

# The growth of topography during sputtering of amorphous solids

## Part 4 A generalized theory

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Theories of topographic surface development during ion bombardment fall broadly into two categories, one based upon erosion of intersecting planes [1] and the other on a point by point erosion basis [2-4]. A recent paper by Barber *et al* [5] has shown how, in semiquantitative fashion, an earlier theory by Frank [6] on chemical dissolution or growth of crystals, can be developed to encompass the ion sputtering case. This theory itself is based upon the kinematic wave equation outlined by Lighthill and Whitham [7, 8] and applies to problems of river flooding [7] and traffic flow [8]. In the present communication, the earlier topographic development theories are shown to fit precisely and analytically into the Frank development of the kinematic wave treatment and it is also shown how the occurrence of sharp angled cones formed on surfaces can be analytically and unequivocally predicted.

### 1. Introduction

It has been well known for a number of years that, during ion bombardment of the surfaces of solids, well-defined surface topographical features are developed. In crystalline solids these can usually be associated [9] with the generation of defects below but close to the surface and the interaction of the complex defect forms, which are produced, with the surface [10]. Even with amorphous solids, however, in which such interactions should not be present, regular features such as cones, pits and furrows are generated and it is generally believed that their development results from the fact that the sputtering rate is a non-monotonic function of the angle of ion incidence to each point on the surface. Such a non-monotonic dependence of sputtering rate upon angle of incidence has been well established for amorphous glass [11]. Two theories for the development of topographical features have been developed. The first by Stewart and Thompson [1] follows the rectilinear motion of a pair of intersecting surface planes, whilst the second by Carter *et al* [2-4] describes the differential motion of any point on a surface. These treatments are not exclusive and in fact lead to identical conclusions.

In a more recent semiquantitative analysis of the erosion by ion sputtering problem, Barber *et al* [5] have made use of the solutions to the formally identical problem of crystal dissolution by chemical etching evaluated by Frank [6]. Frank's treatment of this problem is based upon earlier work by Lighthill and Whitham [7, 8] who derived the kinematic wave equation relating flux and concentration of a quantity when there exists a functional relation between these parameters. In the case of crystal dissolution the flux is equated to the rate of passage of crystal steps past a fixed point in space and is, therefore, clearly related to the removal of surface material or erosion and progression of a target surface during ion bombardment.

In the present communication it is shown, analytically, how the earlier theories of topographic development are complementary and fit within the theoretical framework of kinematic wave processes and their application to crystal dissolution processes.

### 2. Theoretical considerations

#### 2.1. The kinematic wave equation

According to Lighthill and Whitham's arguments [7, 8], if a quantity (e.g. concentration)  $k$

varies in space and time, and the flux of this quantity is  $q$ , then in one dimension one can write:

$$-dq \cdot dt = dk \cdot dx \quad \text{or} \quad \frac{dq}{dx} + \frac{dk}{dt} = 0. \quad (1)$$

If the flux  $q$  is a function of  $k$ , then one can define a wave velocity  $C = |(\partial q)/\partial k|_x = \text{constant}$  which is to be compared with the point velocity  $v = q/k$ . Multiplying Equation 1 by  $C = (\partial q)/\partial k$  leads to the relation

$$\frac{dq}{dt} + C \frac{dq}{dk} = 0 \quad (2)$$

which indicates that  $q$  is a constant for waves travelling past a point with velocity  $C$ . It is also evident that

$$C = \frac{d}{dk}(vk) = v + k \frac{dv}{dk} \quad (3)$$

Such kinematic waves are non-dispersive but can suffer changes of form due to non-linearity (i.e. dependence of  $C$  upon  $q$ ) and discontinuities may develop due to interference between waves. These discontinuities may be regarded as kinematic shock waves. If on one side of the shock wave the values of  $k$  and  $q$  are  $k_1$  and  $q_1$ , and on the other side are  $k_2$  and  $q_2$ , then if the velocity of the shock wave is  $U$ , then the quantity crossing the shock front per unit time is either  $q_1 - Uk_1$  or  $q_2 - Uk_2$  then

$$U = \frac{q_2 - q_1}{k_2 - k_1}. \quad (4)$$

If  $q$  is a function of  $x$  and  $t$ , only through its functional dependence upon  $k$ , then  $q$  is constant on waves of constant velocity  $C$ , which is given by the slope of the tangent to the  $q/k$  function. Thus, in a space-time diagram, the waves of constant  $q$  (or  $k$ ) are straight lines, parallel to the tangent of the  $q/k$  characteristic. However, these tangents may intersect, and where they do so (on the space-time diagram) indicates the generation of a discontinuity or shock wave. At such a point a new wave of velocity given by Equation 4 results.

