

# Analytical and graphical evaluation of local quasi-stable angular points during ion bombardment at oblique incidence

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An implied analytical condition, connecting the incidence angles  $\theta_0$  and  $\theta_e$  between the two intersecting microfacet normals and the ion beam direction, has been inferred for the existence of local quasi-stable intersections (angular points) during ion erosion. This condition, which can also be deduced on the basis of the erosion slowness curve, leads to a higher degree algebraic equation with a parameter, applicable for any dependence  $S = S(\theta)$ , expressed as an algebraic polynomial expression in  $\cos \theta$ . A new graphical method for evaluation of orientations  $\theta_e$  compatible with a given orientation  $\theta_0$ , based on a known polar diagram cursor-type, has also been proposed.

## 1. Introduction

In some previous works [1–5] it has been shown that, during the evolution of surface microtopography subjected to ion erosion, some recently formed or pre-existing edges on the initial profile, defined by surface–surface, surface–plane or plane–plane intersections, can temporarily have a linear trajectory. These intersections (angular points) could be eventually defined as locally quasi-stable since they are completely stable provided that they do not become absorbed with near surface morphology elements, especially by the time regression of other adjacent angular points.

The local quasi-stable angular points can be found by computational methods or graphically on the basis of erosion slowness curve [1–4]. A good agreement between theoretically predicted angular points and experimental observations has been found for the particular case of ion erosion of steps in silicon [2]. Later, the variation of slope angles at quasi-stable angular points as a function of oblique incidence angle between the ion beam

and the adjacent microfacet normal has been calculated for a specific dependence  $S = S(\theta)$  [3].

Recently, a three-dimensional treatment of the evolution of surface topography, based on the method of characteristic trajectories [6], has been extended to the appearance and development of edges and facets upon amorphous and crystalline surfaces undergoing ion bombardment, in order to include the effects of stationary points, present in the angular dependence of the sputtering yield [5].

The importance of angular point evaluation in the theoretical study of the surface topography formed during ion etching and ion-induced surface roughening, for the improvement of depth profiling used in surface analysis and in the generation and delineation of fine-geometry patterns used in microelectronics, have been pointed out in several works mentioned earlier [1–6].

The present work describes an attempt to calculate, by algebraic means, for any dependence  $S = S(\theta)$ , the slope angles  $\theta_e$  of any curves (sur-

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faces) which form local quasi-stable intersections with a line (plane) bombarded by an ion beam at an oblique incidence angle  $\theta_0$ . Although the analytical condition for the existence of a local quasi-stable angular point can be inferred on the basis of the double condition, earlier given by Ducommun *et al.* [2], leading finally to a higher degree equation with a parameter, this direct method for obtaining the dependence  $\theta_e = f(\theta_0)$  provides a much more simple approach in comparison with the earlier proposed computational manner based on a relatively tedious erosion model [3]. Similar algebraic equations have been recently proposed for the evaluation of some other angular values, important for ion erosion [7].

The calculation performed for three different dependences  $S = S(\theta)$ , allows the comparison of results depending on the exact form of the chosen corresponding function  $S(\theta)$ . A general discussion, valid for any function  $S = S(\theta)$ , of the found dependence relationship between the incidence angles  $\theta_e$ ,  $\theta_0$ , associated with a quasi-stable intersection, will be published later [8].

Furthermore, an alternative graphical method for evaluation of incidence angles associated with local quasi-stable intersections is given, presenting more valuable advantages as compared to an earlier proposed graphical method [2–4].

## 2. Theoretical background

### 2.1. Analytical condition for the existence of a local quasi-stable angular point

We consider the intersection of two curved surfaces (or of a plane and an arbitrary surface) subjected to an ion beam incident at the angles  $\theta_0$  and  $\theta_e$  upon the planes tangent along the intersection line of the two surfaces (Fig. 1).

In the two-dimensional case, the simultaneous double condition for angular point local quasi-

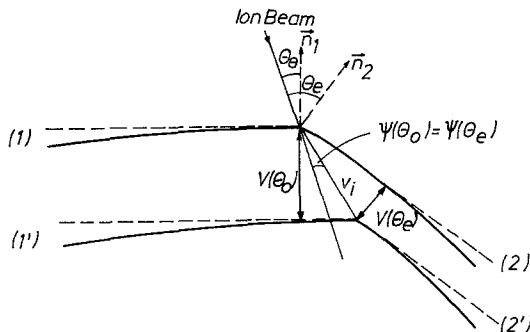


Figure 1 Evolution by ion erosion of a local quasi-stable angular point.

stability (recession linear trajectory), given by Ducommun *et al.* [2], imposes an overlapping of the motion directions of the curve's ending points at the intersection and also an equal velocity for these points (Fig. 1):

$$\psi(\theta_0) = \psi(\theta_e) = \psi \quad (1)$$

and

$$v_i = \frac{V(\theta_0)}{\cos[\theta_0 + \psi(\theta_0)]} = \frac{V(\theta_e)}{\cos[\theta_e + \psi(\theta_e)]} \quad (2)$$

where the angle  $\psi(\theta)$  is formed between the linear trajectory of the quasi-stable angular point and the ion beam direction,  $v_i$  is the recession velocity of the quasi-stable angular point, and  $V(\theta)$  is the ion erosion rate of a plane bombarded at an incidence angle  $\theta$ :

$$V(\theta) = \frac{\Phi}{n} S(\theta) \cos \theta \quad (3)$$

where  $\Phi$  is the ion beam current density and  $n$  is the target number density.

