Letters

The Equilibrium Topography of Sputtered Amorphous Solids III. Computer Simulation

When a non-planar amorphous target is bombarded by a uniform beam of ions, sputtering will occur at different rates at various points across the surface, due to both the variation of beam density with incident angle and the variation of sputtering coefficient with angle. As a result, the original surface contour will begin to change and, in so doing will present different angles to the ion beam, so that a continuous modification of the surface profile will occur until, it may be anticipated, an equilibrium profile will remain. Recent interest in the technique of sputtering surfaces for analysis of target materials, for polishing samples, or for thinning samples for electron microscopy, has made the understanding of the mechanism of the development of rough surfaces during bombardment of tantamount importance and attempts have been made in earlier publications [1, 2] to treat the surface development analytically. It was shown in [2] that the equation governing the time dependence of the surface angle to the beam was analogous to the wave equation and had the form,

$$\frac{\partial \theta}{\partial t} = -\frac{\Phi}{n}\frac{\partial S}{\partial \theta}\cos^2\theta\,\frac{\partial \theta}{\partial x} \qquad (1)$$

Here the surface contour was represented by a curve $y = f(x)$ and bombardment was by a uniform beam of Φ ions/second in the negative y-direction. θ is the angle of incidence of the beam, with respect to the normal to any point on the target surface, S the sputtering coefficient (which is a function of θ of the form shown in fig. 1) and n the atomic density of the target.

Solution of equation 1 to give a time dependent variation of the contour is not generally possible but final equilibrium contours may be predicted and are those for which

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

This condition represents the case where a contour will repeat itself after sputtering but may move at constant speed in the positive or negative x-directions. For the contour to remain stationary, the condition is

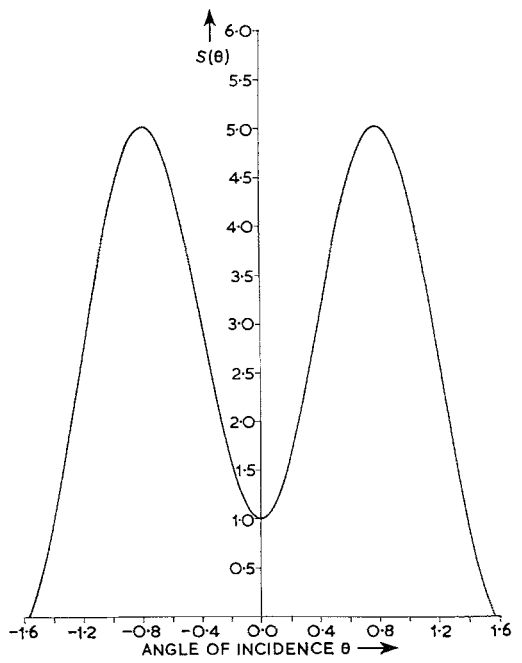

Figure 1 The function $S(\theta) = 3.2696\cos\theta + 13.1059\cos^2\theta - 15.3755\cos^4\theta$ which was used to represent the variation of sputtering yield with angle of incidence.

$$\frac{\Phi}{n}\frac{\partial S}{\partial \theta}\cos^2\theta = 0 \qquad (3)$$

Thus a contour containing only vertical and horizontal elements would reproduce directly below its original position and would be completely stable.

It was clearly of interest to find some method of following the development of a general surface contour to the equilibrium condition. For this reason, the present computer program was devised.

For preliminary studies, an infinite sinusoidal surface of the form $y = a\sin 2\pi x/\lambda$ was selected, bombarded in the negative y-direction by a uniform ion beam of intensity Φ ions per second. The computer was instructed to record the initial co-ordinates (x, y) of 100 equally spaced x points (at $\lambda/100$ intervals). From earlier work, it is clear that the erosion of any point in the negative y-direction is proportional to the value of $S(\theta)$ at that point, so that the computer was next instructed to reduce each of the 100

