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Ripple structures on ion bombarded surfaces arising from the sputter yield dependence on incidence angle

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ABSTRACT

It is shown that ripple structures on oblique incidence ion bombarded surfaces can be stable features under ion erosion without the necessity to invoke mass redistribution, surface diffusion or micro-roughening due to surface curvature dependent energy deposition. Instead the patterns are predicted to be a natural consequence of non-linear effects due to the dependence of the sputtering yield on the angle of incidence.

1. Introduction

Ion-induced ripple pattern formation on semiconductor surfaces under oblique incidence low energy impact is an important phenomenon which has been used to fabricate reproducible patterns in nanotechnology for a number of years [1] but even now the basic formation mechanism is still not fully understood. One of the earliest models of ripple pattern formation was due to Bradley and Harper [2] and since then many other models have been proposed [3–10]. Some of these models assume that ripple patterns could form as a result of the competing effects of surface diffusion (smoothing) and micro-roughening following the Sigmund model [11]. In the Sigmund model roughening occurs because energy is deposited closer to a surface in regions where there are troughs on a surface compared to regions of positive curvature. Sigmund was able to argue that this meant that cones should preferentially form on ion bombarded surfaces as a result.

However this curvature dependent energy deposition should be a second order effect compared to the first order effect of the sputtering yield dependence on the incidence angle. If the primary effect of incidence angle dependence only is taken into account, then work in the 1970s and 1980s [12–15] showed that although cones and edges can form on surfaces subjected to normal incidence ion beams, the surfaces would ultimately flatten due to the sides of the cones eroding at a faster rate than the surrounding flat surface. This is in direct contradiction to the Sigmund's micro-roughening argument.

Carter and Vishnyakov [3] first proposed that instead of the micro-roughening proposal, mass redistribution could be the mechanism by which surface features may be formed and this argument has also been used by Madi et al. [17] and by Numazawa and Smith [18] to show that ripple features can arise purely as a result of mass redistribution alone without even the necessity to use erosion in the argument. In the case of [18] a travelling wave solution was found for a specific incidence angle for the non-linear equations of motion, in the form of a cycloid which matched experimental observations very well.

In this paper an even simpler two-dimensional model is introduced which shows that stable patterns can arise purely as a result of the non-linear dependence of sputtering yield on the ion incidence angle and without the need to invoke any other physical property. This effect was overlooked in the 1970s and 1980s when the theory of surface erosion was first developed because the models were generally formulated by assuming that the ion beam was incident in the direction of the average surface normal. Here we reformulate the equations for non-normal incidence and apply the model to illustrate how stable ripple-like patterns can arise.

2. The model

The co-ordinate system is defined in Fig. 1a. The Cartesian $x-y$ system defines directions respectively parallel and perpendicular to the average surface tangent. The gradient of the surface is given by $\tan\theta$, where θ is also the angle between the surface normal and the y-direction; ϕ is the angle between the ion beam and the surface normal while the angle ψ defines the angle between the ion

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beam and the y-direction. In Fig. 1b the sputter yield dependence on incidence angle ϕ is plotted with a fit to 1 keV ion bombardment of silicon [19]. Although this dependence is typical for many amorphous and semiconductor materials, for metals there are many more maxima and minima due to channelling [20] and also metals retain their crystallinity under ion bombardment [21] whereas silicon becomes amorphous.

If it is assumed that the rate of erosion in the ion beam direction is given by $S(\phi)$ where the flux and atom density are assumed incorporated into a non-dimensionalised time, then it easy to show, following the methodology given in [22] and [13] that the erosion can be described by two first order quasi-linear partial differential equations for θ given by

$$\frac{\partial\theta}{\partial t} + (\sin\psi S(\psi-\theta) - \cos\theta\cos(\psi-\theta)S'(\psi-\theta))\frac{\partial\theta}{\partial x} = 0 \tag{1}$$

and

$$\frac{\partial\theta}{\partial t} - (\sin\theta\cos(\psi-\theta)S'(\psi-\theta) + \cos\psi)S(\psi-\theta)\frac{\partial\theta}{\partial y} = 0. \tag{2}$$

where the primes denote differentiation. In the first equation the partial differential with respect to t means at constant x, whereas in the second equation y is kept constant. These equations have been intensively investigated for the case $\psi = 0$ [12–15] but in the case of ripple formation $\psi \neq 0$. The equations are of a form first investigated by Lagrange [22] and in the 1950s a similar set was used by Lighthill and Whitham [23] to model the flow of traffic. The method of solution involves integration along the characteristic curves [22] but since the right hand sides of the equations are zero, the characteristic curves define straight lines of constant surface orientation ($\theta = const$). The characteristic curves are given in the usual way [22] by the equations

$$\frac{dx}{dt} = \sin\psi S(\psi-\theta) - \cos\theta\cos(\psi-\theta)S'(\psi-\theta) \tag{3}$$

and

$$\frac{dy}{dt} = -\sin\theta\cos(\psi-\theta)S'(\psi-\theta) - \cos\psi S(\psi-\theta) \tag{4}$$

