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A θ-L Formulation-Based Finite Element Method for Solving Axisymmetric Solid-State Dewetting Problems

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Abstract. We propose a θ-L formulation-based finite element method for the sharp-interface model of solid-state dewetting with axisymmetric geometry. The model describes the film/vapor interface using the radial curve in cylindrical coordinates, and is governed by a fourth-order geometric partial differential equation with complex boundary conditions at the moving contact lines. By introducing an appropriate tangential velocity, we derive an equivalent system for the original sharp-interface model. This gives the kinetic equation for the tangential angle θ and the total length L of the radial curve. The new formulation can alleviate the stiffness of the original model and help to maintain mesh equidistribution during the evolution. We present an efficient finite element method for solving the resulting θ-L formulation based on its weak form. Numerical examples are reported to demonstrate the accuracy and efficiency of the numerical scheme.

AMS subject classifications: 65M60, 74H15, 65Z99

Key words: Solid-state dewetting, surface diffusion, moving contact line, θ-L formulation, finite element method.

1. Introduction

Solid thin films deposited on the substrate are usually metastable or unstable in the as-deposited state and can exhibit complex morphological evolutions even when the temperature is well below the film material melting point. This phenomena, known as solid-state dewetting, has been widely observed in many thin film/substrate systems [23]. Recently,

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solid-state dewetting problems have attracted increasing attention not only because of the arising scientific problems in physics, applied mathematics and scientific computing, but also due to its wide applications in industrial technologies such as sensors [1], carbon catalysts [20] and semiconductor nanowire growth [21]. For more details about experimental observations and underlying applications, the readers may refer to the recent review papers [19,23]. Therefore, a better understanding of the underlying mechanisms of solid-state dewetting is necessary.

In general, surface diffusion is recognised as the dominant mass transport of the solid-state dewetting — cf. [14–16, 24, 25, 28]. In addition, as the film-vapor interface evolves, it generates a contact line (where the film, substrate and vapor phases meet with each other) that migrates along the substrate. Surface diffusion and contact line migration constitute two important kinetic features of the solid-state dewetting problem. Progress has been made in modeling and simulation for solid-state dewetting problems by using sharp-interface models [15, 16, 22, 24, 26–28], phase-field models [9, 12, 14], and other models [7, 29].

In this work, we focus on the sharp-interface model proposed by Zhao [26]. This model is a fourth-order geometric partial differential equation (PDE) for simulating the solid-state dewetting of thin films with weakly anisotropic surface energies under the assumption of the axisymmetric geometry. In the model, the film-vapor interface is described by a radial curve in the cylindrical coordinate. The dynamic of the curve is governed by a high-order nonlinear geometric PDE, which generates numerous issues in the development of numerical methods.

There are various numerical methods for simulating the evolution of a closed or open curve governed by surface diffusion — cf. [2,4,10], including "marker-particle" methods [8, 24,25] and parametric finite element methods [3,27,28]. Nevertheless, since the governing equation is highly nonlinear and of high order, explicit numerical schemes often suffer from a severe stability constraint on the time step [24, 25]. Besides, traditional front-tracking methods for the interface evolution generally suffer from mesh distortion and need to rely on mesh regularisation/smoothing algorithms [2, 18, 24, 28] in order to preserve the good mesh quality. Barrett *et al.* [4, 6] proposed a parametric finite element method based on a novel weak formulation which allows implicit tangential velocities. By using semi-implicit method in time and piecewise linear element in space, a full discretisation of the weak formulation can result in unconditional energy stability and good mesh quality. We also note a fully implicit approximation in [5] based on the weak formulation. It can realise the mesh equidistribution but a system of nonlinear algebraic equations needs to be solved at each time step. Unfortunately, these numerical methods are limited to the case when the surface energy is isotropic or takes the specific form.

In this work, we propose an efficient and accurate θ-L formulation for solving the axisymmetric sharp-interface model in [26]. This approach is based on the θ-L formulation proposed by Hou *et al.* [11] for the simulation of interfacial flows with surface tension. Here, the local orientation (the tangential angle) θ, and the curve length L are used as the frame of reference to describe the interface curve and a prescribed tangential velocity is introduced to ensure the equal mesh property. This helps to remove the stiffness arising