By substituting Equations 1 and 3 into Equation 2, the analytical condition for the existence of a local quasi-stable angular point is given by an expression identical to that obtained by Ducommun *et al.* [2]:

$$\frac{S(\theta_0) \cos \theta_0 \cos(\psi + \theta_e)}{S(\theta_e) \cos \theta_e \cos(\psi + \theta_0)} = 1. \quad (4)$$

From Condition 4 we easily obtain the relation:

$$\tan \psi = \frac{[S(\theta_e) - S(\theta_0)] \cos \theta_e \cos \theta_0}{S(\theta_e) \cos \theta_e \sin \theta_0 - S(\theta_0) \cos \theta_0 \sin \theta_e} \quad (5a)$$

leading to the well-known result of Stewart and Thompson [9] for the direction of motion of the intersection point between two planes with different orientations:

$$\tan \psi = \frac{S(\theta_e) - S(\theta_0)}{S(\theta_e) \tan \theta_0 - S(\theta_0) \tan \theta_e} \quad (5b)$$

Equations 5a and b are perfectly symmetrical in  $\theta_0$  and  $\theta_e$ , so that:

$$\psi(\theta_0, \theta_e) = \psi(\theta_e, \theta_0) \quad (6)$$

This result shows that the direction of the angular point during ion erosion is invariant as against the reversing of intersecting microfacet orientation with respect to the ion beam (Fig. 2).

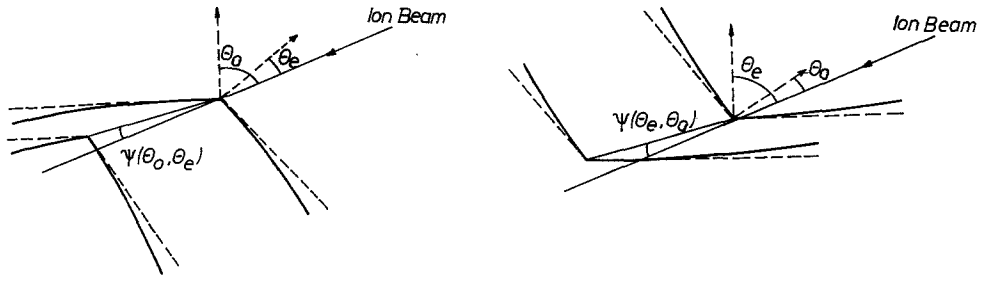


Figure 2 The invariance of the direction of angular point during ion erosion as against the reversing of intersecting microfacet orientation with respect to the ion beam:  $\psi(\theta_0, \theta_e) = \psi(\theta_e, \theta_0)$ .

Carter *et al.* [4] have shown that the behaviour of the intersecting line between two surfaces (angular point between two curves) during ion erosion can be seen as a special case of the general differential erosion theory leading to the erosion slowness curve. Thus, if in Equation 5a,  $\theta_0 \rightarrow \theta$  and  $\theta_e \rightarrow \theta + d\theta$ , this equation is readily shown to lead to an earlier inferred well-known expression:

$$\tan \psi = \frac{\cos^2 \theta \frac{dS}{d\theta}}{\sin \theta \cos \theta \frac{dS}{d\theta} - S} \quad (7)$$

Equation 5a, representing the slope of the quasi-stable angular point trajectory with respect to the ion beam direction, must be equal to the differential expression of  $\tan \psi(\theta_e)$ , related to the angle between the trajectory of the point of  $\theta_e$  orientation and the ion beam direction:

$$\begin{aligned} & \frac{[S(\theta_e) - S(\theta_0)] \cos \theta_e \cos \theta_0}{S(\theta_e) \cos \theta_e \sin \theta_0 - S(\theta_0) \cos \theta_0 \sin \theta_e} \\ &= \frac{\cos^2 \theta_e \frac{dS}{d\theta} \Big|_{\theta=\theta_e}}{\sin \theta_e \cos \theta_e \frac{dS}{d\theta} \Big|_{\theta=\theta_e} - S(\theta_e)} \end{aligned} \quad (8)$$

Further simplification finally results in:

$$\frac{dS}{d\theta} \Big|_{\theta=\theta_e} = \frac{\cos \theta_0 [S(\theta_0) - S(\theta_e)]}{\cos \theta_e \sin(\theta_0 - \theta_e)} \quad (9a)$$

Equation 9a represents an implicit interconnection between the incidence angles  $\theta_0$  and  $\theta_e$  associated with a local quasi-stable angular point, depending solely on the exact shape of  $S(\theta)$ . By using this equation, the incidence angles  $\theta_e$  associated with any curve, forming a quasi-stable angular

point with another curve (line) whose normal to the tangent in the intersection point is inclined at a given angle  $\theta_0$  to the ion beam direction, can be easily calculated.

An equivalent condition, where the role of angles  $\theta_0$  and  $\theta_e$  is reversed, can be obtained by identifying Equation 5a with the differential expression of  $\tan \psi(\theta_0)$ , on the basis of Equation 1:

$$\frac{dS}{d\theta} \Big|_{\theta=\theta_0} = \frac{\cos \theta_e [S(\theta_e) - S(\theta_0)]}{\cos \theta_0 \sin(\theta_0 - \theta_e)} \quad (9b)$$

Evidently, the solution of Equations 9a and b leads to:

$$\theta_e = f(\theta_0) \quad (10a)$$

$$\theta_0 = f(\theta_e) \quad (10b)$$

where the dependence  $f$  must be equal to its inverse:

$$f(\theta) = f^{-1}(\theta) \quad (11)$$

which is a result supported by the possible interchangeability between the angles  $\theta_0$  and  $\theta_e$  in Equations 9a and b.