### 2.2. Application to crystal dissolution

Frank [6] describes a crystal surface in terms of a succession of surface steps, and considers, during dissolution, the rate of passage of these steps past a fixed spatial point. If  $k$  is the step density each

of unit height (number of steps per unit length in the  $x$  direction and thus analogous to concentration), and  $q$  is the rate of passage of steps past a fixed spatial point, in the  $y$  direction, and thus analogous to flux, then the slope of the surface at any fixed time is

$$k = \left| \frac{\partial y}{\partial x} \right|_t = \tan \theta \quad (5a)$$

and the dissolution rate in the  $y$  direction is

$$q = - \left| \frac{\partial y}{\partial t} \right|_x. \quad (5b)$$

If the dissolution rate is a function of step density, then one can write as before  $(\partial q)/\partial k = C$  and Equation 1 as

$$\frac{dq}{dk} \cdot \frac{\partial k}{\partial x} + \frac{\partial k}{\partial t} = 0$$

or

$$C \cdot \frac{\partial k}{\partial x} + \frac{\partial k}{\partial t} = 0. \quad (6)$$

Thus, in the  $(x, t)$  plane a point of given slope ( $k$ ) moves with a constant velocity  $C = (\partial q)/\partial k = (dx)/dt$  along a straight line trajectory called a "characteristic". In the  $(x, y)$  plane

$$\frac{dy}{dx} = \left| \frac{\partial y}{\partial x} \right|_t + \left| \frac{\partial y}{\partial t} \right|_x \frac{dt}{dx}$$

or

$$\frac{dy}{dx} = k - \frac{q}{C} \quad (7)$$

which shows that a point, of given slope  $k$  (and hence given  $q$  and  $C$ ) also follows a straight line trajectory since  $k - q/C$  is a constant for this point.

Corresponding to the kinematic shock wave described earlier, when there is a discontinuity of slope at a point, which geometrically defines an edge in two dimensions, the velocity is given by

$$\frac{dx}{dt} = \frac{q_2 - q_1}{k_2 - k_1}$$

and the trajectory of this edge is defined by

$$\frac{dy}{dx} = k_1 - q_1 \left( \frac{k_2 - k_1}{q_2 - q_1} \right) = k_2 - q_2 \left( \frac{k_2 - k_1}{q_2 - q_1} \right) \dots \dots (8)$$

The trajectory of this edge is not necessarily straight.

The dissolution rate measured normal to the actual macroscopic surface is  $q/(\cos \theta) = q(1 + k^2)^{-\frac{1}{2}}$  and the vector  $\mathbf{d}$  whose magnitude is the reciprocal of this rate and the direction of which is normal to the macroscopic surface is given by

$$\mathbf{d} = q^{-1}(k\mathbf{i} - \mathbf{j}) \tag{9}$$

where  $\mathbf{i}$  and  $\mathbf{j}$  are unit vectors in the  $x$  and  $y$  directions.

If one plots the polar diagram of  $\mathbf{d}$  as a function of  $k$ , then the slope of the tangent to this polar diagram is

$$\frac{d(\mathbf{d})}{dk} = -Cq^{-2} \left\{ \left( k - \frac{q}{C} \right) \mathbf{i} - \mathbf{j} \right\}. \tag{10}$$

According to Equation 7 the trajectory in the  $(x, y)$  plane of a point of given slope  $k$  is parallel to the direction,

$$\mathbf{i} + \left( k - \frac{q}{C} \right) \mathbf{j} \tag{11}$$

which is clearly orthogonal to the direction of the tangent given by Equation 10.

The meaning of this is that the direction of motion of a surface point of given orientation (tangential angle) is parallel to the normal to that point on the reciprocal normal dissolution rate polar diagram which has the same angle as the surface point considered. Frank enunciated these results in several theorems as follows:

1. The locus of a point on the crystal surface with a given orientation is a straight line (Equations 6 and 7) called a dissolution trajectory.
2. If the reciprocal of the dissolution rate normal to the surface is plotted in polar form as a function of surface orientation, then the trajectory of a point on the crystal surface of a given orientation is parallel to the normal to the polar diagram at the point of corresponding orientation (Equations 9, 10 and 11).

A corollary to these theorems is that at a discontinuity (an edge) the dissolution trajectory is parallel to the normal to the chord in the polar diagram joining the points corresponding to the orientations of points at either side of the edge (this follows from Equation 8).

