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Error Estimate of a Second Order Accurate Scalar Auxiliary Variable (SAV) Numerical Method for the Epitaxial Thin Film Equation

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Abstract. A second order accurate (in time) numerical scheme is analyzed for the slope-selection (SS) equation of the epitaxial thin film growth model, with Fourier pseudo-spectral discretization in space. To make the numerical scheme linear while preserving the nonlinear energy stability, we make use of the scalar auxiliary variable (SAV) approach, in which a modified Crank-Nicolson is applied for the surface diffusion part. The energy stability could be derived a modified form, in comparison with the standard Crank-Nicolson approximation to the surface diffusion term. Such an energy stability leads to an H^2 bound for the numerical solution. In addition, this H^2 bound is not sufficient for the optimal rate convergence analysis, and we establish a uniform-in-time H^3 bound for the numerical solution, based on the higher order Sobolev norm estimate, combined with repeated applications of discrete Hölder inequality and nonlinear embeddings in the Fourier pseudo-spectral space. This discrete H^3 bound for the numerical solution enables us to derive the optimal rate error estimate for this alternate SAV method. A few numerical experiments are also presented, which confirm the efficiency and accuracy of the proposed scheme.

AMS subject classifications: 35K30, 35K55, 65K10, 65M12, 65M70

Key words: Epitaxial thin film equation, Fourier pseudo-spectral approximation, the scalar auxiliary variable (SAV) method, Crank-Nicolson temporal discretization, energy stability, optimal rate convergence analysis.

1 Introduction

In this article we consider a slope-selection (SS) epitaxial thin film growth equation, which corresponds to the L^2 gradient flow associated with the following energy func-

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tional

$$E(\phi)=\int_\Omega\left(\frac{1}{4}(|\nabla\phi|^2-1)^2+\frac{\varepsilon^2}{2}|\Delta\phi|^2\right)d\mathbf{x}, \tag{1.1}$$

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 [23,38–40,54], 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 [39,49]. In turn, the chemical potential becomes the following variational derivative of the energy

$$\mu:=\delta_\phi E=-\nabla\cdot\left(|\nabla\phi|^2\nabla\phi\right)-\Delta\phi+\varepsilon^2\Delta^2\phi, \tag{1.2}$$

and the PDE stands for the L^2 gradient flow

$$\partial_t\phi=\nabla\cdot\left(|\nabla\phi|^2\nabla\phi\right)-\Delta\phi-\varepsilon^2\Delta^2\phi. \tag{1.3}$$

Meanwhile, another epitaxial thin film model has also been extensively studied, with the following energy functional

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

and the dynamical equation is formulated as

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

This model is referred to as the no-slope-selection (NSS) equation. In fact, the slope-selection energy (1.1) could be viewed an a polynomial approximation to the no-slope-selection energy (1.4), under a small-slope assumption that $|\nabla\phi|^2\ll 1$; see the related discussions in [36, 37, 39, 49]. A solution to (1.3) exhibits pyramidal structures, where the faces of the pyramids have slopes $|\nabla u|\approx 1$; meanwhile, the no-slope-selection equation (1.5) exhibits mound-like structures, and the slopes of which (on an infinite domain) may grow unbounded [39,59]. 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 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 [1, 11, 26, 35, 46, 50–53, 55, 59, 61, 64], etc. In particular, the linear schemes have attracted a great amount of attentions among the energy stable numerical approaches, due to its simplicity of implementation. For the NSS equation (1.5), there have been extensive works of linear, energy stable numerical schemes [5, 7, 8, 10, 13, 33, 35, 44, 48], with up to the third order accuracy in time. Such a nonlinear energy stability