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Surface Diffusion on Stressed Solid Surface

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Abstract. The surface diffusion of an axi-symmetric solid, a whisker, subject to applied uniaxial stress, is studied numerically based on a new boundary integral formulation for periodic stress configurations. An efficient semi-implicit time-stepping scheme is developed to treat the serve stiffness due to high-order derivatives. When the initial perturbation is small the effect of the stress on the motion of the whisker is found to agree with the linear stability analysis. Numerical simulations of a fully nonlinear case are also presented, and a potential break-up of the whisker is observed.

AMS subject classfications: 74B20, 65N38

Key words: Surface diffusion, elastic stress, boundary integral method, semi-implicit scheme.

1 Introduction

When a solid is heated, the atoms on the outer surface diffuse to form a thermodynamically lower energy configuration. Such a surface diffusion motion of a thin solid rod, a whisker, driven by surface energy only, was first studied by Nichols and Mullins [8]. They derive the Rayleigh criteria for stability of a cylinder, i.e., it is unstable to axi-symmetric perturbations whose wavelength exceeds the circumference of the unperturbed cylinder. This result is analogous to the classical Rayleigh instability of a cylinder of a fluid under surface tension. In both cases, the instability causes the cylinder to pinchoff forming a chain of spheres that minimizes the surface energy for a fixed volume. Through second- and higher-order perturbation arguments and finite-element calculations, Coleman *et al.* [2, 3] have shown that a cylinder is unstable to perturbations of

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certain combination of linearly stable wavelengths. The surface diffusion and the self-similar axi-symmetric pinchoff of a cylinder have been examined using asymptotic, numerical and analytical methods by several authors. For a review and the references, see Bernoff *et al.* [1].

The effect of elastic stress on the morphological instability of a whisker has been studied by linear stability analysis in Colin *et al.* [4] and Kirill *et al.* [6]. The results show that short-wavelength instability can develop when the applied stress is beyond a critical value and non-axisymmetric modes can be excited under certain conditions.

In this work, we investigate the fully nonlinear evolution of an axi-symmetric whisker when the stress is present. In Section 2, we state the problem in which the whisker is periodic in one direction and subject to a periodic applied stress. In Section 3, two equivalent boundary integral formulations of the problem are derived, enabling the sharp-interface numerical simulation.

The nonlinear evolution equation for the whisker involves surface diffusion of the interface curvature. This fourth-order derivative term puts a severe constraint on the time-step when explicit temporal schemes are used. On the other hand, any fully implicit schemes require solving nonlinear systems at every time-step, and it is extremely expensive. In this paper, we present an efficient semi-implicit temporal scheme for interfaces in axi-symmetric geometry based on the local decomposition technique [9,11,15]. Realizing that the meridian term in the mean curvature for an axi-symmetric interface dominates the stability property of a temporal scheme, we express it in terms of the tangent angle of the interface. As a result, the most stiff term reduces to a fourth-order derivative of the tangent angle, and it becomes linear in Fourier space. We treat this term implicitly and the rest of the nonlinear terms in low-oder derivative explicitly. A detailed description of the numerical methods is presented in Section 4. In Section 5, our formulation of the problem and numerical methods are validated using the results from linear stability analysis and the effect of elastic stress is investigated in nonlinear evolution region.

2 Governing equations

Consider an infinite cylinder, periodic on the x-direction with period L_p, as shown in Fig. 1. Denote the cylinder by Ω, its boundary/surface by $\partial\Omega$, and its outward unit normal by $\mathbf{n}$. Let $\partial\Omega_l$ be a cross section of the cylinder with a plane perpendicular to x-axis, and $\partial\Omega_r$ be the first periodic image of $\partial\Omega_l$ to the right. $\partial\Omega_p$ is the one-period section of cylinder surface that is between $\partial\Omega_l$ and $\partial\Omega_r$.

The surface of the cylinder evolves due to surface diffusion which minimizes the sum of the surface energy and elastic energy. Its normal velocity is given by ([6] and references therein)

$$v_n = \frac{\partial \mathbf{x}}{\partial t}\cdot\mathbf{n} = \nabla_s^2(\beta g^{el} - \kappa), \tag{2.1}$$

where $\kappa = \boldsymbol{\nabla}\cdot\mathbf{n}$ is the sum of the principle curvatures, g^{el} is the elastic energy density,