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The Equilibrium Topography of Sputtered Amorphous Solids II

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The sputtering of an amorphous solid is considered analytically and the equations of motion of the changing surface topography derived.

These equations are solved to show that a steady state is reached only in conditions where the surface topography consists of planes aligned, either parallel or perpendicular to the direction of sputtering ion incidence.

1. Introduction

In an earlier communication [1], a theoretical model for the generation of an equilibrium topography of an amorphous, isotropic solid, sputtered by a beam of uniform density energetic heavy ions was developed. This model assumed that, for such a solid, the sputtering coefficient was only a function of the angle of incidence of the ion flux to the normal to the surface at any point on the surface, but a restriction was placed upon the motion of the surface perpendicular to the ion beam, in that pinning regions (e.g. dislocations, vertical generators, surface contamination, etc.) were included to inhibit the surface motion. In the present work, this restriction has been removed and the development of surface contours in an infinite surface are studied. In particular, the equilibrium states of the contour are defined.

2. Theoretical Model

As in the earlier study, we are considering the erosion of a solid amorphous, isotropic substance, as a result of the ejection of atoms from the surface by an energetic heavy ion beam, or the phenomenon known as sputtering. The atomic details of the sputtering process are, at this stage, unimportant to the development of an erosion model, but again it must be pointed out that the model discounts surface rearrangement effects due to local irregularities in atomic density (ingrown occlusions), surface diffusion processes and redeposition of sputtered material.

A sputtering coefficient S, is defined as the number of atoms of a solid ejected per incident ion. S depends on ion species and energy, target material and other parameters, but once these are fixed S is a function only of θ (the angle between the beam direction and the surface normal).

S has a form which typically increases from S_0 at $\theta = 0$, to a maximum at $\theta = \pm\, \theta_p$ and declines to zero at $\theta = \pm\, \pi/2$.

Consider a beam of ϕ ions/sec striking an area A of a surface, at an angle θ to the normal. Let n = atomic density of target.

In a time δt, let the surface erode by a distance δr, in a direction perpendicular to the surface.

Then the number of atoms ejected $= nA\delta r$ and, the number of atoms incident $= \phi\delta t$. By definition,

$$S = \frac{nA\,\delta r}{\phi\,\delta t} = \frac{nA\cos\theta\,\delta r}{\phi\cos\theta\,\delta t} = \frac{n\,\delta r}{\Phi\cos\theta\,\delta t}$$

where Φ is the incident flux density.

$$\therefore\ \frac{\delta r}{\delta t} = \frac{\Phi}{n}\,S_\theta\cos\theta \tag{1}$$

We now consider, for simplicity, the erosion of a surface generator lying in the $x0y$ plane, with the beam of ions incident in the $0y$ direction.

Let A and B be two adjacent points on an eroding surface with centre of curvature at O, which erode to A', B' where AA' and BB' are perpendicular to the tangents at A, B. (See fig. 1.)

Then $AA' = \Phi/n\,(S\cos\theta)_1\,\delta t$ and $BB' = \Phi/n\,(S\cos\theta)_2\,\delta t$. If $A'C$ is drawn parallel to AB, then

$$CB' = \frac{\Phi}{n}\frac{\partial}{\partial\theta}(S\cos\theta)\frac{\partial\theta}{\partial x}\,\delta t.\delta x$$

and $A'C \simeq R\,\partial\theta/\partial x.\delta x$.

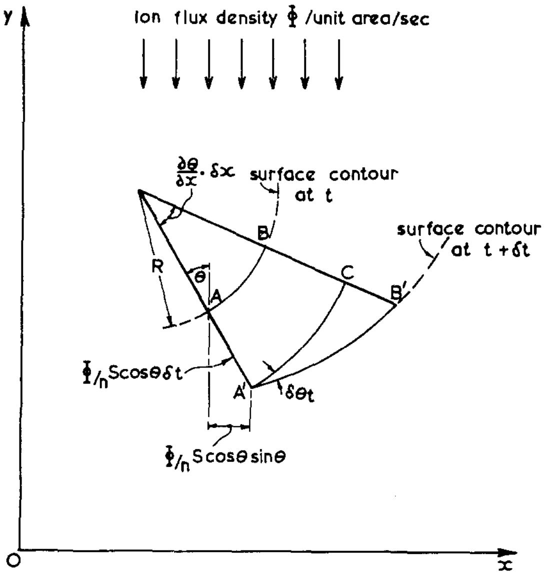

Figure 1 Erosion of a surface generator by an ion flux.