### 2.3. Application to sputtering

Consider an element of surface  $AB$  shown in two-dimensional space in Fig. 1, exposed to a uniform flux of energetic ions  $\phi$  per unit area per sec incident in the  $0y$  direction. One considers that erosion of this surface is due to removal, by

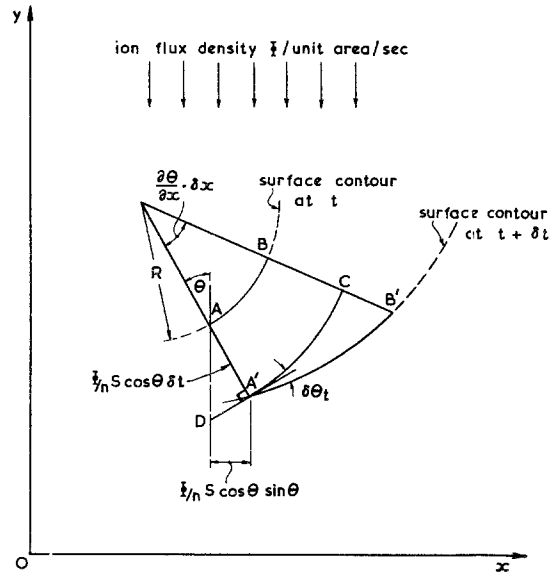


Figure 1 Erosion of a surface generator by an ion flux.

sputtering, of surface atoms and that any resulting changes in topography are due only to the macroscopic variations in the sputtering rate with angle of ion incidence  $\theta$  to the normal to the surface. Thus one excludes effects such as surface atomic migration, local non-uniformities of sputtering owing to impurities or only partial development of the ion generated displacement cascade near the surface, flow of atoms from below to the surface, etc. One defines the sputtering coefficient  $S$  as the number of atoms removed from the surface per incident ion, so that if the target density is  $n$ , the depth eroded normal to a surface, per incident ion per unit area is just  $S/n$ . The generally observed functional relationship between  $S(\theta)$  and  $\theta$  for an amorphous target in the range  $-\pi/2 < \theta < \pi/2$  is that  $S(\theta)$  is symmetric in  $\theta$  about  $\theta = 0$ , experiencing a minimum value of  $S(0)$  at  $\theta = 0$ , rising to a maximum at  $\theta = \pm \theta_p$  and declining to zero at  $\theta = \pm \pi/2$ .

For the element  $AB$  in Fig. 1 the tangential angle increases from  $\theta$  at  $A$  to  $\theta + (\partial\theta/\partial x) dx$  at  $B$ , so that, in a flux of  $\phi$  ions per unit area per sec, the rate of erosion normal to the curve at  $A$  and  $B$  increases from  $(\phi/n) S(\theta) \cos \theta$  to  $(\phi/n) S(\theta + d\theta) \cos(\theta + d\theta)$ . The reciprocals of the ratio of those rates to the value at  $\theta = 0$ , is given by the form  $S(0)/(S \cos \theta)$  where  $S$  is written for  $S(\theta)$  and may be defined, following Barber *et al*, as the "erosion slowness" for a given orientation. By analogy with the chemical

dissolution process,  $S(0)/(S \cos \theta)$  is the normalized normal recession rate of the surface. This function plotted in polar form, now allows deduction of the characteristic trajectories in the  $yOx$  plane, along which points of constant orientation move. This is effected by determining the normal to each point on the polar erosion slowness curve and allowing a point on the real surface, having an equivalent orientation, to move in a direction parallel to this normal and with a velocity determined (according to Barber *et al*) by the relative sputtering rate at that orientation.

Barber *et al* have used these erosion slowness curves to follow, successfully, the progress of erosion of hemispherical protuberances and troughs and sinusoidal geometry features on a surface, using also, Frank's theorem that when trajectories intersect an edge (or shock front) is produced which follows a new trajectory parallel to the normal to the chord joining the original orientations on the erosion slowness curve.

There can be no doubt that this treatment of the topographic development process is the most elegant reported to date. In fact, this treatment can be shown to include, within its framework, the earlier analyses reported by Stewart and Thompson and by Carter *et al*, and this we now propose to elucidate. In the Carter *et al* studies, the relative movement of the two points  $A$  and  $B$  to  $A'$  and  $B'$  respectively was considered as a result of sputtering for a time  $dt$ . Assuming that  $S$  increases with  $\theta$ ,  $BB'$  exceeds  $AA'$  by an amount  $(\phi/n)(d/d\theta)(S \cos \theta)(\partial\theta/\partial x) dt \cdot dx$  which in Fig. 1 is equal to  $CA'$  where  $CA'$  is parallel to  $AB$ . If the radius of curvature of  $AB$  is  $R$ , and the change in tangential angle from  $A$  to  $A'$  is  $d\theta_t$ , then it is readily shown from the triangle  $CA'B'$  that

$$- d\theta_t = \frac{\phi}{n} \frac{d}{d\theta} (S \cos \theta) \frac{dt}{R} \quad (12)$$

However

$$d\theta = \left| \frac{\partial\theta}{\partial n} \right| dx + \left| \frac{\partial\theta}{\partial t} \right|_x dt \quad (13)$$

so that

$$\frac{d\theta}{dt} = \left| \frac{\partial\theta}{\partial x} \right|_t \frac{dx}{dt} + \left| \frac{\partial\theta}{\partial t} \right|_x \quad (14)$$

