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# An Efficient and Unconditionally Energy Stable Scheme for Simulating Solid-State Dewetting of Thin Films with Isotropic Surface Energy†

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**Abstract.** In this paper, we propose highly efficient, unconditionally energy-stable numerical schemes to approximate the isotropic phase field model of solid-state dewetting problems by using the invariant energy quadratization (IEQ) method. The phase field model is governed by the isotropic Cahn-Hilliard equation with degenerate mobilities and dynamic contact line boundary conditions. By using the backward differential formula to discretize temporal derivatives, we construct linearly first- and second-order IEQ schemes for solving the model. It can be rigorously proved that these numerical schemes are unconditionally energy-stable and satisfy the total mass conservation during the evolution. By performing numerical simulations, we demonstrate that these IEQ-based schemes (including the first-order IEQ/BDF1, second-order IEQ/BDF2) are highly efficient, accurate and energy-stable. Furthermore, many interesting dewetting phenomena (such as the hole dynamics, pinch-off), are investigated by using the proposed IEQ schemes.

**AMS subject classifications**: 74K35, 65M06, 65M12, 35K55

**Key words**: Solid-state dewetting, surface diffusion, phase-field model, degenerate Cahn-Hilliard equation, invariant energy quadratization, unconditionally energy-stable.

## 1 Introduction

Solid-state dewetting of thin films on substrates is a ubiquitous phenomenon in thin film technologies and materials science, which has been observed in a wide range of systems

†Dedicated to Professor Jie Shen on the occasion of his 60th birthday.
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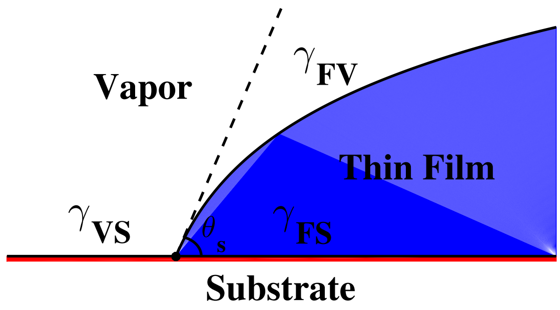


Figure 1: A schematic illustration of the three interfaces which meet with each other at the contact point/line in solid-state dewetting, where $\theta_s$ is Young's contact angle.

and is of considerable technological interest [1–6] (e.g., see the recent review papers by C. V. Thompson [7] and F. Leroy *et. al.* [8]). Nowadays, the solid-state dewetting has been widely used in thin film solar cells [9], optical and magnetic devices [10], sensor devices [11], catalyzing the growth of carbon nanotubes [12], semiconductor nanowires [13], etc. Especially, in recent years, the solid-state dewetting has attracted increasing attention both because of interest in the underlying pattern formation physics and its potential technology applications [14–19].

The dewetting of thin solid films deposited on substrates is very similar to the dewetting phenomena of liquid films on substrates, which has been investigated in numerous theoretical and experimental studies [20–24] and recently reviewed in [25]. For example, for both the phenomena, dewetting and pinch-off may happen when an initially continuous and long thin film is bonded to a rigid substrate and eventually an array of isolated particles will form. However, they have many important major differences. For example, their mass transport processes are totally different, while the solid-state dewetting is usually dominated by surface diffusion rather than fluid dynamics. The solid-state dewetting can be modeled as a type of interface-tracking problem for the evolution via surface diffusion flow, coupled with contact line migration [16,26–30]. More specifically, the contact line is a triple line (where the film, substrate, and vapor phases meet, shown in Fig. 1) that migrates as the curve/surface evolves.

In general, the dewetting problem belongs to a more general class of capillarity-controlled interface/surface evolution problems. The solid-state dewetting problem is mainly studied by using two different mathematical models, i.e., sharp-interface model and phase-field model. Behind these models, surface diffusion flow and contact line migration have been recognized as the two main kinetic processes during the solid-state dewetting evolution. The first sharp-interface model for solid-state dewetting was proposed by Srolovitz and Safran [31] to investigate the hole growth during the dewetting under the assumption of isotropic surface energy, small slope profile and cylindrical symmetry. Subsequently, the sharp-interface model was numerically solved without the small-slope assumption by using "marker particle method" (i.e., finite differ-