JOURNAL OF MATERIALS SCIENCE 16 (1981) 3021–3024

On the ion bombardment induced cone/pyramid apex angle

L. A. TANOVIĆ
Faculty for Electrical Engineering, University of Sarajevo, 71000 Sarajevo, Yugoslavia

The cone/pyramid apex angle dependence on ion energy has been measured on 20 to 80 keV argon-sputtered copper having well-defined initial surface orientation. It has been found that the present experimental data are contained within the limits predicted by the various theoretical models. Our experiments have shown that the cone/pyramid apex angle is dependent not only on the ion–target combination and the ion energy but also on the crystal orientation of the bombarded sample. A critical assessment of the published formulae for estimating cone angles has been made.

1. Introduction

In the earliest experiments in which cone-like features were seen to develop on ion bombarded targets [1], the dependence of the cone apex angle on the target material was noticed. Further experiments showed that this angle was dependent not only on the ion–target combination, but also on the energy of the incident ions [2–5].

It has been suggested that if a substrate becomes completely covered with such cone-like features, than they may be stable against shape change with the increasing ion flux [6]. The existence of such stability was predicted to occur only for a specific angle, θ, at which the ion beam is directed relative to the normal to the cone sides. The relation between the anle, θ, and the cone apex angle, α, is obvious from Fig. 1:

$$\alpha = \pi - 2\theta = 2\phi. \tag{1}$$

In order for these features to remain at least temporarily "stable" against shape change, the angle θ should be equal to the angle θ' at which the sputtering yield reaches a maximum, observed as a function of the ion incidence angle with respect to the surface normal (Fig. 2) as origianlly suggested by Stewart and Thompson [3] and developed by other authors [2,4].

Another author [7], however, has suggested that for cone formation it is important that the angle θ corresponds to the angle θ'' in Fig. 2 at which the sputtering yield is greately reduced due to reflection of the incident ions from the cone sides. It was argued [7] that for $\theta = \theta'$, the ions strike the cone surface causing the most effective sputtering and thus, even if formed with such angle, cones would sputter away very rapidly and thus not exist as a stable form. For $\theta = \theta''$, however, the incident ions are unable to overcome the surface atomic potential barrier and their contribution to the erosion of the surface is minor.

Existing experimentally-measured values of the cone angle do not easily resolve this dilemma as to whether to relate θ to θ' or to θ'' since the uncertainty in the measurement of the cone angles is relatively large compared to the small difference between the angles θ' and θ''.

2. Discussion

Theoretical predictions of the variation of the cone angle with the incident ion energy, adopting the model that $\theta = \theta''$, have been made by relating the angle, θ'', at which the ion reflection occurs, to the phenomenon of planar channeling [3,4,7]. This relationship is derived from studies by Lindhard [8] of the influence of crystal lattice effects on the charged energetic particle movement in which he calculated the critical continuum scattering angle. Assuming the plane in which the atoms are distributed as a two-dimensional liquid or random gas, Lindhard gives a formula for the continuum potential, $Y(z)$, as a function of the numerical value z:

0022–2461/81/113021–4$02.40/0 © *1981 Chapman and Hall Ltd.*

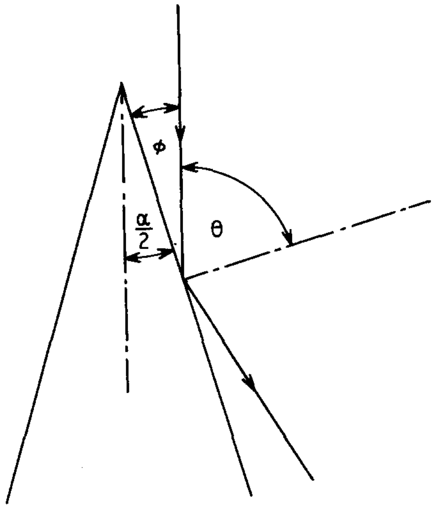

Figure 1 Schematic illustration of the relation between the cone angle, α, and the ion beam incidence angle, θ.

$$Y(z) = n^{2/3} \int_0^\infty 2\pi r \, \mathrm{d}r \, V(z^2 + r^2)^{1/2}, \quad (2)$$

where n is the atom density of the atomic plane, z is the distance from the plane and $V(R)$ is the ion–atom potential for a separation R.