If the direction considered is along the normals at  $A$  or  $B$ , then  $(dx)/dt$  represents the time rate of change of the  $x$  co-ordinate of  $A$ , and is equal to  $(\phi/n) S \cos \theta \sin \theta$ . Substitution of this expres-

sion into Equation 14 and subsequently combining Equations 12 and 14 leads to the identity derived by Carter *et al*

$$\left| \frac{\partial\theta}{\partial t} \right|_x = - \left| \frac{\partial\theta}{\partial x} \right|_t \frac{dS}{d\theta} \cos^2 \theta \cdot \frac{\phi}{n} \quad (15)$$

Carter *et al* recognized that this defined a wave nature for variations of  $\theta$  with  $x$  and  $t$ , but did not associate this with the kinematic wave process outlined by Lighthill and Whitham. In terms of the kinematic wave equation, the meaning of Equation 15 now becomes clear in that it defines the motion of points of constant orientation in  $x, t$  space. Thus

$$\left| \frac{\partial\theta}{\partial t} \right|_x = \left| \frac{dx}{dt} \right|_\theta = - \frac{\phi}{n} \frac{dS}{d\theta} \cos^2 \theta \quad (16)$$

which indicates that the rate of motion of points of constant orientation in the  $x$  direction is equal to  $-(\theta/n)(dS/d\theta) \cos^2 \theta$ .

Equation 13 can equally be cast in terms of  $y$  co-ordinates by using the fact that the velocity of motion of the point  $A$  in the  $y$  direction is  $(\phi/n) S \cos^2 \theta$ , thus an analogous equation to Equation 16 in terms of  $y$  can be derived, i.e.

$$\left| \frac{\partial\theta}{\partial t} \right|_y = \left| \frac{dy}{dt} \right|_\theta = - \frac{\phi}{n} \left| \frac{dS}{d\theta} \sin \theta \cos \theta - S \right| \cdot \dots \quad (17)$$

Thus the rate of motion of points of constant orientation in  $y, t$  space is

$$\frac{\phi}{n} \left\{ \frac{dS}{d\theta} \sin \theta \cos \theta - S \right\}.$$

Division of Equations 16 and 17 yields the slope of the trajectory in  $(x, y)$  space, of points of constant orientation, i.e.

$$\left| \frac{dy}{dx} \right|_\theta = \frac{(dS/d\theta) \sin \theta \cos \theta - S}{(dS/d\theta) \cos^2 \theta} \quad (18)$$

The polar plot of  $S(0)/(S \cos \theta)$ , is effectively a Cartesian plot of  $S(0)/S$  as a function of  $(S(0)/S) \tan \theta$  and it is readily shown that the slope of the normal to this curve is

$$\frac{d(\tan \theta/S)}{d(1/S)} = - \left\{ \frac{(dS/d\theta) \sin \theta \cos \theta - S}{(dS/d\theta) \cos^2 \theta} \right\}.$$

This establishes the fact that the trajectory of

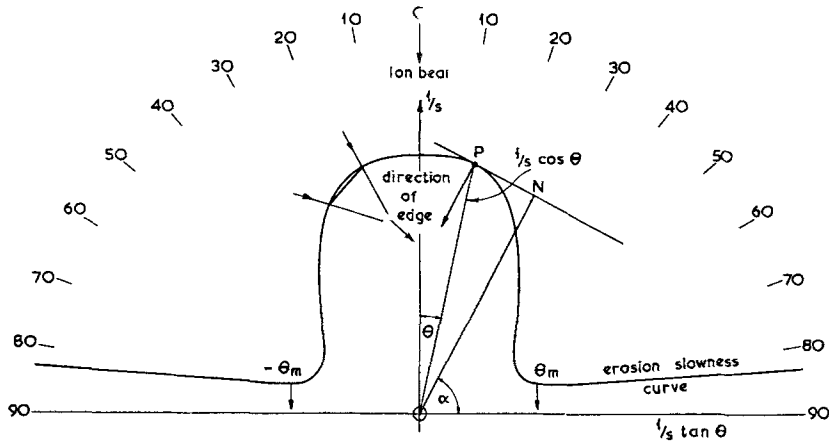


Figure 2 The non-normalized erosion slowness curve, depicting the direction and velocity of motion of a point  $P$  at orientation  $\theta$  and the direction of motion of an edge, following the intersection of two point trajectories.

points of constant orientation on the sputtered surfaces is parallel to the normal to the polar erosion slowness curve.

It is important to note that the Barber *et al* result, derived from Frank's earlier treatment, is based upon motion of surface steps, i.e. effectively considering finite motion whereas the present treatment has considered infinitesimal point by point or continuum motion of a curved surface. It is encouraging that the results are identical, and in fact must be expected to be so since both treatments clearly lie within the framework of the kinematic wave theory. In this respect one identifies the velocity

$$C \left( = \frac{dq}{dk} = \left| \frac{dx}{dt} \right|_{\theta} \right)$$

from Equations 2 and 16 as  $(dS/d\theta) \cos^2 \theta$ .