y-values by amounts proportional to the S value at these points. It should be pointed out that this procedure is not forcing motion of a curve in the y-direction only but stimulates motion in both x and y directions. The reason for this is that a point P on a curve moves along the surface normal by a distance $\Phi/n\, S \cos\theta\, \delta t$ in a time δt and the x and y co-ordinates of the point are thereby changed by $\Phi/n\, S \cos\theta \sin\theta\, \delta t$ and $\Phi/n\, S \cos^2\theta\, \delta t$, respectively. Every point on the original curve produces a new point on a new curve and there will be one such point Q having the same x-co-ordinate as the point P.The change in y co-ordinates between P and Q, Δy, is thus given by

$$\Delta y = \frac{\Phi}{n}\,(S\cos^2\theta\,\delta t + S\sin\theta\cos\theta \tan(\theta + \delta\theta)\,\delta t)$$

It is readily shown that as $\delta t \to 0$, $\Delta y \to \Phi/n\, S\, \delta t$ indicating that, at constant x, the change in the y co-ordinates is as used in the simulation.

Having calculated the new y co-ordinates, the new slopes were evaluated at the selected 100 points and the process repeated, the resulting increment in y-erosion being added to any previous increment at each step. When the y changes are all identical to those in the last step, the programme stops and equilibrium has been reached. In this simulation, it is not necessary to use actual values of sputtering coefficient, ion beam density or target density, since these form a normalisation coefficient upon the actual rate of surface atom removal in real time. In general, an erosion rate was chosen such that an amount 0.01 times the original amplitude "a" was removed from the $\theta = 0$ parts of the curve at each stage, although larger speeds of $0.06a$ gave results of almost the same accuracy. End effects were eliminated by using points $x = 99\lambda/100$ and $x = \lambda/100$ to interpolate the new slopes at $x = 0$.

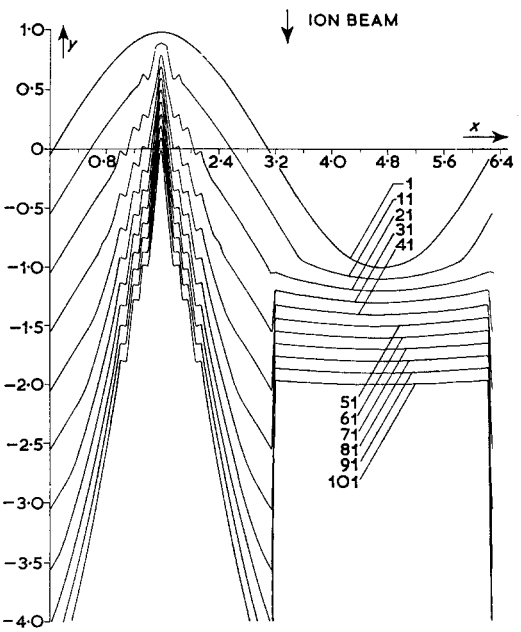

Figure 2 Initial changes of a sinusoidal surface of the form $y = a \sin(2\pi x)/\lambda$ for which $\lambda = 2\pi a$ and $a = 1$. The scale factor β is 1.657, i.e. all y values are shown 1.657 times their true values. (The numbers on the contours indicate the number of steps calculated, each step corresponding to a removal of 0.01 times the original amplitude at the points where the beam hits the curve normally.)

To produce the equilibrium profile, it was necessary to provide the computer with information on the variation of S with θ. From available data of Wehner [3] it was clear that $S(\theta)$ increases with θ, reaches a maximum of about 4 to 5 times the $S(0)$ value at approximately 50° to 70° and returns to an apparent zero at $\theta = 90°$. Curves vary for different materials and a typical curve is given empirically by

$$S(\theta) = 3.2696\cos\theta + 13.1059\cos^2\theta - 15.3755\cos^4\theta \qquad (4)$$

This is shown in fig. 1 and it is clear that the maximum yield occurs at $\theta = 45°$ and is 5.02 times the $S(0)$ value. Also, the $S(\theta)$ curve returns to the same value as $S(0)$ at $\theta = \theta_n = 79° 36\frac{1}{2}'$.