In the various theoretical predictions of $\alpha(E)$ (where E is the energy in keV) dependence which associate the cone apex angle, α, with the angle θ'', i.e., with the critical continuum scattering angle, ϕ, the major differences arise mainly because of the different selections of the ion–atom potential $V(R)$ used in Equation 2. Additionally, there appear to be some errors and doubtful assumptions in some of these predictions (see Appendix).

If we apply the various published formulae for the cone angle, α, in the case of Ar-ion bombarded

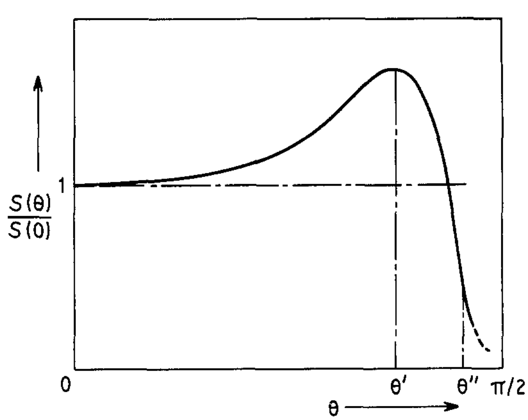

Figure 2 Schematic illustration of the angular dependence of the sputtering yield.

copper targets ($Z_1 = 18$, $Z_2 = 29$), the following expressions may be deduced.

Stewart–Thompson [3]:

$$\alpha = 69.75\,E^{-1/2}; \quad (3)$$

Improved Stewart–Thompson (see Appendix):

$$\alpha = 139.5\,E^{-1/2}; \quad (4)$$

Witcomb I [4], Chadderton [7]:

$$\alpha = 109.076\,E^{-1/2}; \quad (5)$$

Witcomb II [4]:

$$\alpha = 267.35\,E^{-1/4}; \quad (6)$$

Witcomb III [4]:

$$\alpha = 401.2\,E^{-1/4}; \quad (7)$$

Witcomb IV [4]:

$$\alpha = 77.942\,E^{-1/2}; \quad (8)$$

where E is in keV and α is in degrees.

A plot of values of $\alpha(E)$ derived from Equations 3 to 8 in the energy range 20 to 80 keV, together with experimental results of $\alpha(E)$ measured in the recent studies by the author [5] is shown in Fig. 3. It should be emphasized here that all of our measured values of the cone/pyramid angles shown, were determined on the surface of a (1 1 6) orientated Cu single crystal.

The importance of using only one crystal orientation for $\alpha(E)$ determination becomes clear by inspection of Fig. 4 which shows the experimentally-determined values of α for a single ion energy for four different crystal orientations. It is evident that for $E = 40$ keV a very pronounced dependence is observed for the cone/pyramid angle on the crystal orientation. From Fig. 4 one observes that the cone/pyramid angle, α, decreases with the opacity of the initial surface plane.

3. Conclusions

It is clear from our experiments that the cone/pyramid apex angle is dependent not only on the ion–target combination and the ion energy but also on the crystal orientation of the bombarded sample. This suggests strongly that in the experimental measurements of the cone/pyramid apex angle, α, one should be careful to perform such measurements with the variation of only one parameter which may influence the cone/pyramid angle and that in studies using the polycrystalline substrates for example, the grain orientation, upon which

