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Convex Splitting Method for Strongly Anisotropic Solid-State Dewetting Problems in Two Dimensions

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Abstract. A novel sharp-interface model for the solid-state dewetting problem in the two-dimensional case is proposed. Instead of incorporating the Willmore energy or an L_2-curvature regularization term as is done in previous studies, we add an L_1-curvature regularization to the interfacial energy functional in order to make this problem well-posed. Experiments show that such regularization improves the computational efficiency. In strongly anisotropic case, we consider a new numerical scheme based on the convex-splitting idea. This approach remarkably relax the restriction on the time step. In addition, we present the theoretical analysis of the scheme. Numerical results demonstrate the high efficiency and accuracy of the method.

AMS subject classifications: 65M10, 78A48

Key words: Strongly anisotropic, convex-splitting, solid-state dewetting, parametric finite element method.

1. Introduction

In material science and engineering, the solid thin film is viewed as a basic building component in the construction of micro- and nanoscale devices. Driven by capillarity effects, solid thin films sitting on a substrate are rarely stable and can exhibit complex morphological changes — e.g. faceting, edge retraction, pinch-off, and fingering instabilities. In general, they will dewet or agglomerate to disjoint islands with the temperature increase. This phenomenon is called the solid-state dewetting.

Unlike to the fluid dynamics in the liquid-state dewetting, the dominant influence in solid-state thin films is surface diffusion. This force compels thin films to minimize the total energy of the free surfaces of the film, the substrate, and the film-substrate interface. Meanwhile, it was noted that the driving force increases with the film thickness decrease. Dewetting can be used in order to form the shape of nanoscale particles in sensors and optical magnetic devices. On the other hand, it can influence the nanodevice performance

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due to the instability. Therefore, it is important to characterize the patterns of thin films when dewetting occurs. Due to the complicated evolution of interface and difficulties in numerical simulations, the problem has attracted considerable interest and has been widely studied by experimental and theoretical methods [25,36].

From a mathematical perspective, we want to determine a connected equilibrium shape Ω of an island/film on a substrate, which minimizes the total interfacial energy functional of the system

$$\min_{\Omega} W = \int_{\Gamma_{FV}} \gamma_{FV}\, d\Gamma_{FV} + \int_{\Gamma_{FS}} \gamma_{FS}\, d\Gamma_{FS} + \int_{\Gamma_{VS}} \gamma_{VS}\, d\Gamma_{VS} \tag{1.1}$$

assuming that the total volume $|\Omega|$ of the tin film Ω is constant — cf. Fig. 1, [16,21].

Note that Γ_{FV}, Γ_{FS}, and Γ_{VS} respectively denote the film/vapor, film/substrate, and vapor/substrate interfaces and γ_{FV}, γ_{FS}, and γ_{VS} are the corresponding interfacial energy densities. Following typical solid-state dewetting problems, we assume that γ_{FS} and γ_{VS} are constants. For a crystalline film, γ_{FV} is a function of the surface normal θ to the film/vapor interface — i.e. $\gamma_{FV} = \gamma(\theta) \in C^0[-\pi,\pi]$ is a positive periodic function. In two dimensions, θ is the angle between the outer surface normal and the y-axis. For constant γ_{FV} the problem is isotropic but if it depends on the orientation of the interface (free surface), we have an anisotropic problem. It is called weakly anisotropic if the surface stiffness satisfies the condition

$$\tilde{\gamma}(\theta) = \gamma(\theta) + \gamma''(\theta) > 0 \quad \text{for all} \quad \theta \in [-\pi,\pi].$$

Otherwise, we say that it is strongly anisotropic.

The equilibrium shape of an island on the substrate is often called Winterbottom shape [39] and can be determined by the Wulff-Kaischew construction [18], i.e. a Wulff shape truncated by a flat substrate plane in two/three dimensions, which depends on $\gamma_{VS} - \gamma_{FS}$. The Winterbottom construction [19,22,47] only describes the film shapes corresponding to global minimizers of the free energy — i.e. the solution to (1.1). However, various experiments show that final shapes are not always consistent with the Winterbottom shape and the island shapes trap in metastable free energy — i.e. in local minimizers to problem (1.1). This local minimizers appear in strongly anisotropic cases because the free energy functional is not convex [23,27]. Bao *et al.* [2] proposed a generalization of the Winterbottom construction to determine all possible stable equilibria, including local and global

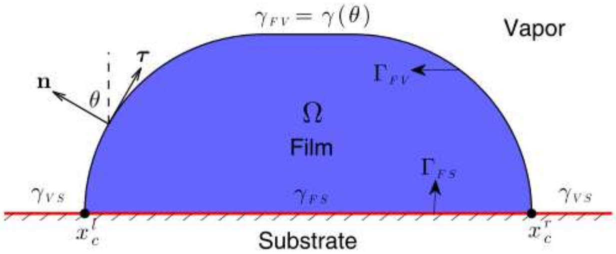

Figure 1: A illustration of a film on a flat.