The spatial velocity of points of constant orientation is given, from Equations 16 and 17 as

$$\left\{ \left| \frac{dx}{dt} \right|_{\theta}^2 + \left| \frac{dy}{dt} \right|_{\theta}^2 \right\}^{\frac{1}{2}} = \frac{\phi}{n} \left\{ \left( \frac{dS}{d\theta} \sin \theta \cos \theta - S \right)^2 + \left( \frac{dS}{d\theta} \cos^2 \theta \right)^2 \right\}^{\frac{1}{2}} \quad (19)$$

If one plots, as in Fig. 2, the non-normalized erosion slowness curve (i.e.  $1/S \cos \theta$ ) in polar form, or  $1/S$  as a function of  $(1/S) \tan \theta$  in Cartesian form), then the vector  $OP$  to a point of given orientation is the reciprocal of the velocity of the point normal to the real surface at that orientation. Constructing the tangent to  $P$  and forming the normal to this tangent from the

origin, then the length of this normal  $ON$  is given by

$$ON = OP \cos (90 - \alpha - \theta)$$

where  $\alpha$  is defined in Fig. 2 as the slope of the normal at  $N$  and thus at  $P$ . Since

$$\tan \alpha = \frac{(dS/d\theta) \cos^2 \theta}{-(dS/d\theta) \sin \theta \cos \theta + S}$$

and

$$OP = \frac{1}{S \cos \theta}$$

it is readily shown that

$$ON = \{ [(dS/d\theta) \sin \theta \cos \theta - S]^2 + [(dS/d\theta) \cos^2 \theta]^2 \}^{-\frac{1}{2}} \quad (20)$$

Identifying Equations 19 and 20 indicates that the reciprocal of the spatial velocity of points of constant orientation is proportional to the length of the normal from the origin of the erosion slowness curve to the tangent at the point of constant orientation considered.

This result, which was not given by Barber *et al*, indicates that, in obtaining the actual time progression of a sputtered surface, not only is the direction of motion of constant orientation defined by the normal to the erosion slowness curve, but also the actual velocity of these points is defined by the reciprocal length of the normal from the origin of the erosion slowness curve to the tangent at the orientation considered. The extreme value of the erosion slowness curve becomes even more evident.

Lighthill and Whitham, Frank and Barber *et al* showed that when the constant orientation trajectories intersect, a new edge trajectory ensues with a direction of motion parallel to the normal to the chord joining the original points of constant orientation on the erosion slowness curve. This is illustrated in Fig. 3 for two points  $P_1$  and  $P_2$  on the erosion slowness curve. If  $ON$  is now drawn as the normal from the origin to the chord  $P_1P_2$  then the above authors suggest that this defines the direction of motion of the edge produced when the trajectories of the points on the real sputtered surface, corresponding to the orientations at  $P_1$  and  $P_2$  intersect. If the co-ordinates of the points  $P_1$  and  $P_2$  are  $(\tan \theta_1/S_1, 1/S_1)$  and  $(\tan \theta_2/S_2, 1/S_2)$  then the slope of the normal  $ON$  is given by

$$-\frac{\delta(1/S \tan \theta)}{\delta(1/S)} = \frac{S_1 \tan \theta_2 - S_2 \tan \theta_1}{(S_2 - S_1)} \quad (21)$$

Stewart and Thompson considered the sputtering erosion of two infinite intersecting planes, inclined at angles  $\theta_1$  and  $\theta_2$  to the  $x$ -axis and showed that the direction of motion of the intersection, was given by

$$\frac{dy}{dx} = \tan \beta = - \left\{ \frac{S_1 \tan \theta_2 - S_2 \tan \theta_1}{(S_2 - S_1)} \right\} \quad (22)$$

One can readily identify Equations 21 and 22 so that it is clear that the direction of motion of the intersection of sputtered planes is totally identical to the direction of motion of the edge trajectory in the treatment of Frank and Barber *et al*.

Furthermore Stewart and Thompson show that the velocity of the intersection point  $v$  is given by the relation

$$\frac{1}{v} = \frac{n}{\phi} \cdot \frac{1}{S_1 \cos \theta_1} \cos(\beta - \theta_1) \quad (23)$$

Referring to Fig. 3 it is evident that

$$ON = \frac{1}{S_1 \cos \theta_1} \cos(\beta - \theta_1)$$

thus one identifies the reciprocal of the length  $ON$  with the velocity of the edge (or intersection). Clearly this normal relaxes to the normal to the tangent at a point  $P$  when the points  $P_1$  and  $P_2$  coincide.

