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EFFICIENT LINEAR SCHEMES WITH UNCONDITIONAL ENERGY STABILITY FOR THE PHASE FIELD MODEL OF SOLID-STATE DEWETTING PROBLEMS*

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Abstract

In this paper, we study linearly first and second order in time, uniquely solvable and unconditionally energy stable numerical schemes to approximate the phase field model of solid-state dewetting problems based on the novel "scalar auxiliary variable" (SAV) approach, a new developed efficient and accurate method for a large class of gradient flows. The schemes are based on the first order Euler method and the second order backward differential formulas (BDF2) for time discretization, and finite element methods for space discretization. The proposed schemes are proved to be unconditionally stable and the discrete equations are uniquely solvable for all time steps. Various numerical experiments are presented to validate the stability and accuracy of the proposed schemes.

Mathematics subject classification: 65N38, 65N30.
Key words: Phase field models, Solid-state dewetting, SAV, Energy stability, Surface diffusion, Finite element method.

1. Introduction

Solid-state dewetting of thin films plays an important role in many engineering and industrial applications, such as microelectronics processing, formation of patterned silicides in electronic devices, production of catalysts for the growth of carbon and semiconductor nanowires [1, 3–7, 18, 19, 28]. In general, solid-state dewetting can be modeled as interfacial dynamic problems where the morphological evolution is controlled by the surface diffusion.

To understand the process of solid-state dewetting, many mathematical models have been developed, and numerical simulations based on these models have been carried out (cf. [1, 2, 28,

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29] and the references therein). During the evolution, the film/vapor interface may experience complicated topological changes such as pinch-off, splitting and fattening, all of them make a great difficulty in the simulation of this interface evolution problem. A phase field model that can naturally captures the topological changes that occur during the morphological evolution and can be easily extended to high dimension spaces is presented in [1], where the spectral method with stabilized scheme is employed.

The idea of phase field approach dates back to the pioneering work of [22] and [30]. It has been successfully employed in many fields of science and engineering ever since. The phase field method uses an auxiliary variable ϕ (phase field function) to localize the phases and describe the interface by a layer of small thickness. The phase field function takes two different values (e.g., $+1$ and -1) in each of the two phases and varies smoothly across the interface. In the phase field model, the interface is considered as a transition layer over which a continuous, but steep change of some physical quantities occurs. The phase field model can be naturally derived from the variational principle, i.e., via minimizing the free energy of the total system. As a result, the derived system satisfies an energy dissipation law, which justifies its thermodynamic consistency and leads to a mathematically well-posed model. Moreover, the presence of the energy law serves as a guideline for the design of energy stable numerical schemes. The phase field method now becomes one of the major modeling and computational tools for the study of interfacial phenomena (cf. [8–13, 20, 25, 26]), and the references therein).

From the numerical perspective, for phase field models, one main challenge in the numerical approximation is how to design unconditionally energy stable schemes which keep the energy dissipative in both semi-discrete and fully discrete forms. The preservation of the energy dissipation law is particularly important, and is critical to preclude the nonphysical numerical solutions. In fact, it has been observed that numerical schemes which do not respect the energy dissipation law may lead to large numerical errors, particular for long time simulation, so it is specially desirable to design numerical schemes that preserve the energy dissipation law at the discrete level. Another focus of developing numerical schemes to approximate the phase field models is to construct higher order time marching schemes. Under the requests of some degree of accuracy, higher order time marching schemes are usually preferable to lower order time marching schemes when we want to use larger time marching steps to achieve long time simulation. This fact motivates us to develop more accurate schemes. Moreover, it goes without saying that linear numerical schemes are more efficient than the nonlinear numerical schemes because the nonlinear schemes are expensive to solve.

In this paper, we study linearly first and second order accurate in time, uniquely solvable and unconditionally energy stable numerical schemes for solving the phase field model of solid-state dewetting problems based on the SAV approach which is applicable to a large class of gradient flows [15, 16]. The schemes for gradient flows that introduce auxiliary variables are first presented in [23, 24] known as the invariant energy quadratization (IEQ) approach, where the auxiliary variable is a function. The essential idea of the SAV approach is to split the total free energy $\mathcal{E}(\phi)$ of gradient flows into two parts, written as

$$\mathcal{E}(\phi) = \frac{1}{2}(\phi, \mathcal{L}\phi) + \mathcal{E}_1(\phi), \tag{1.1}$$

where $\mathcal{L}$ is a symmetric non-negative linear operator contains the highest linear derivative terms in $\mathcal{E}$, and $\mathcal{E}_1(\phi) \geq C > 0$ is the nonlinear term but with only lower order derivative than $\mathcal{L}$. Then the SAV approach transforms the nonlinear term $\mathcal{E}_1$ into quadratic form by introducing