Growth Dynamics of Sputter Deposition

Karunasiri, Bruinsma, and Rudnick[1] recently proposed an equation of motion for the height $h(x,t)$ of a one-dimensional solid-on-solid film growing under conditions of sputter deposition.[1] Their intent was to include the effects of nonlocal shadowing of the incident flux, surface diffusion, and noise. The purpose of this Comment is to point out that a more complete treatment of the deposition term completely changes the morphological evolution of the surface from that obtained in Ref. 1.

Every point on the surface is presumed to receive flux from the vapor phase from all angles of incidence which are not geometrically shadowed by other parts of the surface (see Fig. 1 of Ref. 1). This deposition contributes to growth [in the direction of the local surface normal $\mathbf{n}(x)$] at a rate $v_{\mathbf{n}}(x)$ given by the *projection* of this flux $\mathbf{J}(\alpha) = -(R/2)[\mathbf{i}\cos\alpha + \mathbf{j}\sin\alpha]$ along $\mathbf{n}(x)$ integrated over the total opening angle. Surface diffusion contributes to the normal growth at a rate proportional to the second derivative of the local surface curvature $K(x)$ with respect to the arc length s.[2] Thus, neglecting shot noise in the deposition flux,

$$v_{\mathbf{n}}(x) = -\int_{\phi_R(x)}^{\pi-\phi_L(x)} \mathbf{J}(\alpha)\cdot\mathbf{n}(x)d\alpha + D\frac{\partial^2 K(x)}{\partial s^2}. \quad (1)$$

In this expression, $\phi_R(x)$ and $\phi_L(x)$ are acute angles which define the angular limits for flux arrival at a point x. Note that these angles are actually functionals of the entire surface profile $h(x)$ and $\phi_L(x)+\phi_R(x)+\theta(x)=\pi$ with the definition of $\theta(x)$ in Ref. 1.

Figure 1 exhibits the evolution of a small-amplitude sinusoid as determined numerically from Eq. (1) for $D/R=0.1$. The growth is unstable but evidently differs substantially from the dynamics found in Ref. 1. When $h(x,t)$ is single valued we may write[2] $\partial h/\partial t = v_{\mathbf{n}}(x) \times [1+(\partial h/\partial x)^2]^{1/2}$ so that, for $D=0$,

$$\frac{\partial h}{\partial t} = \frac{R}{2}\left\{\frac{\partial h}{\partial x}[\sin\phi_R(x) - \sin\phi_L(x)] + [\cos\phi_R(x)+\cos\phi_L(x)]\right\}. \quad (2)$$

This is exact. To understand the evolution of a small-amplitude wave, it is sufficient to expand Eq. (2) to second order in the angles $\phi_L(x)$ and $\phi_R(x)$,

$$\frac{\partial h}{\partial t} = R + \frac{R}{2}\frac{\partial h}{\partial x}[\phi_L(x)-\phi_R(x)] - \frac{R}{4}[\phi_R^2(x)+\phi_L^2(x)]. \quad (3)$$

Let $h=0$ correspond to the maxima of the initial surface at $t=0$. In the vicinity of these maxima it is clear that one of the shadow angle limits is nearly zero while the other is approximately $\partial h/\partial x$. Then, from Eq. (3), evolution proceeds according to $\partial h/\partial t = R + (R/2)(\partial h/\partial x)^2$. A particular solution of this equation is $h(x,t) = Rt - a_0 x^2/(1+a_0 Rt)$, where a_0 is a constant. The surface thus advances at an average rate of R while local

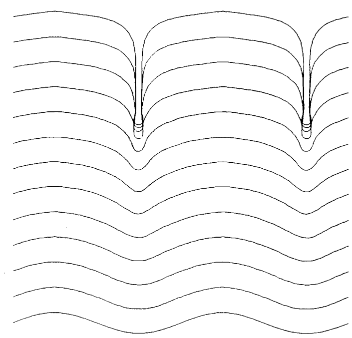

FIG. 1. Evolution of a small-amplitude, periodic initial surface obtained by numerical evolution of Eq. (1) for $D/R=0.1$.

maxima evolve toward inverted parabolas which flatten out as growth proceeds. Similarly, in the immediate vicinity of the local minima of $h(x,t)$, $|\phi_L(x)| = |\phi_R(x)| \simeq h/(\lambda/2)$, where λ is the wavelength of $h(x,t)$. Equation (3) then yields $\partial h/\partial t = R - 2R(h/\lambda)^2$ and the minima steadily evolve toward grooves. Observe that there is no *linear* instability; morphological evolution is nonlinear from the outset.

So far, we have been unable to establish analytically that a groove, once formed, continues to propagate parallel to itself as is clearly observed in Fig. 1. On the other hand, it is easy to show that an established groove will not pinch off at a point far down from the top due to the small flux that it continues to receive from the vapor. Moreover, one can show directly from Eq. (2) that if a surface possesses a unique absolute maximum (unlike a sinusoid), the maximum evolves according to Huygens' principle (in a frame moving at velocity $R/2$) and spreads out like an optical wave front. This result, coupled with the shadowing evident in Fig. 1, is sufficient to construct a quantitative alternative to "natural selection" models[3] for the columnar microstructure observed in many cases of thin-film growth. This work, along with the smoothing effects of surface diffusion, will be presented in full elsewhere.

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G. S. Bales and A. Zangwill
School of Physics
Georgia Institute of Technology
Atlanta, Georgia 30332

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