If $\delta\theta_t$ is the change in tangential angle from A to A' in time δ_t, then

$$-\delta\theta_t = \frac{CB'}{A'C} = \Phi/n \frac{\partial}{\partial\theta}(S\cos\theta)\frac{\delta t}{R}$$

or

$$\frac{\delta\theta_t}{\delta t} = -\frac{\Phi}{nR}\frac{\partial}{\partial\theta}(S\cos\theta) \qquad (2)$$

This expresses the rate of change of tangential angle, in the direction of the surface normal.

Now consider θ to be a function only of x and time. Then

$$\delta\theta = \left(\frac{\partial\theta}{\partial x}\right)_t \cdot \delta x + \left(\frac{\partial\theta}{\partial t}\right)_x \cdot \delta t$$

$\therefore$ $\delta\theta/\delta t$ in any chosen direction

$$= \left(\frac{\partial\theta}{\partial x}\right)_t \cdot \frac{\delta x}{\delta t} + \left(\frac{\partial\theta}{\partial t}\right)_x$$

$$= \frac{1}{R\cos\theta} \cdot \frac{\delta x}{\delta t} + \left(\frac{\partial\theta}{\partial t}\right)_x$$

Let the chosen direction be the normal direction

$$\therefore \text{ from equation 2 } -\frac{\Phi}{nR}\frac{\partial(S\cos\theta)}{\partial\theta}$$

$$= \frac{1}{R\cos\theta}\frac{\delta x}{\delta t} + \left(\frac{\partial\theta}{\partial t}\right)_x$$

But from equation 1, the rate of change in the x co-ordinate of the point A is given by

$$\frac{\delta x}{\delta t} = \frac{\Phi}{n} S\cos\theta\sin\theta$$

$$\therefore \left(\frac{\partial\theta}{\partial t}\right)_x = -\frac{\Phi}{nR}\frac{\partial(S\cos\theta)}{\partial\theta} - \frac{\Phi}{nR} S\sin\theta$$

$$= -\frac{\Phi}{nR}\cos\theta\frac{\partial S}{\partial\theta} \qquad (3)$$

This gives the apparent change of tangential angle with time in the beam direction. Substituting for R yields the identity,

$$-\left(\frac{\partial\theta}{\partial t}\right)_x = \frac{\Phi}{n}\cos^2\theta\frac{\partial S}{\partial\theta}\left(\frac{\partial\theta}{\partial x}\right)_t$$

or

$$\left(\frac{\partial\theta}{\partial t}\right)_x \Big/ \left(\frac{\partial\theta}{\partial x}\right)_t = -\frac{\Phi}{n}\cos^2\theta\frac{\partial S}{\partial\theta} \qquad (4)$$

Now the contour of surface considered in the $x0y$ plane can equally well be converted to a surface contour in a θ/x frame of reference, and equation 4 indicates how the tangential angle varies with both spatial co-ordinate x and time t.

Equation 4 is of the form of a progressive wave, with a velocity defined by the ratio on the left hand side and can, in principle, be solved for θ as a function of x and t, in which the wave velocity given by $(\Phi/n)(\partial S/\partial\theta)\cos^2\theta$ is itself a spatial and time dependent function. Such solution requires a precise knowledge of the $S - \theta$ function and a solution technique would be to cast the velocity function in an appropriate Fourier (or Legendre) expansion and use transform methods, together with the initial conditions of θ, as a known function of x and t, to derive the transient solution. If the surface contour is to be reproducible in space however, i.e. an equilibrium topography, then the velocity of the progressive wave must be constant for all x and t and one arrives at the condition for such equilibrium as

$$-\frac{\Phi}{n}\cos^2\theta\frac{\partial S}{\partial\theta} = \text{constant} \qquad (5)$$

This still indicates, however, that θ progresses with time in the x direction, i.e. the surface topography moves in a direction with a component perpendicular to the direction of ion incidence.

One can state the more rigid requirement for equilibrium that the surface must be immobile in the perpendicular direction, so that to a viewer, the only topographical change is parallel to the beam direction and none parallel to the surface. This condition requires that the constant velocity of progression in equation 5 is equal to zero, i.e.

$$-\frac{\Phi}{n}\cos^2\theta\,\frac{\partial S}{\partial\theta}=0 \qquad (6)$$

This result is immediately seen to be identical to that in the earlier work, where artificial suppressors of surface motion (e.g. pinning regions), were introduced.

