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A Third Order BDF Energy Stable Linear Scheme for the No-Slope-Selection Thin Film Model

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Abstract. In this paper we propose and analyze a (temporally) third order accurate backward differentiation formula (BDF) numerical scheme for the no-slope-selection (NSS) equation of the epitaxial thin film growth model, with Fourier pseudo-spectral discretization in space. The surface diffusion term is treated implicitly, while the nonlinear chemical potential is approximated by a third order explicit extrapolation formula for the sake of solvability. In addition, a third order accurate Douglas-Dupont regularization term, in the form of $-A\Delta t^2\Delta_N^2(u^{n+1}-u^n)$, is added in the numerical scheme. A careful energy stability estimate, combined with Fourier eigenvalue analysis, results in the energy stability in a modified version, and a theoretical justification of the coefficient A becomes available. As a result of this energy stability analysis, a uniform in time bound of the numerical energy is obtained. And also, the optimal rate convergence analysis and error estimate are derived in details, in the $\ell^\infty(0,T;\ell^2)\cap\ell^2(0,T;H_h^2)$ norm, with the help of a linearized estimate for the nonlinear error terms. Some numerical simulation results are presented to demonstrate the efficiency of the numerical scheme and the third order convergence. The long time simulation results for $\varepsilon=0.02$ (up to $T=3\times10^5$) have indicated a logarithm law for the energy decay, as well as the power laws for growth of the surface roughness and the mound width. In particular, the power index for the surface roughness and the mound width growth, created by the third order numerical scheme, is more accurate than those produced by certain second order energy stable schemes in the existing literature.

AMS subject classifications: 35K30, 35K55, 65L06, 65M12, 65M70, 65T40

Key words: Epitaxial thin film growth, no-slope-selection, third order backward differentiation formula, energy stability, optimal rate convergence analysis.

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1 Introduction

In this article we consider a no-slope-selection (NSS) epitaxial thin film growth equation, which corresponds to the L^2 gradient flow associated with the following energy functional

$$E(u):=\int_\Omega \left(-\frac{1}{2}\ln(1+|\nabla u|^2)+\frac{\varepsilon^2}{2}|\Delta u|^2\right)\mathrm{d}\mathbf{x}, \tag{1.1}$$

where $\Omega=(0,L_x)\times(0,L_y)$, $u:\Omega\to\mathbb{R}$ is a periodic height function, and ε is a constant parameter of transition layer width. In more details, the first nonlinear term represents the Ehrlich-Schwoebel (ES) effect [14,26–28,40], which results in an uphill atom current in the dynamics and the steepening of mounds in the film. The second higher order quadratic term represents the isotropic surface diffusion effect [27,35]. In turn, the chemical potential becomes the following variational derivative of the energy

$$\mu:=\delta_u E=\nabla\cdot\left(\frac{\nabla u}{1+|\nabla u|^2}\right)+\varepsilon^2\Delta^2 u, \tag{1.2}$$

and the PDE stands for the L^2 gradient flow

$$\partial_t u=-\mu=-\nabla\cdot\left(\frac{\nabla u}{1+|\nabla u|^2}\right)-\varepsilon^2\Delta^2 u. \tag{1.3}$$

Meanwhile, under a small-slope assumption that $|\nabla u|^2\ll 1$, the energy functional could be approximated by a polynomial pattern

$$E(u)=\int_\Omega \left(\frac{1}{4}(|\nabla u|^2-1)^2+\frac{\varepsilon^2}{2}|\Delta u|^2\right)\mathrm{d}\mathbf{x}, \tag{1.4}$$

and the dynamical equation is formulated as

$$\partial_t u=\nabla\cdot\left(|\nabla u|^2\nabla u\right)-\Delta u-\varepsilon^2\Delta^2 u. \tag{1.5}$$

This model is referred to as the slope-selection (SS) equation [24,25,27,35]. A solution to (1.5) exhibits pyramidal structures, where the faces of the pyramids have slopes $|\nabla u|\approx 1$; meanwhile, the no-slope-selection equation (1.3) exhibits mound-like structures, and the slopes of which (on an infinite domain) may grow unbounded [27,42]. On the other hand, both solutions have up-down symmetry in the sense that there is no way to distinguish a hill from a valley. This can be altered by adding adsorption/desorption or other dynamics.

The numerical schemes with high order accuracy and energy stability have been of great interests, due to the long time nature of the gradient flow coarsening process. There have been many efforts to devise and analyze energy stable numerical schemes for both the SS and NSS equations; see the related references [6,8,17,23,29,31,36–39,41–43,45,47], etc. In particular, the linear schemes have been attracted a great amount of attentions