It is interesting that this result is also readily derivable from Equations 7 and 8 for the dissolution process. From these equations, by division, it is found that

$$\left| \frac{dy}{dt} \right|_{\theta} = \frac{q_2 k_1 - q_1 k_2}{k_2 - k_1}$$

so that the velocity of an edge characteristic trajectory is given by

$$\left\{ \left| \frac{dx}{dt} \right|_{\theta}^2 + \left| \frac{dy}{dt} \right|_{\theta}^2 \right\}^{\frac{1}{2}} = \frac{\phi}{n} \{ (q_2 - q_1)^2 + (q_2 k_1 - q_1 k_2)^2 \}^{\frac{1}{2}} \cdot (k_2 - k_1)^{-1} \quad (24)$$

In the dissolution process,  $q$ , is the rate of passage of steps (of unit length) past a fixed  $x$  co-ordinate point, and so in the analogous sputtering process  $q$  is equated to the equivalent distance moved by the surface in the  $Oy$  direction for a given  $x$  co-ordinate. Referring to Fig. 1, since the point  $A$  moves to  $A'$ , a distance  $(\phi/n) S \cos \theta dt$ , the movement of the surface below  $A$  is to  $D$  where

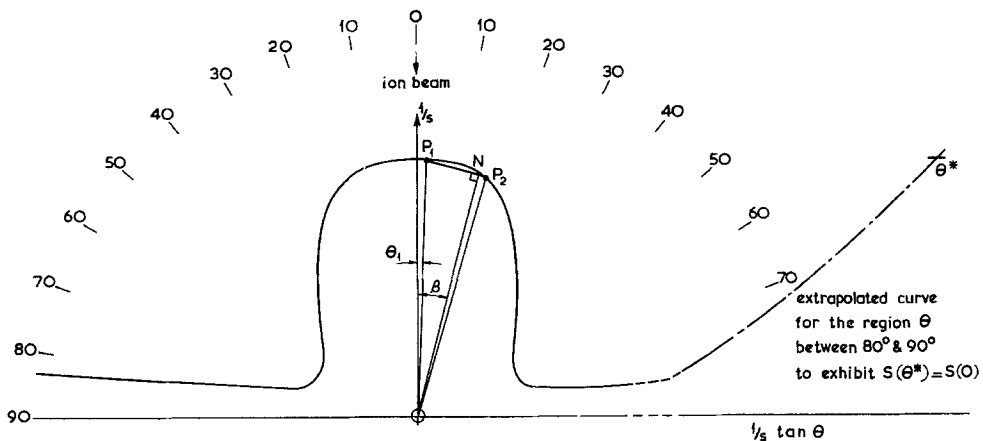


Figure 3 The non-normalized erosion slowness curve, depicting the direction of motion and velocity of an edge.

$$AD \cos \theta = \frac{\phi}{n} S \cos \theta dt.$$

Thus the rate of motion of the surface, at fixed  $x$ , in the  $y$ -direction is  $(\phi/n) S$ , so one identifies  $q$  with this quantity and  $k$  is already defined in both the step and continuum cases as equivalent to  $\tan \theta$ . The velocity of an edge is thus given by

$$v = \frac{\phi}{n} \{ (S_2 - S_1)^2 + (S_2 \tan \theta_1 - S_1 \tan \theta_2)^2 \}^{\frac{1}{2}} \tan \theta_2 - \tan \theta_1^{-1}. \quad (25)$$

Referring again to Fig. 3

$$ON = \frac{\cos(\beta - \theta_1)}{S_1 \cos \theta_1} = \frac{(\cos \beta - \sin \beta \tan \theta_1)}{S_1}. \quad (26)$$

Substituting for  $\sin \beta$  and  $\cos \beta$  from Equation 21 for the slope of the normal ( $\tan \beta$ ) it is readily shown that

$$ON = \{ (S_2 - S_1)^2 + (S_2 \tan \theta_1 - S_1 \tan \theta_2)^2 \}^{\frac{1}{2}} (\tan \theta_2 - \tan \theta_1)$$

again showing that  $ON$  is indeed proportional to the reciprocal of the edge velocity  $v$ . If one proceeds to the limit where  $\theta_2 - \theta_1 \rightarrow \delta\theta$  and  $S_2 - S_1 \rightarrow \delta S$  it is again readily proved, from Equation 25, that the velocity  $v$  is given by

$$v = \frac{\phi}{n} \left\{ \left( \frac{dS}{d\theta} \sin \theta \cos \theta - S \right)^2 + \left( \frac{dS}{d\theta} \cos^2 \theta \right)^2 \right\}^{\frac{1}{2}}$$

the result already given in Equation 19.

One, therefore, concludes that the continuum approach of Carter *et al* and the intersection plane approach of Stewart and Thompson both fall within the general framework of Barber *et al*'s extension of the Frank theory of crystal dissolution. It also becomes evident that the use of the erosion slowness curve provides a very elegant and straightforward method of determining the spatial progress of points of constant orientation on a sputtered surface, since not only are the directions of motion of such points determined to be parallel to the normal to the erosion slowness curve at the corresponding orientation, but also the velocity of such points is determined by the reciprocal length of the normal from the origin to the tangent to the erosion slowness curve at that orientation. Furthermore, when trajectories of the surface points intersect, an edge forms, the velocity and direction of motion of which are now given by the

normal from the origin to the chord joining corresponding orientations on the erosion slowness curve.