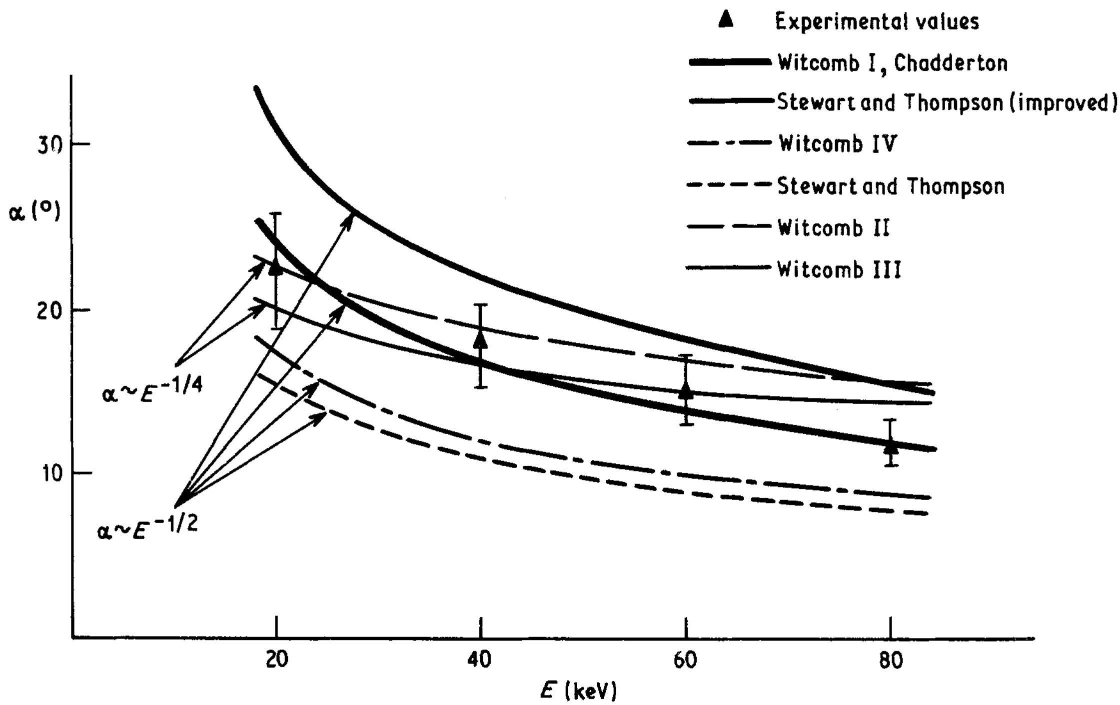

Figure 3 Comparison of the measured pyramid angles on (1 1 6) Cu with the theoretical predictions for the different ion energies.

cones/pyramids are observed, should be determined.

Our experiments showed only a very weak dependence of the cone/pyramid apex angle on the incident ion energy in the interval 20 to 80 keV (Fig. 3). It is also clear from Fig. 3 that the present data for a well-defined initial surface orientation, are contained within the limits predicted by the various theoretical models of Equations 3 to 8; but, since the variation of $\alpha(E)$ is so weak, the data cannot be taken to support any one model, or indeed confirm whether those models which associate α with θ'' are valid.

We observed a much stronger dependence of the pyramid apex angle on the crystal orientation of (1 0 0), (1 1 1), (1 1 6) and (11 3 1) Cu surfaces bombarded with a 40 keV argon ion beam (Fig. 4). This observation confirms our conclusion published elsewhere [9,10,11] that the final pyramid form is largely dictated by the crystallographic habit.

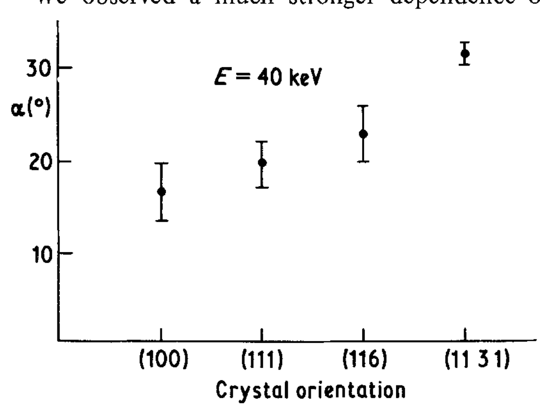

Figure 4 The dependence of the pyramid apex angle on the crystal orientation of the bombarded sample.

Acknowledgements

The author wish to acknowledge with gratitude the help of Dr. J. L. Whitton and Professor G. Carter.