These lines have gradient given by

$$\frac{dy}{dx} = (-\sin\theta\cos(\psi-\theta)S'(\psi-\theta) - \cos\psi S(\psi-\theta))/(\sin\psi S(\psi - \theta) - \cos\theta\cos(\psi-\theta)S'(\psi-\theta)). \tag{5}$$

Thus the surface evolution can be plotted graphically in the same way as the Huyghen's wave front construction in geometrical optics, except that now the wavefront does not propagate isotropically. Instead parts of the surface expand into facets, whereas other parts of the surface contract into edges or shocks (discontinuities in θ). The shocks are equivalent to caustic curves in geometrical optics [24]. To examine which parts of the surface expand and which parts contract, consider a small element of the initial surface δs_0. After time t, using Eqs. (3) and (4) it is possible to evaluate how δs_0 evolves. After some algebra the corresponding element, δs, on the evolved surface can be calculated as

$$\delta s^2 = \delta s_0^2(1 + 2t\kappa[\cos(\psi-\theta)S''(\psi-\theta) - 2\sin(\psi-\theta)S'(\psi-\theta)]) \times [1 + t\kappa[\cos(\psi-\theta)S''(\psi-\theta) - 2\sin(\psi-\theta)S'(\psi-\theta)]. \tag{6}$$

Here κ is the curvature of the surface and is a function of θ. Thus expansion waves occur when the function $g(\theta,\psi)$ is positive where

$$g(\theta,\psi) = \kappa[\cos(\psi-\theta)S''(\psi-\theta) - 2\sin(\psi-\theta)S'(\psi-\theta)]. \tag{7}$$

Eq. (7) was also derived in [12] when $\psi = 0$ and an equivalent expression by Budil and Hobler [16].

3. Results and discussion

One can now see why this formulation is in contradiction to the micro-roughening argument of Sigmund for normally incident ion beams ($\psi = 0$) by using a specific example. Consider a surface initially described by a simple sinusoidal curve subject to erosion by a normally incident beam shown in Fig. 2 for different times. One can see how the surface maxima evolve into discontinuities due to the collapse of surface elements ($\kappa < 0$), whereas the bottom of the valleys expand ($\kappa > 0$). The sides of the 'cones' evolve into facets corresponding to the maxima ($g_\theta = 0$) in Eq. (7) before the surface eventually flattens due to these facets eroding more quickly than the flat concave areas of the surface. This rather remarkably depends on the third derivative (the maximum occurs when $g_\theta = 0$) of the sputtering yield with respect to the incidence angle and the surface curvature defines whether or not locally flat regions either sharpen (tops of ridges) or expand (bottoms of valleys). Facets therefore do not always form corresponding to planes where the sputtering yield is a maximum as was predicted over 40 years ago by Stewart and Thompson [25]. Conical structures do form and persist on ion-bombarded surfaces due to crystallinity effects such as grain boundaries or due to impurities shielding parts of a surface that erode at a faster rate. Indeed similar structures can also be seen in geology such as at Tent Rocks in New Mexico. However any initially flat surface under bombardment by a normally incident beam with the sputtering yield-angle of incidence dependence as given in Fig. 1b will remain flat since any perturbations in the surface height will flatten as the result in Fig. 2 demonstrates.

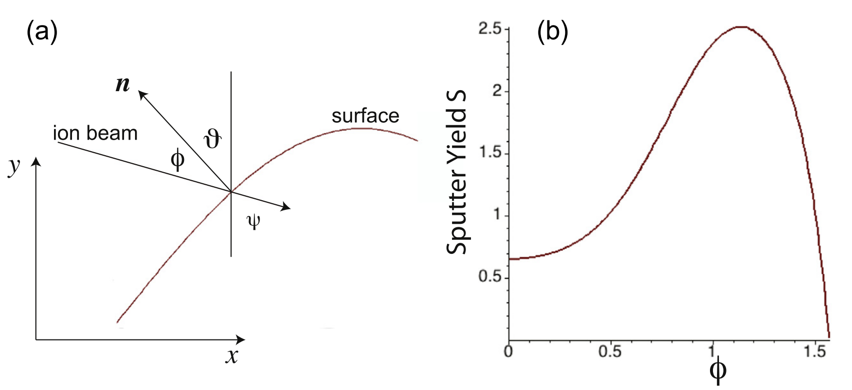

Fig. 1. (a) A description of the co-ordinate system and angles used in the calculation. The y direction defines the normal to the originally flat surface. (b) The dependence of sputtering yield S (atoms ejected per incident ion) on incidence angle for 1 keV Ar bombardment of Si taken from [19]. The value of ϕ corresponding to the maximum sputtering yield is defined as ϕ_{max} which for many materials is an angle between 50° and 70°.