Taking into account the evident properties of the dependence  $S = S(\theta)$ :

$$S(\theta) = S(-\theta) \quad (12a)$$

$$\frac{dS}{d\theta} \Big|_{\theta=-\theta_e} = -\frac{dS}{d\theta} \Big|_{\theta=\theta_e} \quad (12b)$$

$$\frac{dS}{d\theta} \Big|_{\theta=-\theta_0} = -\frac{dS}{d\theta} \Big|_{\theta=\theta_0} \quad (12c)$$

it is easy to see that Equations 9a and b are invariant to a simultaneous sign change of variables  $\theta_0$  and  $\theta_e$  ( $\theta_e \rightarrow -\theta_e$ ,  $\theta_0 \rightarrow -\theta_0$ ). Therefore, in a coordinate system  $(\theta_0, \theta_e)$ , the graphical representation of the function  $f$  will be symmetrical about the origin  $\theta_0 = \theta_e = 0^\circ$ .

## 2.2. Algebraic equations associated with the analytical condition for local quasi-stable angular points

Generally, the angular dependence of sputtering yield can be described by a polynomial expression in  $\cos \theta$  [1–5, 10–12]:

$$S(\theta) = \sum_{k=1}^n a_k \cos^k \theta \quad (13)$$

where  $a_k$  are numerical coefficients, so chosen that the function  $S(\theta)$  shall fit the experimentally observed angular dependence for a given energy and ion-target combination.

Experimentally, the function  $S(\theta)$  increases from  $S(0^\circ)$ , at  $\theta = 0^\circ$ , and reaches a maximum value of  $S(\theta_p)$  at an angle  $\theta = \theta_p$ . Then,  $S(\theta)$  decreases with increasing angle of incidence until  $\theta \rightarrow \pi/2$  (grazing incidence) when  $S(\theta) \rightarrow 0$  [4].

The substitution of expressions for  $S(\theta_0)$ ,  $S(\theta_e)$  and of the first derivative  $dS/d\theta|_{\theta=\theta_e}$ :

$$\left. \frac{dS}{d\theta} \right|_{\theta=\theta_e} = (-\sin \theta_e) \sum_{k=1}^n k a_k \cos^{k-1} \theta_e \quad (14)$$

in Equation 9a leads to a trigonometric equation in  $\cos \theta_e$  and  $\sin \theta_e$  containing the parameter  $\theta_0$ :

$$\begin{aligned} & -\cos \theta_0 \sum_{k=1}^n k a_k \cos^{k+2} \theta_e - \sin \theta_0 \sin \theta_e \\ & \times \sum_{k=1}^n k a_k \cos^{k+1} \theta_e + \cos \theta_0 \sum_{k=1}^n (k+1) a_k \cos^k \theta_e \\ & = \sum_{k=1}^n a_k \cos^{k+1} \theta_e. \end{aligned} \quad (15a)$$

The same equation can be also written as:

$$\begin{aligned} & \sum_{k=1}^n a_k \cos^k \theta_e [(k+1) \cos \theta_0 - k \sin \theta_0 \sin \theta_e \\ & \times \cos \theta_e - k \cos \theta_0 \cos^2 \theta_e] = \sum_{k=1}^n a_k \cos^{k+1} \theta_e \end{aligned} \quad (15b)$$

Since the Equations 15a and b contain not only terms in  $\cos \theta_e$  but also a linear term in  $\sin \theta_e$ , the solution is possible by the substitution  $t = \tan \theta_e/2$ , which leads to an algebraic equation of  $2n+4$  degree:

$$\begin{aligned} & \sum_{k=1}^n a_k \frac{(1-t^2)^k}{(1+t^2)^{k+2}} \{ \cos \theta_0 [1 + 2(1+2k)t^2 + t^4] \\ & - \sin \theta_0 2kt(1-t^2) \} = \sum_{k=1}^n a_k \cos^{k+1} \theta_e \end{aligned} \quad (16)$$

which allows us to find the angles  $\theta_e$  for any given angle  $\theta_0$ .

In the particular case of normal incidence ( $\theta_0 = 0^\circ$ ) to one intersecting microfacet at the angular point, Equation 9a becomes:

$$\left. \frac{dS}{d\theta} \right|_{\theta=\theta_e} = \frac{S(\theta_e) - S(0^\circ)}{\sin \theta_e \cos \theta_e}. \quad (17)$$

The substitution of Equations 13 and 14 into Equation 17 gives:

$$\sum_{k=1}^n a_k [-kx^{k+2} + (k+1)x^k - 1] = 0 \quad (18)$$

which is an algebraic equation of  $n+2$  degree in  $x = \cos \theta_e$ . The same result is obtained from Equations 15 or 16 for  $\theta_0 \rightarrow 0^\circ$ .

Generally, this equation has four roots in the range  $\theta_e \in [-90^\circ, +90^\circ]$  noted as  $\pm \theta_{i_1}, \pm \theta_{i_2}$ .

Assuming a well defined initial angular dependence  $S = S(\theta)$ , the incidence angles  $\theta_e$  for a given angle  $\theta_0$  can be easily calculated from the algebraic Equations 16 and 18 respectively (for the particular case  $\theta_0 = 0^\circ$ ), both angles characterizing a local quasi-stable intersection during ion erosion.

