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AN ENERGY-STABLE PARAMETRIC FINITE ELEMENT METHOD FOR SIMULATING SOLID-STATE DEWETTING PROBLEMS IN THREE DIMENSIONS*

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Abstract

We propose an accurate and energy-stable parametric finite element method for solving the sharp-interface continuum model of solid-state dewetting in three-dimensional space. The model describes the motion of the film/vapor interface with contact line migration and is governed by the surface diffusion equation with proper boundary conditions at the contact line. We present a weak formulation for the problem, in which the contact angle condition is weakly enforced. By using piecewise linear elements in space and backward Euler method in time, we then discretize the formulation to obtain a parametric finite element approximation, where the interface and its contact line are evolved simultaneously. The resulting numerical method is shown to be well-posed and unconditionally energy-stable. Furthermore, the numerical method is generalized to the case of anisotropic surface energies in the Riemannian metric form. Numerical results are reported to show the convergence and efficiency of the proposed numerical method as well as the anisotropic effects on the morphological evolution of thin films in solid-state dewetting.

Mathematics subject classification: 74H15, 74S05, 74M15, 65Z99.
Key words: Solid-state dewetting, Surface diffusion, Contact line migration, Contact angle, Parametric finite element method, Anisotropic surface energy.

1. Introduction

A thin solid film deposited on the substrate will agglomerate or dewet to form isolated islands due to surface tension/capillarity effects when heated to high enough temperatures but well below the thin film's melting point. This process is referred to as the solid-state dewetting (SSD) [1] since the thin film remains solid. In recent years, SSD has been found wide applications in thin film technologies, and it is emerging as a promising route to produce well-controlled patterns of particle arrays used in sensors [2], optical and magnetic devices [3], and catalyst formations [4]. A lot of experimental (e.g., [5–11]) and theoretical efforts (e.g., [12–21]) have been devoted to SSD not just because of its importance in industrial applications but also the arising scientific questions within the problem.

In general, SSD can be regarded as a type of open surface evolution problem governed by surface diffusion [22] and moving contact lines [23]. When the thin film moves along the solid substrate, a moving contact line forms where the three phases (i.e., solid film, vapor and substrate) meet. This brings an additional kinetic feature to this problem. Recently, different

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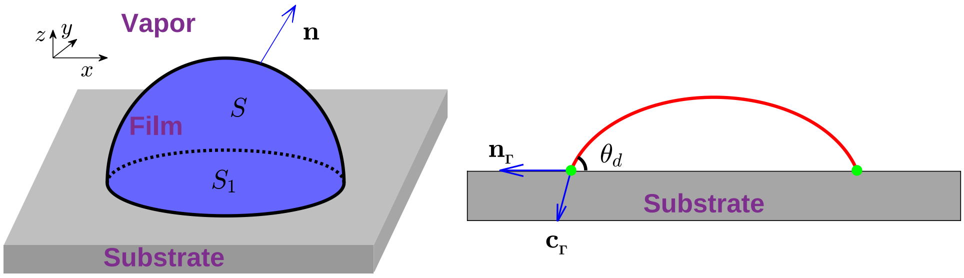

Fig. 1.1. Left panel: A geometric setup of SSD, where a thin film (shaded in blue) is deposited on a flat rigid substrate (shaded in gray), S is the film/vapor interface and S_1 is the film/substrate interface. Right panel: configuration of the contact angle: $\theta_d = \cos^{-1}(\mathbf{c}_\Gamma \cdot \mathbf{n}_\Gamma)$ at the contact line (green).

mathematical models and simulation methods have been proposed to study SSD, such as sharp-interface models [14,19,23,24], phase-field models [12,25–27] and other models including the crystalline formulation [28,29], discrete chemical potential method [18] and kinetic Monte Carlo method [30].

In this work, we will restrict ourselves to the model in [24]. It is a sharp-interface model in three dimensions (3D) and was developed based on the thermodynamic variation. As illustrated in Fig. 1.1(a), we consider the case when a thin film is deposited on a flat substrate. The evolving film/vapor interface is described by a moving open surface $S(t)$ with mapping given by (with $\mathbf{X} = (x,\ y,\ z)^T$ or $\mathbf{X} = (x_1,\ x_2,\ x_3)^T$)

$$\mathbf{X}(\boldsymbol{\rho},\ t) = \Big(x_1(\boldsymbol{\rho}, t),\ x_2(\boldsymbol{\rho},\ t),\ x_3(\boldsymbol{\rho}, t)\Big)^T : S^0 \times [0,\ T] \to \mathbb{R}^3, \tag{1.1}$$

where $S^0 = S(0)$ is the initial surface. The film/substrate interface is a flat surface, i.e., a two-dimensional moving domain and denoted by $S_1(t)$. The two interfaces intersect at the contact line and form a closed curve $\Gamma(t) := S(t) \cap S_1(t)$. We assume $\Gamma(t)$ is a simple closed curve and positively orientated with the mapping given by: $\Gamma(t) := \mathbf{X}_\Gamma(\boldsymbol{\rho},\ t),\ \boldsymbol{\rho} \in \Gamma^0 = \Gamma(0)$.

Some relevant geometric parameters are defined as follows: $\mathbf{n}$ and $\mathcal{H}$ are the unit outward normal vector and mean curvature of $S(t)$, respectively; $\mathbf{c}_\Gamma$ and $\mathbf{n}_\Gamma$ represent the outward unit conomral vector of $S(t)$ and $S_1(t)$, respectively, and ∇_s is the surface gradient operator defined in (A.1). The sharp-interface model of SSD in 3D can be stated as [24]:

$$\partial_t \mathbf{X} = \Delta_s \mathcal{H}\, \mathbf{n}, \tag{1.2a}$$
$$\mathcal{H} = -\,(\Delta_s \mathbf{X}) \cdot \mathbf{n}, \tag{1.2b}$$

where $\Delta_s = \nabla_s \cdot \nabla_s$ is the surface Laplacian operator. The above equations are supplemented with the following conditions at $\Gamma(t)$:

(i) The contact line condition

$$x_3(\cdot,\ t)\big|_\Gamma = 0, \qquad t \geq 0. \tag{1.3a}$$

(ii) The relaxed contact angle condition

$$\partial_t \mathbf{X}_\Gamma = -\eta\,(\mathbf{c}_\Gamma \cdot \mathbf{n}_\Gamma - \cos\theta_Y)\,\mathbf{n}_\Gamma, \qquad t \geq 0. \tag{1.3b}$$

(iii) The zero-mass flux condition

$$(\mathbf{c}_\Gamma \cdot \nabla_s \mathcal{H})\big|_\Gamma = 0, \qquad t \geq 0. \tag{1.3c}$$