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A tangent-plane marker-particle method for the computation of three-dimensional solid surfaces evolving by surface diffusion on a substrate

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ABSTRACT

We introduce a marker-particle method for the computation of three-dimensional solid surface morphologies evolving by surface diffusion. The method does not use gridding of surfaces or numerical differentiation, and applies to surfaces with finite slopes and overhangs. We demonstrate the method by computing the evolution of perturbed cylindrical wires on a substrate. We show that computed growth rates at early times agree with those predicted by the linear stability analysis. Furthermore, when the marker particles are redistributed periodically to maintain even spacing, the method can follow breakup of the wire.

1. Introduction

Capillarity-driven morphological instabilities and evolution of solid micro and nanostructures [29,27,28,5] are important in many branches of materials science and engineering, such as electronic materials processing, crack healing in ceramics, and densification of powder particles during sintering. For a microelectronic or optoelectronic device to function properly, the structural integrity of the thin films must be maintained [18,15,35,36]. This requirement becomes more stringent as the component size of integrated circuits decreases. Thus, characterization of thin film deformation is becoming one of the more important issues in the reliability of integrated circuits.

Several methods have been proposed for direct computation of 3D solid deformation by surface diffusion. The level-set methods were developed by Smereka [33] and Smith et al. [34], the finite-element methods by Burger [3], Bänsch et al. [1], Hausser and Voigt [14], Mayer [21], and Deckelnick et al. [9], and the finite-difference method by Zhang [44]. Most of these methods allow for surface topology changes and for implicit time stepping, and some allow for strong crystalline anisotropy and associated formation of corners and cusps. However, with the exception of Ref. [34], all cited methods are for closed or open periodic surfaces freely suspended in space. The method of Ref. [34] is capable of computing the deforming contact lines, but it requires $N-1$ level set functions if N phases are present, plus complicated and delicate procedure to prevent formation of vacuum or overlaps at junctions of phases. All cited methods employ gridding of either the surface,

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or of the three-dimensional space (as in the level set method). The level set and the finite-difference methods require numerical differentiation. The finite-element methods usually require complex mesh regularization and triangulation's angle control, at least at large times.

In this paper we describe a meshless particle method for computing evolving solid surfaces which are in contact with a material boundary (substrate) at all times [42,20,19]. In crystal growth such setup is universal, since all methods for thin film growth rely on deposition from the vapor phase or by means of atomic beams. We choose to model a cylindrical solid wire on a substrate as it evolves by surface diffusion. It is assumed that the wire has been pre-grown in such a way that its axis is parallel to the substrate. In the following, we call such wire *supported*, while one that is free of contact with any material boundary is called a *free* wire. The cross-sectional shape of the wire is a part-circle with small perturbations imposed in the axial and circumferential directions. We assume isotropic surface energy in this paper.

The surface and the three-phase contact lines formed among the film, substrate and air are explicitly tracked. We make no assumption as to the smallness of the surface slope and allow any values of a contact angle α in $(0,\pi)$. Surface overhangs are handled naturally in our method. The method uses biquadratic interpolation for the computation of the surface normal and (mean) curvature, and the surface Laplacian of mean curvature. We perform most of the computations in the local tangent-plane coordinate system where the surface Laplacian is greatly simplified (Front-tracking methods employing marker particles have been long in use (and proved very successful) for direct numerical simulations of multiphase fluid flows and solidification. The very extensive list of contributors and bibliography can be found in the review paper by Tryggvason et al. [38]).

The linear stability of supported circular wires with isotropic surface energy was considered by McCallum et al. [22], and with anisotropic surface energy by Gurski et al. [13]. The linear stability of free circular wires with isotropic surface energy, with respect to axial or circumferential perturbations was examined by Nichols and Mullins [30]. Surface energy anisotropy was factored in the linear stability analysis of free wires by Cahn [4] and Gurski and McFadden [12] (In a related study, Kan and Wong [16] considered the three-dimensional linear stability of a two-dimensional profile of a retracting edge of a film on a substrate (assuming isotropic surface energy) [15,8,43] and found one unstable mode of perturbation; thus the edge becomes wavy when perturbed. They determined the growth rate of the perturbation as a function of the wavelength of the perturbation and the speed of the receding edge).

This problem of stability of cylindrical wires can be traced back to Plateau and Lord Rayleigh [31,32]. Rayleigh found that free, inviscid, capillary liquid threads are unstable to small axisymmetric perturbations whose wavelengths are greater than the circumference of the undisturbed thread. Under the action of instability, the thread would tend to decompose in isolated liquid droplets [25]. These conclusions hold also for the solid, free cylindrical wires with isotropic surface energy [30]. For such wires, all purely non-axisymmetric disturbances decay. Rayleigh instability of supported copper, gold and platinum nanowires was experimentally demonstrated [37,17,45]. The kinetic Monte Carlo simulations of instability development due to axisymmetric perturbation (in a free wire) were performed by Muller et al. [26] and gave predictions consistent with the Nichols and Mullins analysis.

This paper aims to present the new method and to validate it by computing the evolution of perturbed surfaces to equilibrium, which could be wires if the perturbation is stable or drops if the perturbation is unstable. Physical implications/discussion will be presented elsewhere. It must be noted that we do not restrict the perturbation to axisymmetric form (Stability and dynamics in the axisymmetric case for free cylindrical wires have been extensively studied using analytical and numerical methods; most notably, see Refs. [7,6,41,2]).

2. Problem formulation

When a solid film evolves by capillarity-driven surface diffusion, the film surface displaces with a normal velocity that obeys [29]

$$V_n^* = B(\nabla_s^* \cdot \nabla_s^*)\kappa^*, \tag{1}$$

where ∇_s^* is the surface gradient operator, $\kappa^* = \nabla^* \cdot \mathbf{n}$ is the surface mean curvature (termed simply "curvature" below), $\mathbf{n}$ is the unit outward normal to the surface, and B is a material constant. Superscript * denotes dimensional variables. This equation is derived using the fact that the chemical potential varies linearly with the curvature of the solid film surface. If the surface curvature is not uniform, then a gradient in chemical potential exists. This gradient drives a surface flux, which redistributes mass along the solid surface. The net effect is that the solid surface moves in the normal direction.

To demonstrate the tangent-plane method, we simulate the evolution of a supported wire with the cross-sectional shape of a part-circle (Fig. 1). The radius of the circle is R_0 which is used as the length scale. Time is made dimensionless by R_0^4/B. In dimensionless variables, Eq. (1) reads

$$\frac{d\mathbf{r}}{dt} \cdot \mathbf{n} = V_n = \nabla_s^2(\nabla \cdot \mathbf{n}), \tag{2}$$

where $\mathbf{r}(t) = x(t)\mathbf{i} + y(t)\mathbf{j} + z(t)\mathbf{k}$ is the position vector of a point on a surface. The Cartesian coordinates (x, y, z) are defined with y pointing in the axial direction and z pointing upward, as shown in Fig. 1. These coordinates form the global coordinate system. The governing, fourth-order Eq. (2) is subject to the following boundary conditions. At the contact line $x = x_c(y)$, the