Equation 6 clearly indicates that for true equilibrium to have been achieved, then either $\cos\theta = 0$ ($\theta = \pm\,\pi/2$) or $\partial S/\partial\theta = 0$ ($\theta = 0$ or $\pm\,\theta_p$). The meaning of these results is that final equilibrium can be achieved only with planar surfaces at $\theta = \pi/2$ (vertical surface), $\theta = 0$ (horizontal surface) or $\theta = \pm\,\theta_p$ (plane inclined at θ_p to the horizontal). Final equilibrium is not achieved however, by an arbitrary combination of these values of θ. Thus a combination of $\theta = 0$ and $\theta = \pi/2$ (horizontal and vertical steps) is an equilibrium situation as is a combination of $\theta = \pi/2$ and $\theta = \theta_p$ (a cone on a cylinder or conical pit below a cylindrical hole in three dimensions), but a simultaneous combination of $\partial S/\partial\theta = 0$ values ($\theta = 0$ and θ_p, e.g. horizontal surfaces with a plane or cone or conical pit of angle θ_p) is not an equilibrium situation, since although the plane at θ_p alone remains constant in slope (i.e. the θ/x contour does not move in space) it does have a velocity in the $x0y$ plane of $\Phi/n\; S(\theta_p)\cos\theta_p \sin\theta_p$ which is unequal to the velocity (zero) of a horizontal plane. Thus the combination of a horizontal plane and a plane at θ_p will move in the x direction and a trough with sides at angles θ_p will tend to widen, whilst a plateau with sides at θ_p will contract as the inclined planes move in opposite directions.

In the absence of pinning regions, therefore, one concludes that only a horizontal, or a vertical plane or a combination of these, represents true equilibrium. The presence of pinning regions (such as dislocations, surface contamination) however, may lead to at least transitory surface structure, such as cones and pits. These results are summarised in fig. 2.

It is to be noted that, if one defines equilibrium as allowing for progression of the surface in a direction perpendicular to the beam, then the criterion for this form of equilibrium is (Φ/n) $(\partial S/\partial\theta)$ $\cos^2\theta$ = constant. The $\partial S/\partial\theta$ $\cos^2\theta$ function is readily constructed from a given $S - \theta$ function and is a curve which crosses the θ axis at $\theta = \pm\,\pi/2, 0, \pm\,\theta_p$. For (Φ/n) $(\partial S/\partial\theta)$ $\cos^2\theta$ to be equal to an arbitrary constant indicates horizontal cuts on this curve, in turn meaning that several values of θ simultaneously satisfy the criterion. Thus, sets of intersecting planes (at values of θ specified by the horizontal cuts) are equilibrium situations in this context, but as already noted these will sweep across the surface in the x direction.

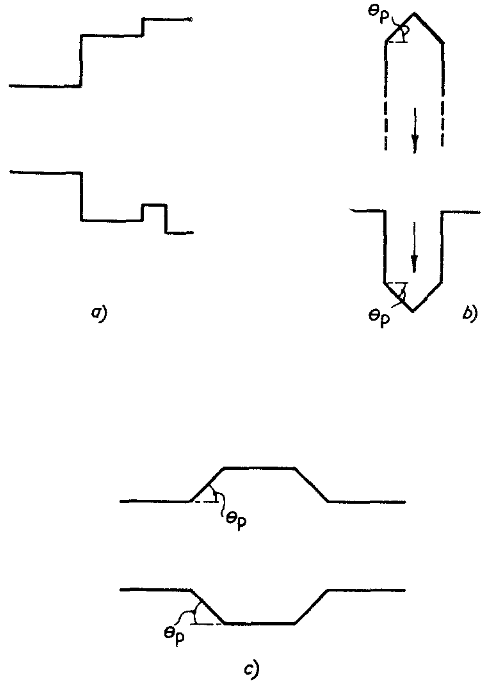

Figure 2 Stable and unstable surface configurations. (a) and (b) are stable, (c) unstable.

It is interesting to note that recently Bayly, in an unpublished study of the sputter etching of amorphous glass surfaces, has indeed observed the development of terraced (horizontal and vertical planes) structures and the enlargement of troughs as predicted by the above theory.

Reference

1. M. J. NOBES, J. S. COLLIGON, and G. CARTER, *J. Mater. Sci.* 4 (1969) 730.

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