As noted earlier, Barber *et al* have applied the erosion slowness curve to determine the topographical changes in various surface forms. In particular it was shown that a hemispherical surface protuberance developed a conical form, a hemispherical hollow develops into a flat-bottomed cylinder, a hollow of the shape of the cap of a hemisphere tends to enlarge along the surface plane but becomes shallower, finally disappearing so that a flat surface develops, whilst it was also suggested that a sinusoidal topographic feature also developed towards planity. All these developments are readily explained in terms of the erosion slowness curve and the behaviour of the normals at each point on this curve, but Barber *et al* appear to have missed the significant behaviour of a particular point on the erosion slowness curve, where  $\theta = \pm \theta_p$ , the points of maximum sputtering coefficient in the  $S/\theta$  function. One notes in Fig. 2 that all inward drawn normals will have points of intersection provided that  $\theta < \pm \theta_m$ , where  $\pm \theta_m$  are the values of  $\theta$  for which the normals are mutually parallel to the  $1/S$  axis. For values of  $\theta > \pm \theta_m$ , the normals always diverge but intersect with the normals for  $\theta = \pm \pi/2$ . The significance of this behaviour is that for all orientations  $\theta < \pm \theta_m$  on a real surface with angles symmetrically distributed about  $\theta = 0$  (which is true for the hemispherical protuberance and sinusoidal cases treated by Barber *et al*), edges will develop, in such a manner that for a protuberance the smaller  $\theta$  values disappear first and the larger  $\theta$  values disappear last. The value of  $\theta = \pm \theta_m$  cannot disappear at all, however, since no other normal (even a chord normal) from  $\theta = 0$  to  $\pm \theta_m$  can intersect this. Consequently, the  $\theta = \pm \theta_m$  configuration increases in importance and a conical shape develops.

The value of  $\theta = \pm \theta_m$  is determined when the slope of the tangent to the erosion slowness curve

$$\frac{d(S(0)/S)}{d(S(0) \tan \theta/S)}$$

is zero, i.e. when

$$\frac{(dS/d\theta) \cos^2 \theta}{(dS/d\theta) \sin \theta \cos \theta - S} = 0.$$

This gives the conditions  $dS/d\theta = 0$ ,  $\cos \theta = 0$

( $\theta = \pi/2$ ). The sputtering coefficient  $S$  as a function of  $\theta$  characteristic exhibits values of  $dS/d\theta = 0$  at  $\theta = 0$  and  $\pm \theta_p$ . One readily identifies, therefore,  $\theta_p$  with  $\theta_m$ , with the concomitant result that cones of half angle  $\pi/2 - \theta_p$  will develop upon a surface possessing protuberances in which  $\theta_p$  exists. This latter qualification is crucial since the erosion slowness curve shows that no orientations greater than the initial orientations can ever ensue, thus cones of half angle  $\pi/2 - \theta_p$  can only develop provided that there exists a  $\theta_p$  value in the initial surface contour. This growth of cones of half angle  $\pi/2 - \theta_p$  has already been inferred in the work of Stewart and Thompson and Carter *et al* but it had not been previously possible to determine quantitatively the conditions for such growth.

The result which identifies  $\theta_m$  with  $\theta_p$  can also be readily derived by noting that  $\theta_m$  occurs where there is no change of  $1/S$  (the Cartesian  $y$  co-ordinate) with polar angle  $\theta$ , i.e.

$$\frac{d(1/S)}{d\theta} = 0$$

which again leads to the condition  $dS/d\theta = 0$ , and defines the motion of the  $\theta_p$  orientation as parallel to the ion beam ( $Oy$ ) direction. Of course, a further angle, of some significance, exists, in which there is no motion parallel to the  $Oy$  direction, and which is defined where the *tangent* to the erosion slowness curve is parallel to the  $Oy$  direction. This condition is met by the statement that  $d(\tan \theta/S)/d\theta = 0$  indicating that if such a condition is satisfied on the erosion slowness curve and such orientations exist on a real surface, there will only be motion of these orientations perpendicular to the direction of ion incidence.

