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Artificial Regularization Parameter Analysis for the No-Slope-Selection Epitaxial Thin Film Model

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Abstract. In this paper we study the effect of the artificial regularization term for the second order accurate (in time) numerical schemes for the no-slope-selection (NSS) equation of the epitaxial thin film growth model. In particular, we propose and analyze an alternate second order backward differentiation formula (BDF) scheme, with Fourier pseudo-spectral spatial discretization. The surface diffusion term is treated implicitly, while the nonlinear chemical potential is approximated by a second order explicit extrapolation formula. A second order accurate Douglas-Dupont regularization term, in the form of $-A\Delta t\Delta_N^2(u^{n+1}-u^n)$, is added in the numerical scheme to justify the energy stability at a theoretical level. Due to an alternate expression of the nonlinear chemical potential terms, such a numerical scheme requires a minimum value of the artificial regularization parameter as $A=\frac{289}{1024}$, much smaller than the other reported artificial parameter values in the existing literature. Such an optimization of the artificial parameter value is expected to reduce the numerical diffusion, and henceforth improve the long time numerical accuracy. Moreover, 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 and accuracy of the alternate second order numerical scheme. 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.

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

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1 Introduction

The no-slope-selection (NSS) epitaxial thin film growth equation is the L^2 gradient flow associated with the following energy functional

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

in which $\Omega = (0,L_x)\times(0,L_y)$, $u:\Omega\to\mathbb{R}$ is a periodic height function, and ε is a constant parameter of transition layer width. In fact, the first non-quadratic term represents the Ehrlich-Schwoebel (ES) effect, which means that an atom has to overcome a higher energy barrier to stick to a step from an upper rather than from a lower terrace [11,21–23,33]. This 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 [22,27]. 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 dynamical equation stands for the L^2 gradient flow

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

On the other hand, under a small-slope assumption that $|\nabla u|^2 \ll 1$, (1.3) may be approximated as

$$\partial_t u = \nabla\cdot\left(|\nabla u|^2\nabla u\right) - \Delta u - \varepsilon^2\Delta^2 u, \tag{1.4}$$

with the energy functional given by a polynomial approximation

$$E(u) = \int_\Omega \left(\frac{1}{4}(|\nabla u|^2-1)^2 + \frac{\varepsilon^2}{2}|\Delta u|^2\right) d\mathbf{x}. \tag{1.5}$$

This model is referred to as the slope-selection (SS) equation [19,20,22,27]. A solution to (1.4) 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 [22,35]. 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.