Initially, a sinusoidal curve for which $a = \lambda/2\pi$ was selected as the initial surface contour, i.e. $y = a \sin x/a$. For this the maximum value of θ is 45° which is, in fact, the maximum of the $S - \theta$ function. Fig. 2 shows the initial stages 1 to 100 of the change in contour and a most evident feature is the development of rapid oscillations from step 11 onwards. A thorough investigation of these oscillations has shown that they arise from unavoidable errors induced by both approximations of method and non-correctable computer errors. For example, the estimate of the new slope of a curve requires subtraction of two similar numbers, so that figures in the last decimal places become critically important. This approximate slope is then multiplied by large constants to determine the next step in the erosion process. Because the number of multiplications is very large ($n.m$

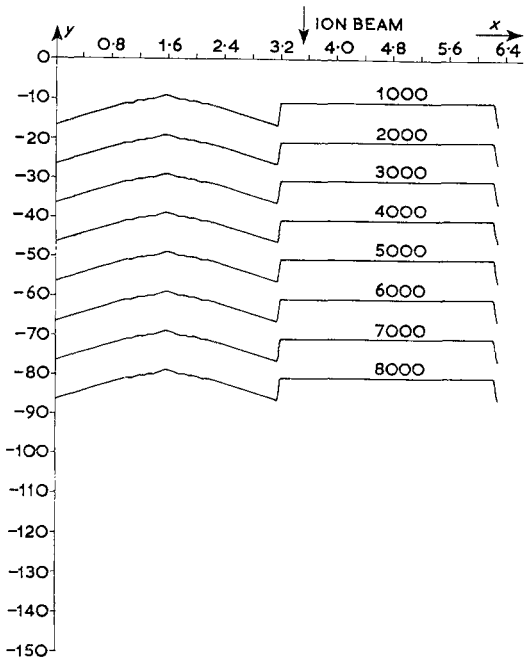

Figure 3 Further development of the surface shown in fig. 2. Slight changes in profile in the region $1.0 < x < 2.0$ occur but are not visible on these graphs. The scale factor β is now 0.0553.

where n = the number of iterations and m = the number of constants accepted), the rounding errors, in the critical points of the sine wave profile, are correspondingly big. From the results obtained with different methods, we are able to make searching comparisons between the accuracy of the various methods of solution and also arrive at practical rules governing the safe but economical number of intervals which need to be used during the computation of the solution. More frequently however, the determination of a strict bound for the general error in the solution requires information which is at least as difficult to obtain as the solution itself.

Generally speaking, the oscillations wash out after a large number of iterations and a smooth curve results, as for example, in fig. 3, which shows the development of $y = a \sin x/a$ up to 8000 steps, at which point, an apparent equilibrium is being approached.

The simulation shows that the apparent equilibrium condition is a triangle which is situated in a vertical-sided pit and a horizontal plateau; the upward pointing section of the sinusoidal contour giving rise to the triangular protrusion and the valley developing into the plateau. The scale factor β on these diagrams is the number of times by which the ordinate scale should be increased to give a true scaled picture, i.e. the triangle has much steeper sides than shown. The angle of the sides of this triangle is, in fact, exactly $79° 36\frac{1}{2}'$, i.e. the value for which the sputtering yield is equal to that for normal incidence. A simple calculation shows that this must be the case if a true equilibrium exists (see fig. 4). It was thought that a more accurate treatment would result from an increase in the number of x-intervals selected from 100 to 1000 and even to 10000. However, the additional computational errors which are introduced cancel out any improvement in the data, so that whilst the results for 1000 intervals are exactly the same, those for 10000 intervals produce much more pronounced oscillations.

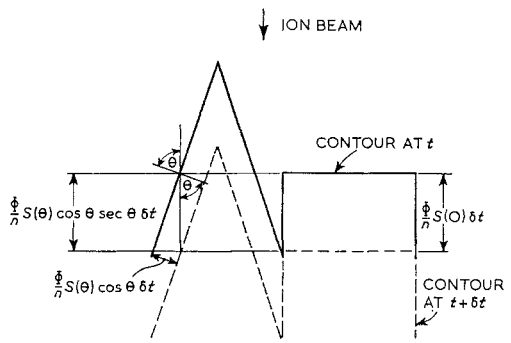

Figure 4 Illustration of the equilibrium condition that $S(\theta)$ must equal $S(0)$.