## 3. Computational results

In this paragraph, the numerical results concerning the dependence  $\theta_e = f(\theta_0)$  will be given. Evaluation has been made on the basis of Equation 16, and eventually for  $\theta_0 = 0^\circ$ , of Equation 18, by using three types of  $S = S(\theta)$  dependences, previously proposed by different authors in specific applications:

$$1. S(\theta) = 3.4142 \cos \theta + 12.7574 \cos^2 \theta - 15.1716 \cos^4 \theta \quad [10].$$

$$2. S(\theta) = 33.5 \cos \theta - 90.9 \cos^2 \theta + 93.0 \cos^3 \theta - 34.6 \cos^4 \theta \quad [12].$$

$$3. S(\theta) = 18.73845 \cos \theta - 64.65996 \cos^2 \theta + 145.19902 \cos^3 \theta - 206.04493 \cos^4 \theta + 147.31778 \cos^5 \theta - 39.89993 \cos^6 \theta \quad [2].$$

Excepting the angular value  $\theta_p$  corresponding to a maximum sputtering yield and the angles  $\theta_{s_1}$  and  $\theta_{s_2}$ , related to the erosion slowness curve

[2], no other angular values important for ion erosion are given in the papers mentioned [2, 10, 12]. Recently, additional data concerning the main angular values connected to ion erosion and associated polar diagrams have been obtained by solving similar higher degree algebraic equations, applied for each specific  $S = S(\theta)$  dependence [7].

A computer program to solve Equations 16 and 18 respectively for each given  $\theta_0$  was devised. The results of the application of this program, by using the mentioned  $S(\theta)$  dependences, are shown in Figs. 3a, b and c for  $\theta_0 \in [-90^\circ, +90^\circ]$  and  $\theta_e \in [-90^\circ, +90^\circ]$ . The algebraic sign attached to the incidence angles is related to the relative position of respective microfacet normals as against the ion beam direction. If  $\theta_0$  and  $\theta_e$  have the same sign, the normals are both at the left or the right side, respectively, of the ion beam, but if these angles have opposite signs, the normals are in opposite regions with respect to the ion beam direction. The variation of incidence angles in the range  $[-90^\circ, +90^\circ]$  corresponds to the physical situation in which the microfacets are not shadowed with respect to the ion beam.

Generally, the dependence  $\theta_e = f(\theta_0)$  has four distinct branches which are noted as  $\theta_{e1}^1, \theta_{e1}^2, \theta_{e2}^1, \theta_{e2}^2$ . The additional branch  $\theta_{e1}^0$ , which corresponds to  $\theta_0\theta_e > 0$ , is linear ( $\theta_{e1}^0 = \theta_0$ ), being associated to a solution without a physical meaning. Indeed, if  $\theta_e = \theta_0$ , the angular point disappears and the microfacets are connected into a plane surface.

Although, in Fig. 3, the dependence  $\theta_e = f(\theta_0)$  is shown for the whole angular range  $[-90^\circ, +90^\circ]$ , the numerical computation can be limited only to  $\theta_0 \in [-90^\circ, +90^\circ]$  and  $\theta_e \in [0^\circ, 90^\circ]$  since the branches for  $\theta_e \in [-90^\circ, 0^\circ]$  could be traced taking into account the symmetry of the function  $f$  about the origin. Indeed, according to Fig. 3, the results obtained for  $\theta_0 \leq 0^\circ$  and  $\theta_e \leq 0^\circ$  are symmetrical about the origin with those corresponding to  $\theta_0 \geq 0^\circ$  and  $\theta_e \geq 0^\circ$ . Also, symmetrical data appear for  $\theta_0 \geq 0^\circ$  and  $\theta_e \leq 0^\circ$  with respect to the values for  $\theta_0 \leq 0^\circ$  and  $\theta_e \geq 0^\circ$ . The invariance of Equations 15 or 16 with the unchanged sign of the product  $\theta_0, \theta_e$  and their modification at the change of sign for  $\theta_0, \theta_e$  can easily explain this behaviour.

#### 4. Graphical evaluation of local quasi-stable angular points

Ducommun *et al.* [2] have proposed a geometrical method based on the erosion slowness curve to

determine the slope  $\theta_e$  of any surfaces (curves) which give quasi-stable intersections with a plane (line) of given orientation  $\theta_0$ . Thus, if from the point A, corresponding to the orientation  $\theta_0$  on the erosion slowness plot, tangents are drawn to the diagram, then the respective orientations associated to all tangent points represent the only orientations  $\theta_e$  compatible with a linear recession of edge intersections (local quasi-stable angular points) (Fig. 4). In Fig. 4, the tangent points  $B_1, C_1, B_2$  and  $C_2$  correspond to the orientations  $\theta_e$  defined as  $\theta_{e1}^1, \theta_{e1}^2, \theta_{e2}^1, \theta_{e2}^2$  associated with quasi-stable intersections. Indeed, the velocity and direction of motion of quasi-stable edges (angular points) are defined by the inverse magnitude and direction of the normals from the origin to the chords tangent at the erosion slowness curve (chords  $AB_1, AC_1, AB_2, AC_2$  in Fig. 4). Also, the same normals to the tangents at the erosion slowness curve in the points of  $\theta_e$  orientation define the velocity and direction of these points on the bounding curve.

The coincidence of the direction and velocity of edge (angular point) and curve boundary of  $\theta_e$  orientation indicates that Equations 1 and 2 for the existence of local quasi-stable angular points are simultaneously satisfied.

