerical simulations are presented to demonstrate the accuracy and efficiency of the proposed numerical schemes.

Mathematics subject classification: 65M06, 65M12.
Key words: The molecular beam epitaxial model, High order stabilized convex splitting BDFk scheme, Discrete gradient structure, Unconditional energy dissipation, L^2 norm convergence analysis.

1. Introduction

The molecular beam epitaxial technique can be used to obtain high-quality crystalline materials and form the structures with very high precision in the vertical direction [25]. In this paper, we consider the molecular beam epitaxial (MBE) model with slope selection [16], that is

$$\partial_t \Phi = -\kappa\mu, \quad \mu = \epsilon^2\Delta^2\Phi - \nabla\cdot[(|\nabla\Phi|^2 - 1)\nabla\Phi], \quad \mathbf{x} \in \Omega, \tag{1.1}$$

which can be regarded as the L^2 gradient flow of the energy functional

$$E[\Phi] = \int_\Omega \left[\frac{\epsilon^2}{2}|\Delta\Phi|^2 + \frac{1}{4}(|\nabla\Phi|^2 - 1)^2\right] \mathrm{d}\mathbf{x}. \tag{1.2}$$

The above mentioned Φ indicates the periodic scaled height function. The chemical potential μ can be seen as the variational derivative of the functional (1.2) and be calculated by $\mu{=}\delta E/\delta\Phi$

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formally. Parameters κ and ϵ^2 are the mobility coefficient and the dissipation coefficient respectively. The fourth order term and the nonlinear second order term model the surface diffusion and the Ehrlich-Schwoebel effect respectively [9,31]. Due to the slope selection in the dynamics evolution, the solution of the model (1.1) is featured by the shape of pyramids or pyramid-like structures.

We consider the model (1.1) with the periodic boundary conditions and the initial condition $\Phi(\mathbf{x},0)=\phi_0(\mathbf{x})$. It reveals that the MBE model with slope selection has the properties of the mass conservation and the energy dissipation. Given $(u,v)=\int_\Omega uv\,\mathrm{d}\mathbf{x}$ is the inner product in $L^2(\Omega)$ and $\|u\|_{L^2(\Omega)}=\sqrt{(u,u)}$ is the corresponding norm. Simple calculation leads to the mass conservation law $(\Phi(t),1)=(\phi_0,1)$ and the energy dissipation law as follows:

$$\frac{\mathrm{d}}{\mathrm{d}t}E[\Phi]=-\kappa\|\partial_t\Phi\|_{L^2}^2\le 0. \tag{1.3}$$

Many efficient and stable numerical methods have been developed and analyzed for the MBE equation with or without slope selection. See the relevant references [1,7,8,11,19,22,27–30,33,35–39], etc. To the best of our knowledge, several effective strategies have been developed to design the unconditional energy stable numerical schemes, such as the stabilized method, the convex splitting method, the invariant energy quadratization (IEQ) method and the scalar auxiliary variable (SAV) method, etc. Among these methods, we focus on the convex splitting strategy in dealing with the temporal approximation. In [35], the convex splitting method was applied to develop the first order unconditionally stable scheme for the MBE model. The second order convex splitting schemes [33] were proposed for the same model. The MBE model with slope selection was solved by a fully discrete finite difference scheme combining the convex splitting strategy [29]. And, the convergence analysis was carried out carefully. The first and second order linear energy stable schemes [2, 4] based on the convex splitting method were devised for a thin film model without slope selection. A second order unconditionally energy stable finite difference scheme [11], which combines the second order backward differentiation formula (BDF) and convex splitting method, was presented and analyzed for the MBE model with slope selection.

The high order energy stable numerical methods are more desirable because of the long time coarsening process of the MBE model, such as that in [3, 13, 15, 17], etc. The third order linear BDF schemes were devised for the MBE model without slope selection in [13, 17], and the modified energy dissipation law and the convergence of the numerical schemes were proved rigorously. Especially, the Douglas-Dupont type stabilization term in the form of $S\tau^2\Delta_h\delta_1\phi^n$, was added to ensure the energy stability for any temporal steps [13]. Recently, the fully implicit BDF methods up to fifth order [15] were studied for the no-slope MBE equation. Under certain temporal step constraints, the modified energy dissipation law and L^2 norm error analysis of the numerical schemes were constructed by using the tools including the discrete gradient structure of k-th order BDF (BDFk) formula and the discrete orthogonal convolution (DOC) kernels. Based on this idea, we proposed the BDF3-5 schemes [18] for the MBE model with slope selection, and analyzed those schemes under the theoretical framework [24]. However, the above proposed BDF3-5 schemes were proved to be uniquely solvable and energy stable under the temporal step constraint $\tau\le 2\epsilon^2\min\{2\sigma_{Lk},b_0^{(k)}\}/\kappa$.

In this work, the unconditionally energy stable high order accurate methods, which remove the temporal step constraint on the energy dissipation law, are concerned for solving MBE model with slope selection. We combine the high order BDF formulas and the convex splitting method to deal with the time approximation in the time evolution process. However, for the