Because the $S - \theta$ characteristic is clearly so important in governing the final contour, a different $S - \theta$ curve was introduced into the programme. This curve had a maximum value for S at $\theta = 67°$ and $S(\theta) = S(0)$ at $\theta = 87°33\frac{1}{2}'$. The programme for $y = \sin(2\pi x)/\lambda$ was repeated with this new $S(\theta)$ function and an identical form of equilibrium is clearly being approached as shown in fig. 5. However, slope of the triangular sections of the curve are now $\theta = 87° 33\frac{1}{2}'$, the new value for which $S(\theta) = S(0)$.

The computed form of the equilibrium contours is as predicted by the previous analytical treatment of the process, [2] in that generators result for which θ is equal to 0°, 90° or some other fixed angle. The computation revealed that the fixed angle was, in fact, θ_n (the angle for which

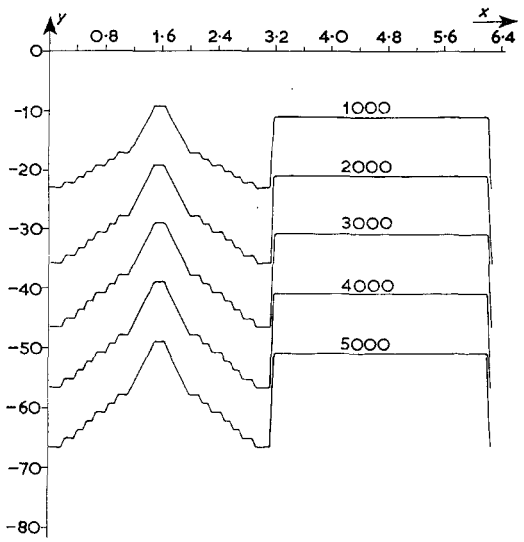

Figure 5 Development of a contour $y = a \sin(2\pi x)/\lambda$ for which $\lambda = 2\pi a$ and $a = 1$ using a new $S - \theta$ function of the form $S = 25(\cos\theta - 1.42\cos^2\theta + 0.46\cos^4\theta)$. The scale factor β is 0.0833.

$S(\theta) = (S0)$). This result is clearly due to the limiting behaviour of the maximum and minimum of the sine wave for which the ion beam is always normal to the simulated surface. Other studies have suggested that the fixed angle should be $\hat{\theta}$ (i.e. the angle for which S is a maximum), since a contour with this angle would tend to develop more rapidly than others and indeed, solution of equation 1 for convex surfaces shows that surfaces at all angles rotate, in equilibrium to $\hat{\theta}$. It appears, however, that the dominant conditions in deciding the final development of the curve is associated with the erosion of that part of the surface which is normal to the beam.

A further interesting feature is the development of the vertical step $x = (n\lambda)/2$. At such points $(\partial\theta)/\partial x$ is initially zero, i.e. inflexion points, and the sputtering rate at both sides of such a point will be either greater than or less than that at the inflexion value. This immediately develops a local maximum and minimum which rapidly becomes a quasi-step. The role of the inflexion point can be further understood, since it represents the transition from a convex to a concave surface, the latter part of which rotates, according to solution of equation 1 towards a vertical or horizontal generator, according as to whether the angle at the inflexion point is greater or less than $\hat{\theta}$.

It should be noted that the present simulation treats the apex of the convex surface, at all times, as lying normal to the beam with a consequent constant erosion rate of $S(0)$. In other estimates of the motion of surfaces [4], the progress of a point of intersection of lines is considered by reference to the motion of the lines remote from the point, so that this point, which is a discontinuity in equation 1 ($[d\theta]/dx = \infty$) is dictated by the motion of the surroundings rather than the reverse, which occurs in the present simulation at the apex. In a practical situation, the sputtering process is dictated by a collision cascade of finite dimensions, so that it is probably unrealistic to consider that the apical point can remain a point unaffected by neighbouring sputtering. This mean that, although the computer simulation *precisely* represents an idealised situation of point by point sputtering, in reality, the special limiting action of the $\theta = 0$ point may not exist. Removing this limitation may then result in formation of cones of angle $\hat{\theta}$, as predicted theoretically and we are currently conducting further simulations, in which the motion of an initially $\theta = 0$ point is dictated by neighbouring points and is excluded itself from dominating the process.