The analytical Condition 9a, satisfied by the incidence angles associated to quasi-stable angular points, can be easily derived on the basis of the geometrical method earlier proposed by Ducommun *et al.* [2]. If we equate the slope of normals at the points of B or C type and the slope of the normal at the chord joining the point A (orientation  $\theta_0$ ) and the points of B or C type (orientation  $\theta_e$ ):

$$\left. \frac{d\left(\frac{1}{S(\theta)} \tan \theta\right)}{d\left(\frac{1}{S(\theta)}\right)} \right|_{\theta=\theta_e} = \frac{\frac{1}{S(\theta_0)} \tan \theta_0 - \frac{1}{S(\theta_e)} \tan \theta_e}{\frac{1}{S(\theta_0)} - \frac{1}{S(\theta_e)}} \quad (19)$$

After rearrangement we have:

$$\begin{aligned} \tan \theta_e - \frac{S(\theta_e)}{\cos^2 \theta_e} \frac{1}{\frac{dS}{d\theta}} \Big|_{\theta=\theta_e} \\ = \frac{S(\theta_e) \tan \theta_0 - S(\theta_0) \tan \theta_e}{S(\theta_e) - S(\theta_0)} \quad (20) \end{aligned}$$

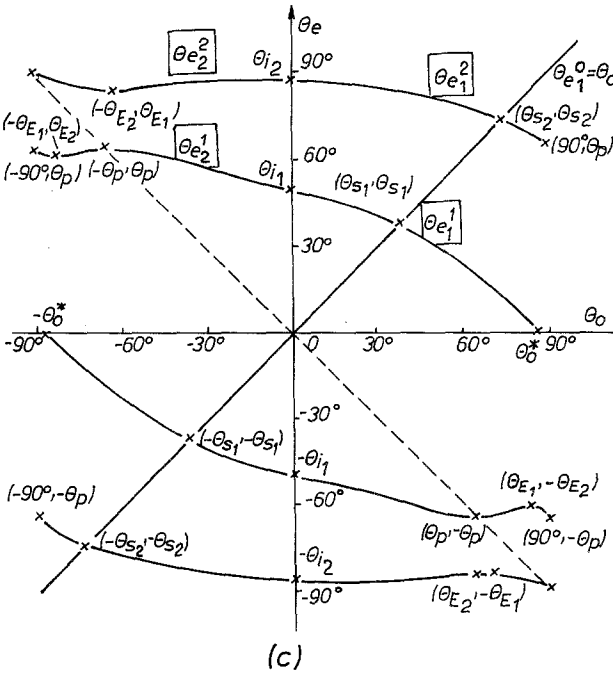
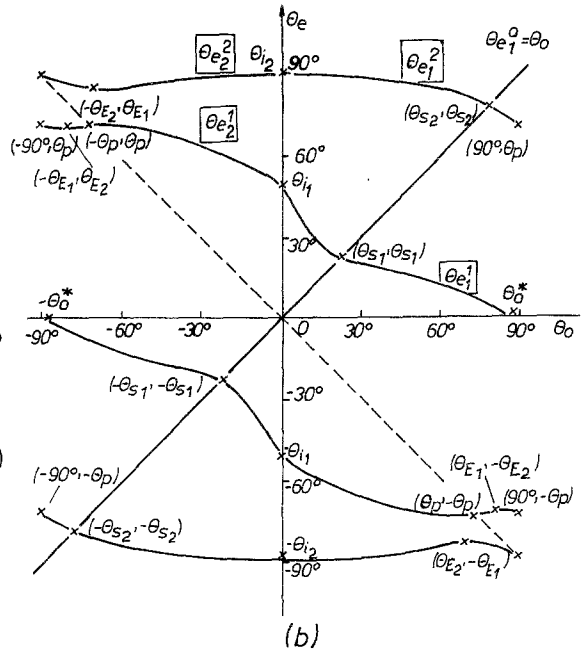
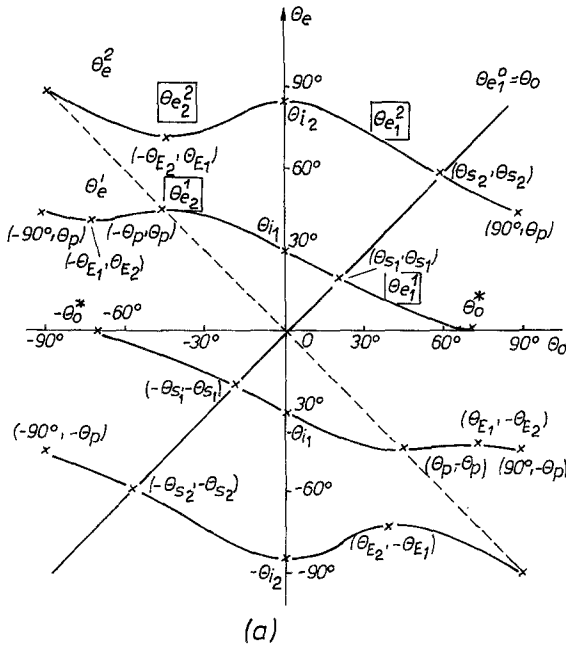


Figure 3 Variation of slope angles  $\theta_e$  associated with local quasi-stable angular points as a function of incidence angle  $\theta_0$ , computed for the following dependences  $S = S(\theta)$ : (a)  $S(\theta) = 3.4142 \cos \theta + 12.7574 \cos^2 \theta - 15.176 \cos^4 \theta$  [10], (b)  $S(\theta) = 33.5 \cos \theta - 90.9 \cos^2 \theta + 93.0 \cos^3 \theta - 34.6 \cos^4 \theta$  [12], (c)  $S(\theta) = 18.73845 \cos \theta - 64.65996 \cos^2 \theta + 145.19902 \cos^3 \theta - 206.04493 \cos^4 \theta + 147.31778 \cos^5 \theta - 39.89993 \cos^6 \theta$  [2].

which easily leads to Condition 9 associated with local quasi-stable angular points having linear trajectories during ion erosion.

A superior graphical method for evaluation of quasi-stable angular points may be obtained from the cursor-type polar diagram of normalized recession velocity  $V(\theta)/V(0^\circ)$  as a function of the associated recession angle  $\psi(\theta)$  for constant orientation trajectories, previously proposed by Carter *et al.* [4] and Lewis *et al.* [13].