Appendix: A critical assessment of the published formulae for estimating cone angles

Stewart and Thompson [3] first used the theoretical approach of Lindhard [8]. It was assumed that the ion–atom potential is $V(r)$ of inverse-square form:

$$V(r) = 2E_R/e(Z_1Z_2)^{5/6}(a_0/r)^2, \quad \text{(A1)}$$

(where the symbols have their usual meaning). These authors presented an expression for cone half-angle, $\alpha/2$, i.e., for the reflection angle ϕ given by:

$$\phi = \alpha/2 = \pi/2 - \theta' = \left\{\frac{5\pi a_0^2 n^{2/3} Z_1 Z_2 E_R}{(Z_1^{2/3} + Z_2^{2/3})E}\right\}^{1/2} \quad \text{(A2)}$$

It is, in fact, not possible, using the potential $V(r)$ from Equation A1 with Bohr's expression for screening radius $a = a_0/(Z_1 Z_2)^{1/6}$, to obtain $(Z_1^{2/3} + Z_2^{2/3})$ in the denominator of Equation A2. We may, however, assume that the authors have used a screening radius a defined by $A = a_0/(Z_1^{2/3} + Z_2^{2/3})^{1/2}$. Still, in the denominator of Equation A2 a further error remains since the expression in brackets should be raised to the exponent $\frac{1}{2}$. Equation A2 was that used by the authors in their comparison of theory with, from $S(\theta)$ curve calculated values for cone angle on the base of Equation 1.

Witcomb [4] suggested four different formulae for the cone angle values determined as a function of the ion energy. The first one is based on the estimate of Lindhard of an effective potential barrier of the atomic plane ($Y_{\text{eff}} = Y(0)/2$) [8]. Using in Lindhard's formula [2] for continuum potential, the standard ion–atom potential, Witcomb deduced the expression for the cone apex angle:

$$\alpha = 694 \left\{ \frac{n^{2/3} Z_1 Z_2}{(Z_1^{2/3} + Z_2^{2/3})^{1/2} E} \right\}^{1/2} \tag{A3}$$

In his second calculation Witcomb assumed a specific case where the incident particle suffered only scattering from a single surface atom in a close-packed row of atoms. As a result of these assumptions, using Equation 2, Witcomb finds:

$$\alpha = \frac{134}{d(Z_1^{2/3} + Z_2^{2/3})^{1/2}} \left\{ \frac{Z_1 Z_2 (Z_1^{2/3} + Z_2^{2/3})^{3/2}}{n^{2/3}\, E} \right\}^{1/4}, \tag{A4}$$

where d is the atom separation in the lattice. Later, without any modifications to the basic theory and using only a slight change in the assumptions, Witcomb deduced two further expressions for cone apex angle:

$$\alpha = 201 \left\{ \frac{Z_1 Z_2}{d^3 (Z_1^{2/3} + Z_2^{2/3}) E} \right\}^{1/4} \tag{A5}$$

and

$$\alpha = 203 \left\{ \frac{A n^{2/3} b^2}{E} \right\}^{1/2}, \tag{A6}$$

where b and A are factors from the Born–Mayer potential.

In Equation A5 the modification to channelling angles for interacting with a single atomic string proposed by Lindhard, was employed, and in Equation A6 the Born–Mayer ion–atom potential in Equation 2 was used for the planar potential.

Chadderton [7] repeated Witcomb's first calculation finding apparently good agreement with the experiment, but making a simple arithmetical error of a factor of 2 in his comparison of the theory with the experiment.

References

1. A. GUNTERSCHULZE and W. TOLMIEN, *Z. Phys.* 119 (1942) 685.
2. I. H. WILSON and M. W. KIDD, *J. Mater. Sci.* 6 (1971) 1362.
3. A. D. G. STEWART and M. W. THOMPSON, *ibid.* 4 (1969) 56.
4. M. J. WITCOMB, *ibid.* 10 (1975) 669.
5. L. TANOVIĆ, J. L. WHITTON and S. KOFOD, Proceedings of the Conference on the Physics of Ionised Gases, Dubrovnik, Yugoslavia, 1978 p. 171.
6. G. CARTER, J. S. COLLIGON and M. J. NOBES, *J. Mater. Sci.* 6 (1971) 115.
7. T. L. CHADDERTON, *Rad. Effects* 33 (1977) 129.
8. J. LINDHARD, *Matt. Fys. Medd. Dan. Vid. Selsk.* 34 (1965) 14.
9. J. L. WHITTON, L. TANOVIĆ and J. S. WILLIAMS, *Appl. Surf. Sci.* 1 (1978) 408.
10. J. L. WHITTON and G. CARTER, Proceedings of the Symposium on Sputtering, Vienna, 1980.
11. L. TANOVIĆ, Ph.D. Thesis, University of Belgrade, 1978.

Received 27 February and accepted 6 April 1981.