It is surprising to note how much "sputtering time" is involved in reaching the equilibrium condition. For the $y = \sin(2\pi x)/\lambda$ contour, approximately 8000 steps, each of magnitude 0.01 of the original amplitude of the sine wave, are required before equilibrium is reached. This means that a depth of over 100 times the original amplitude of the undulation must be removed before attaining equilibrium, so that, if we are dealing with a 1 mm amplitude, 80 mm would have to be removed. Obviously, experimental observations of surface topography will generally compare with contours in the early stages of this computer programme. For example, contour number 21 of fig. 2, where a thickness 0.2 mm has been sputtered away, may be typical. In experimental conditions, this contour will, in fact, be the section through the three-dimensional topography, i.e. it represents a cone in a valley. Such contours have, in fact, been observed on gold by Navinsek [5]. It should be noted that, in this treatment, no account is taken of redeposition of sputtered material. Clearly, the escape of atoms from the bottom of grooves must be restricted, so that one can estimate a filling-in of the valleys and a generally less-ragged equilibrium contour than is predicted. Also, the

effect of ions rebounding at grazing incidence and sputtering in a second collision has been ignored.

The computer programme has successfully followed the development of a sinusoidal surface to an equilibrium form. The angle at which the sputtering coefficient is again equal to the normal incidence value (θ_n) is of extreme importance; in three-dimensional topography, cones will develop with semi-vertical angle ($\pi/2 - \theta_n$). Experimental observation of such cones is unlikely as the equilibrium does not occur until some 100 mm of surface is eroded. Intermediate stages in the progress to equilibrium will, however, be seen and existing obervations support this model.

Although it is believed that the present calculations present the general details of the topographical development, further simulation with different amplitudes to wavelength values and other forms of the $S - \theta$ function are being investigated to study the development of real surfaces.

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Short-term Elevated Temperature Tensile Behaviour in 0° Sapphire Filament

The structure and resulting complicated nature of the slip process in sapphire [1] give this material potential use as a structural material at elevated temperature. At the present time, data exist for the strengths of whisker and bulk forms of sapphire at elevated temperature showing more than an order of magnitude variation in comparative strengths. This note reports studies of the elevated temperature strength of a newer type of bulk material available in very long filament form having room temperature properties approaching the whisker values [2-4].

The first measurements of the high temperature strength of bulk sapphire crystals were carried out in tension, compression and bending by Wachtman and Maxwell [5-7] who demonstrated that macroscopic plastic deformation could be induced above 900° C when the basal plane was favourably oriented for slip. Creep by slip on this system was observed at low resolved stresses, 11 to 12 ksi, at 1000° C. This behaviour was shown qualitatively to be similar to metals at lower temperatures. The same authors [7] also carried out a study of the short term properties in bending of sapphire having the 0 and 45° orientations as a function of temperature up to 1000° C. The strength was shown in both cases to show a minimum value in the range 400 to 600° C. The minimum was lowest in the 0° samples, while the maximum was the greatest in the 45° samples. In the latter case, the 1000° C strength was 90 ksi greater than the room temperature strength. This qualitative behaviour was rationalised by the hypothesis that plastic crack blunting became operative as temperature increased and was most effective in those orientations favouring slip. The minimum strength has been observed by others in experiments carried out in vacuum [8].

More recently, tension tests above 1000° C have demonstrated that sapphire displays a striking yield drop and strain rate effect in tension tests so that, from 1100 to 1500° C, the strain rate as well as the temperature is a significant determinant of fracture stress [9, 10]. The samples in these experiments were 60° rods and were favourably oriented for slip on the basal system.