In Fig. 5, showing this polar diagram in the range  $-90^\circ \leq \theta_0 \leq 90^\circ$ , the orientations  $\theta_e$  associated with a given angle  $\theta_0$  can be determined by intersecting the tangent at polar diagram in the point of orientation  $\theta_0$  with the diagram branches.

The angular values corresponding to the intersection points are just the angles  $\theta_e$ , according to the further demonstration. Indeed, if we draw the tangents to the points of the polar diagram corresponding to the orientations  $\theta_0$  and  $\theta_e$  (for example

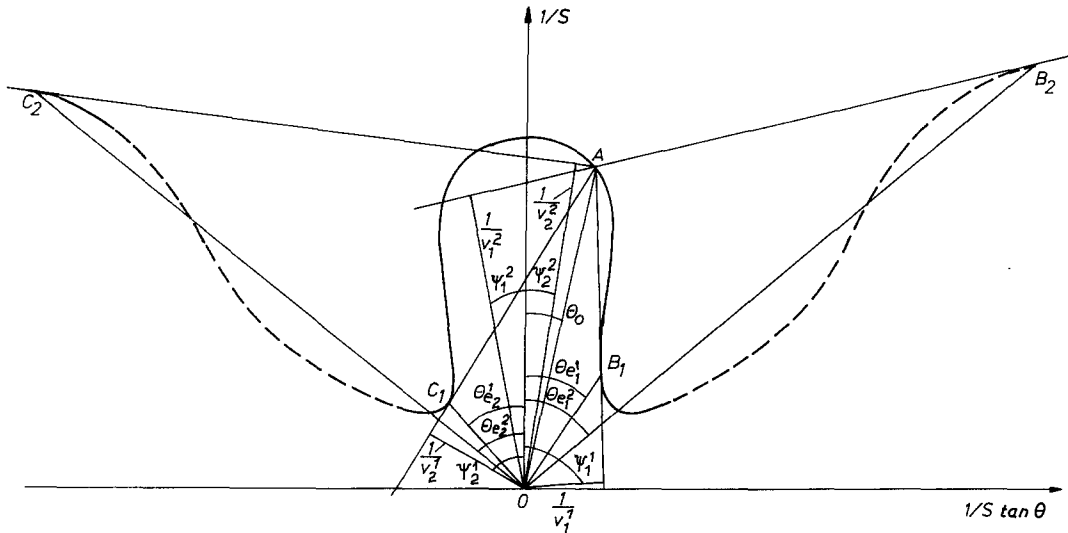


Figure 4 Graphical method according to Ducommun *et al.* [2], for determining the incidence angles  $\theta_{e_i}^k$  ( $\theta_{e_1}^1, \theta_{e_1}^2, \theta_{e_2}^1, \theta_{e_2}^2$ ) corresponding to a given value  $\theta_0$  and associated with the local quasi-stable angular points. The angles  $\psi_i^k$  between the recession directions of quasi-stable intersections and the ion beam direction and the associated recession velocities  $v_i^k$  are also shown.

$\theta_{e_1}^1$ ), from the geometry of Fig. 5, it is easily deduced that:

$$BC = OB - OC = S(\theta_e) - S(\theta_0) \quad (21)$$

and

$$\begin{aligned} BC &= BD - CD \\ &= AD(\tan \theta_e - \tan \theta_0) = \frac{dS}{d\theta} \Big|_{\theta=\theta_e} \\ &\quad \times \cos^2 \theta_e (\tan \theta_e - \tan \theta_0) \end{aligned} \quad (22)$$

since the representation has the remarkable property that a tangent drawn to the polar diagram at the point corresponding to the orientation  $\theta$  has itself the orientation  $\theta$  and intersects the negative Oy-axis at a value  $S(\theta)$  [4].

Further, the defining Condition 9a can be easily inferred by equating Equations 21 and 22.

Evidently, the reversing and self-intersection points of the polar diagram branches having a double tangent will be points of the dependence  $\theta_e = f(\theta_0)$ . In Fig. 3, the reversing points  $(\pm \theta_{s_1}, \pm \theta_{s_1})$ ,  $(\pm \theta_{s_2}, \pm \theta_{s_2})$  and the self-intersection point  $(\pm \theta_p, \mp \theta_p)$  are present for all cases in the representation  $\theta_e = f(\theta_0)$ .

According to a general discussion, valid for any dependence  $S = S(\theta)$ , which will be published elsewhere [8], the lower self-intersection points (and also, eventually, in some special cases, depending on the exact shape of  $S = S(\theta)$  dependence, the higher self-intersection points) between the diagram branches corresponding to the range  $\theta \in$

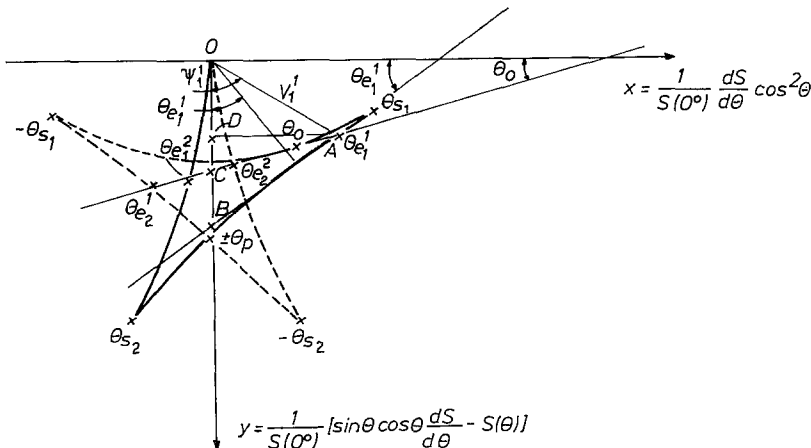


Figure 5 Graphical method based on cursor-type polar diagram, proposed by Carter *et al.* [4], for determining the incidence angles  $\theta_{e_i}^k$  corresponding to a given orientation  $\theta_0$  and associated to the possible quasi-stable angular points ( $\psi_i^k$  and  $v_i^k$ , graphically indicated, have the same meaning as in Fig. 4).

