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A θ-L APPROACH FOR SOLVING SOLID-STATE DEWETTING PROBLEMS*

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Abstract

We propose a θ-L approach for solving a sharp-interface model about simulating solid-state dewetting of thin films with isotropic/weakly anisotropic surface energies. The sharp-interface model is governed by surface diffusion and contact line migration. For solving the model, traditional numerical methods usually suffer from the severe stability constraint and/or the mesh distribution trouble. In the θ-L approach, we introduce a useful tangential velocity along the evolving interface and utilize a new set of variables (i.e., the tangential angle θ and the total length L of the interface curve), so that it not only could reduce the stiffness resulted from the surface tension, but also could ensure the mesh equidistribution property during the evolution. Furthermore, it can achieve second-order accuracy when implemented by a semi-implicit linear finite element method. Numerical results are reported to demonstrate that the proposed θ-L approach is efficient and accurate.

Mathematics subject classification: 65M06, 65M12, 65M60, 75G15, 74H15.
Key words: Solid-state dewetting, Surface diffusion, Moving contact lines, Anisotropic surface energy, θ-L formulation, Finite element method.

1. Introduction

Solid thin films deposited on inert substrates will spontaneously dewet or agglomerate at elevated temperatures which are well below their melting points (i.e., the films are still in solid-state) [23, 26, 27, 39, 45, 51, 53]. This kind of solid-state dewetting has been thought of as a drawback in producing thin film-based devices since it can destroy the film structure and decrease the stability of the devices [26, 45]. However, solid-state dewetting has been recently exploited to provide a simple way for fabrication of well-ordered micro- and nano-structures [26, 45, 47, 51–53] which possess a wide range of applications in sensing [1], catalysis for nanotube and nanowire growth [40,42] and many other nano-technology-related applications [26,45]. These rich applications have led to renewed interests in designing mathematical models [2, 8, 16, 18–20, 22, 37, 43, 48, 49, 56] and efficient numerical methods [3, 4, 8, 18, 48, 49, 55, 56] for simulating solid-state dewetting.

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From modeling point of view, the solid-state dewetting problem belongs to a type of interface evolution problems. The problem is described by the evolution of the film/vapor interface and the migration of contact lines where the film, vapor and substrate phases meet with each other (as shown in Fig. 1.1). For modeling such an interface problem, a sharp-interface model is widely used [19,20,48]. In this model, the evolving film/vapor interface is usually described by surface diffusion flow, since the dominant mass transport process in solid-state dewetting is generally thought of as surface diffusion [32]; the contact line migration is designed to satisfy some physical constraints, such as the mass conservation and total free energy dissipation [20,25,48]. Under isotropic/weakly anisotropic surface energies, solid-state dewetting of thin films can be described by a (dimensionless) sharp-interface model in two dimensions as [3,48]

$$\begin{aligned} &\partial_t \mathbf{X} = V\mathbf{n} = \partial_{ss}\mu\ \mathbf{n}, && 0 < s < L(t), \quad t > 0, \\ &\mu = \widetilde{\gamma}(\theta)\kappa = \big(\gamma(\theta) + \gamma''(\theta)\big)\kappa, && \kappa = -(\partial_{ss}\mathbf{X}) \cdot \mathbf{n} \end{aligned} \tag{1.1}$$

subject to the following three boundary conditions:

(i) contact point condition

$$y(0,t) = 0, \quad y(L,t) = 0, \quad t \geq 0, \tag{1.2}$$

(ii) relaxed contact angle condition

$$\frac{dx_c^l}{dt} = \eta f\left(\theta_d^l; \sigma\right), \quad \frac{dx_c^r}{dt} = -\eta f\left(\theta_d^r; \sigma\right), \quad t \geq 0, \tag{1.3}$$

(iii) zero-mass flux condition

$$\partial_s \mu(0,t) = 0, \quad \partial_s \mu(L,t) = 0, \quad t \geq 0, \tag{1.4}$$

where s is the arc length, t is time, $\mathbf{X} := \mathbf{X}(s,t) = (x(s,t), y(s,t))$ represents the film/vapor interface (shown in Fig. 1.1) which is initially given as $\mathbf{X}(s,0) = \mathbf{X}_0(s)$, $0 \leq s \leq L(0)$, $L := L(t)$ is the total length of the interface curve, $\mathbf{n}$ is the unit outer normal vector, $V := V(s,t) = \partial_{ss}\mu$ denotes the normal velocity with $\mu := \mu(s,t)$ representing the chemical potential, $\kappa := \kappa(s,t)$ is the curvature of the interface curve, $\gamma(\theta)$ represents the surface energy density where $\theta \in [-\pi, \pi]$ is the local orientation (the interfacial normal/tangent angle) defined as the angle between $\mathbf{n}$ and y-axis (or the angle between the unit tangent vector $\boldsymbol{\tau}$ and x-axis), $\widetilde{\gamma}(\theta) := \gamma(\theta) + \gamma''(\theta)$

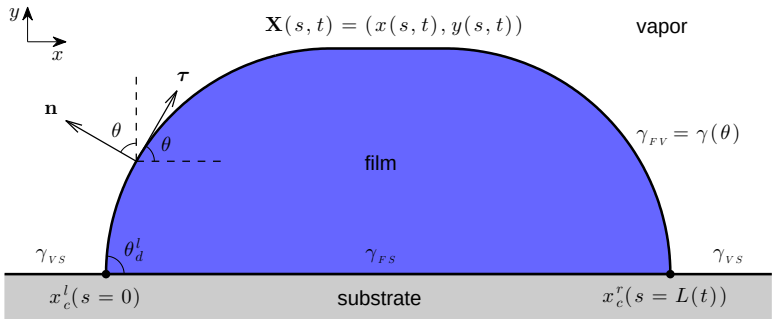

Fig. 1.1. A schematic illustration of an island film lying on a rigid flat substrate in two dimensions.