In the case of hemispherical or hemispherical cap depressions in a surface, the direction of motion of characteristic trajectories of current orientations is (as shown by Barber *et al*) to be along the outward drawn normals from the erosion slowness curve. In such cases the edge trajectories develop first for larger values of  $\theta$  and if  $\theta > \pm \theta_m$  the tendency is to eliminate the smaller values of  $\theta$  and a movement towards the largest values of  $\theta = \pm \pi/2$  is experienced. For orientations  $\theta < \pm \theta_m (= \pm \theta_p)$  the trajectories do not intersect until they approach the  $\theta > \pm \theta$  trajectories and eventually the  $\theta = \pm \pi/2$  trajectories. The result is, therefore, that the smaller orientation parts of the curve grow most rapidly at the expense of the larger orientations

and only the  $\theta = \pm \pi/2$  angle cannot be eliminated and so either a single value of  $\theta = 0$  or a combination of  $\theta = 0$  and  $\pm \pi/2$  for which there is no intersection of the normals results. This is the case of the hemispherical trough treated by Barber *et al*, in which all  $\theta$  values between  $\pm \pi/2$  are included and the form of development is towards a flat base cylinder with  $\theta = 0$  and  $\theta = \pm \pi/2$  whereas for the hemispherical cap trough for which the values of  $\pm \pi/2$  were not included, there was no development towards vertical generators, only a gradual elimination of all the large angle orientations until a flat surface ensued. If, however, values of  $\pi/2 < \theta < \theta_m$  were also included in the initial topography, it would be expected that these angles would relax, by intersection, towards the  $\theta = \pi/2$  geometry.

In the sinusoidal case treated by Barber *et al*, the angles  $\pm \theta_p$  were not included in the positive half of the sinusoid nor could the  $\pm \pi/2$  values be included in the negative half of the sinusoid. Consequently, the final form of the development, as suggested by Barber *et al*, must be a polished flat surface in the  $OX$  plane. However, Barber *et al* do indicate that during erosion of the sinusoid, the positive half cycle develops a triangular shape (a conic section in three dimensions) whilst the negative half assumes a flattened shape. Further they suggest that if a section develops for which the erosion of all points in the  $Oy$  (beam direction) is constant, an equilibrium form can be achieved. Such a form would ensue when the positive half of the cycle formed a triangle of half angle  $\pi/2 - \theta^*$  where  $\theta^*$  is such that sputtering coefficient is equal to  $S(0)$ . The apex of this triangle is then an edge which moves in the  $Oy$  direction with velocity  $S(0)$  since the orientations of the sides of the triangle are  $\pm \theta^*$  and so the chord joining the equivalent orientations in the polar erosion slowness curve is parallel to the  $\theta = \pi/2$  orientation (i.e. parallel to the  $S(0) \tan \theta/S$  axis in Cartesian co-ordinates) and the length of the normal to this chord is just  $S(0)$ . In addition, at the feet of the triangle where the inclined faces meet the flat ( $\theta = 0$ ) plane, the edges formed here also move in the  $Oy$  direction only, since the chords joining the  $\theta = 0$  and  $\theta = \pm \theta^*$  are again parallel to the  $\theta = \pi/2$  direction and the normal from the origin to the chord again equals  $S(0)$ . A triangle of half angle  $\pi/2 - \theta^*$  together with a flat surface was observed to develop in computer simulations of the sputtering of a sinusoid by Catana *et al* in a



case where the orientation  $\theta_m^*$  was included in the sinusoid. It should be noted however, that it is now believed that the topography actually determined in those simulations was somewhat artificially produced because the apex of the upward sinusoid always sputtered with a value  $S(0)$  and not, as has been shown in this paper, a value corresponding to the planes which include the apex. In Barber *et al*'s case the  $\theta^*$  orientation was not included so that no triangle flat configuration would develop.

This example of topographic development illuminates a general rule for the generation of an equilibrium contour which is that for all points on the contour, or all edges, both the direction of motion and velocity must be constant. This means that on the polar erosion curve, the normals from the origin to the tangents or chords of corresponding orientations must be of equal length and parallel. Thus the *only* orientations which could co-exist in equilibrium with a  $\theta = 0$ , flat plane are  $\theta = \pm \theta^*$  orientations and  $\theta = \pm \pi/2$ . A topography consisting of a cone with a generator at  $\theta = \pm \theta_p$  and a flat surface is not in equilibrium, since the erosion rate at the apex ( $S(\theta_p)$ ) is different from that at the foot (obtained by drawing the normal from the origin to chord joining the  $\theta = 0$  and  $\theta = \pm \theta_p$  orientations on the polar erosion curve).

### 3. Conclusions

It has been shown that the theories of topographic surface development proposed by Stewart and Thompson (intersecting plane model) and Carter *et al* (differential surface recession model) can be fitted within the general technique using erosion slowness curves developed by Barber *et al* from Frank's treatment of crystal dissolution. It has been further shown that the erosion slowness

curve not only defines the direction of motion of points of constant orientation on the sputtered surface, but that also the velocity of such points is also readily derived.

The important role of the angle at which maximum sputtering occurs has been analytically determined as have the conditions for equilibrium topographies involving a combination of surface orientations.

It seems that, in view of the many other processes involved in topography development, which have been ignored here, the erosion slowness curve and its application represents as elegant a technique for following surface erosion by sputtering as should be developed.

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