$[0^\circ, 90^\circ]$  and those for  $\theta \in [-90^\circ, 0^\circ]$  have been identified as some extremum points of the dependence  $\theta_e = f(\theta_0)$ . In Fig. 3 these points are noted as  $(\pm \theta_{E_1}, \mp \theta_{E_2})$  and respectively  $(\pm \theta_{E_2}, \mp \theta_{E_1})$ .

Recently, it has been shown that the erosion slowness curve and the diagram mentioned above contain essentially all important angular values related to the ion erosion and the dependence  $S = S(\theta)$ , which can be easily evaluated by higher degree algebraic equations [7].

## 5. Discussion

During ion erosion, an intersection between two surfaces, characterized by the associated incidence angles  $\theta_0$  and  $\theta_e$ , satisfying the inferred analytical Condition 9a, may be infinitely stable only for an ideal situation when no absorption or injection of other orientations, besides those naturally related to its boundary surfaces, are occurring. Generally, in the real case, an edge of this type will be however influenced by the time evolution of the adjacent angular points, so that the respective intersection (angular point) will have only a temporary stability, defined by the instantaneous linear edge motion. Therefore, these local quasi-stable angular points are transient in the surface morphology evolution, not being connected to a real space and time extended stability.

In this work, the mutual variation of slope (incidence) angles  $\theta_0$  and  $\theta_e$ , associated with a local quasi-stable angular point, has been numerically computed for various  $S = S(\theta)$  dependences.

For  $\theta_0 \theta_e > 0$ , the dependence  $\theta_e = f(\theta_0)$  has three distinct branches  $(\theta_{e1}^0, \theta_{e1}^1, \theta_{e1}^2)$  and for  $\theta_0 \theta_e < 0$  only two branches  $(\theta_{e2}^1, \theta_{e2}^2)$ .

The linear branch  $\theta_{e1}^0 = \theta_0$  corresponds to a trivial solution, consisting in the connection of the microfacets forming thus a plane surface without angular point. Mathematically, the respective solution is evident if we make  $\theta_e \rightarrow \theta_0$  in Equation 9a.

Taking into account the symmetry of the dependence  $\theta_e = f(\theta_0)$  about the origin, a qualitative discussion of its behaviour will be given only for  $\theta_e \in [0^\circ, 90^\circ]$ .

The branch noted  $\theta_{e1}^1$ , formed by the connection of the branches  $\theta_{e1}^1(\theta_0 > 0^\circ)$  and  $\theta_{e2}^1(\theta_0 < 0^\circ)$  contains some remarkable points.

1. The absolute maximum point  $\theta_0 = -\theta_p$ ,  $\theta_e = \theta_p$  which is an evident solution of Condition 9a and represents, according to Carter *et al.* [4], a stable intersection plane–plane. This pair  $(-\theta_p, \theta_p)$  corresponds to the regression of the angular point

along the bisector of a ridge bombarded with an ion beam parallel to the respective bisector [13].

2. The point  $\theta_0 = \theta_{s_1}$ ,  $\theta_e = \theta_{s_1}$  is simultaneously contained by the branches  $\theta_{e1}^1$  and  $\theta_{e1}^0$  as a double root, leading to the physically trivial solution mentioned.

3. The point  $\theta_0 = -90^\circ$ ,  $\theta_e = \theta_p$  corresponds to the erosion of an edge, bounded by planar or curved surfaces, making an acute angle with an ion beam perfectly grazing one of microfacets.

4. The point  $\theta_0 = \theta_0^*$ ,  $\theta_e = 0^\circ$  (where  $S(\theta_0^*) = S(0^\circ)$ ) corresponds to metastable intersections of type surface–surface, plane–surface or plane–plane. The angular point between two planes characterized by these incidence angle values is not stable, although a computer simulation of ion erosion for a sinusoidal contour [10] has indicated as a final equilibrium profile a ridge of  $\theta_0^*$  slope lying on a horizontal plane. However, it has been demonstrated theoretically [1] or by computer simulation [11] that such a formation is quasi-stable, relaxing to a ridge having a  $\theta_p$  slope. Some additional information about the metastability of ridges having  $\theta_0^*$  slopes will be given elsewhere [8].

5. The  $\theta_{e1}^1$  dependence also contains a local minimum point of coordinates  $(-\theta_{E_1}, \theta_{E_2})$ . The angles  $\theta_{E_1}$  and  $\theta_{E_2}$  are, in the notation of Carter *et al.* [4], angles with a special meaning for ion erosion, being associated to quasi-stable intersections plane–plane. Applying the graphical method given in Section 4, these angles are related to the lower self-intersecting points of the cursor-type diagram (Fig. 5).

In the ranges  $\theta_0 \in [-90^\circ, -\theta_{E_1})$  and  $\theta_0 \in (-\theta_p, +90^\circ]$ ,  $\theta_{e1}^1$  decreases until  $\theta_{e1}^1 = 0^\circ$  for  $\theta_0 = \theta_0^*$ . In the narrow angular range  $\theta_0 \in (-\theta_{E_1}, -\theta_p)$ ,  $\theta_{e1}^1$  increases. For  $\theta_0 = 0^\circ$ , the solution  $\theta_{e1}^1$  has been noted as  $\theta_{i_1}$ .

The branch  $\theta_{e2}^2$ , consisting of  $\theta_{e1}^2(\theta_0 > 0^\circ)$  and  $\theta_{e2}^2(\theta_0 < 0^\circ)$  also contains the following notable points.

1. The absolute maximum point  $\theta_0 = -90^\circ$ ,  $\theta_e = 90^\circ$  corresponds to the bombardment of a very thin vertical wall with a vanishing thickness.

2. The point  $\theta_0 = \theta_{s_2}$ ,  $\theta_e = \theta_{s_2}$  is a double root, placed at the intersection point of the branches  $\theta_{e1}^2$  and  $\theta_{e1}^0$ , leading to a physically trivial solution.

3. The absolute minimum point  $\theta_0 = 90^\circ$ ,  $\theta_e = \theta_p$  is associated with the quasi-stability of an edge between two planar or curved surfaces making an obtuse angle during ion erosion, the ion beam being perfectly grazing one of microfacets.



4. The local maximum point  $\theta_0 = 0^\circ$ ,  $\theta_e = \theta_{i_2}$  corresponding to the quasi-grazing bombardment of an edge between two quasi-normal planar or curved surfaces. Indeed, the angular values of  $\theta_{i_2}$  are very close to  $90^\circ$  [7].

5. The dependence  $\theta_e^2$  also has a local minimum  $\theta_0 = -\theta_{E_2}$ ,  $\theta_e = \theta_{E_1}$  which is the symmetrical point about the line  $\theta_e = -\theta_0$  of the local minimum point  $\theta_0 = -\theta_{E_1}$ ,  $\theta_e = \theta_{E_2}$  placed on the branch  $\theta_e^1$ . Both the extremum points are associated with the quasi-stable intersections of type plane-plane [4, 7].

In Fig. 3,  $\theta_e^2$  is decreasing in the range  $\theta_0 \in [-90^\circ, \theta_{E_2}]$  and  $\theta_0 \in (0^\circ, 90^\circ]$  and is increasing in the range  $\theta_0 \in (-\theta_{E_2}, 0^\circ)$ . For  $\theta_0 = 0^\circ$ , the solution  $\theta_e^2$  has been noted as  $\theta_{i_2}$ .

The angular values  $\theta_{i_1}$ ,  $\theta_{i_2}$  have been introduced by Ducommun *et al.* [1-3], being important for ion engraving used in microelectronics.

Generally, the values for  $\theta_e^1$  are localized in the range  $(\theta_{i_1}, \theta_p)$  for  $\theta_0 < 0^\circ$  and between  $(0^\circ, \theta_{i_1})$  for  $\theta_0 > 0^\circ$ . The numerical values of  $\theta_e^2$  are not superposed on the angular range of  $\theta_e^1$ , being localized between  $(\theta_{E_1}, 90^\circ)$  for  $\theta_0 < 0^\circ$  and between  $(\theta_p, \theta_{i_2})$  for  $\theta_0 > 0^\circ$ .

The numerical computation results for the three various dependences  $S = S(\theta)$  may be conveniently summarized in terms of  $\theta_e$  root number and location as a function of incidence angle  $\theta_0$ . Assuming an algebraic sign for the incidence angles as a function of the relative position of the associated normals to the ion beam, there are, for a given  $\theta_0$ , four solutions  $\theta_e$  (two positive and two negative) if  $\theta_0 \in [-90^\circ, \theta_0^*]$  and three solutions  $\theta_e$  (one positive and two negative) if  $\theta_0 \in (\theta_0^*, 90^\circ]$ . Two solutions have absolute values lower than  $\theta_p$  ( $0^\circ < |\theta_e| < \theta_p$ ) and the other two higher than  $\theta_p$  ( $\theta_p < |\theta_e| < 90^\circ$ ).

Further aspects concerning the analysis of the general trend of the  $\theta_e = f(\theta_0)$  dependence and the more precise identification of all associated extremum points, valid for any sputtering yield curve  $S = S(\theta)$ , will be discussed elsewhere [8].

## 6. Conclusions

In the present work, a unique analytical condition for the angular point local quasi-stability during ion erosion, implicitly relating the incidence angles  $\theta_0$  and  $\theta_e$  between the intersecting microfacet normals and the ion beam direction, has been inferred. This condition, which can also be deduced on the basis of erosion slowness curve,

leads to a higher degree algebraic equation with a parameter, appropriate for any  $S = S(\theta)$  dependence, described by an algebraic polynomial expression in  $\cos \theta$ .

By solving the algebraic equation obtained, it is possible to evaluate the angles  $\theta_e$  compatible with a given angle  $\theta_0$ . Assuming an algebraic sign for the incidence angles as a function of the relative position of intersecting microfacet normals to the ion beam, numerical computations for three various dependences  $S = S(\theta)$  have shown that there are four solutions  $\theta_e$  (two positive and two negative) if  $\theta_0 \in [-90^\circ, \theta_0^*]$  and three solutions  $\theta_e$  (one positive and two negative) if  $\theta_0 \in (\theta_0^*, 90^\circ]$  for a given  $\theta_0$ .

An alternative graphical method, based on a cursor-type polar diagram, for the determination of the incidence angles  $\theta_e$  compatible with an incidence angle  $\theta_0$  for a local quasi-stable angular point, is also proposed.

A general discussion, valid for any angular dependence of sputtering yield  $S = S(\theta)$ , concerning the interdependence relationship between the incidence angles associated with local quasi-stable intersections during ion erosion, will be published later.

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