THE MODELLING OF SPUTTERING AND ETCHING PROCESSES ON A MICRO COMPUTER

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1. SUMMARY

This paper describes two fairly simple programs, SPUTTER and ETCH, which may be loaded into a micro computer which uses BASIC, to plot graphical output on a television screen or X-Y plotter. These programs will model the metallisation processes of sputtering and etching in two dimensions.

The paper starts with the derivation of the formulae for the growth in each direction. The simple layout of the initial data file which generates the cartesian coordinates, and the logic to find the angles to integrate over for each point are also described. Examples using the SPUTTER program are then given.

The section on ETCHING discusses how points which disappear in practice need to be removed from the computer store to prevent "negative etching", i.e. growth, occurring. This is done with the aid of a discriminant. Four different types of distribution of the etching medium may be used. Examples of the ETCH program using different distributions are given, and other examples using both programs are described.

In conclusion suggestions are made as to the possible development of this work.

2. BASIS OF THE METHOD

The method used to model sputtering is based on a paper by I.A. Blech (1). The following assumptions are made:-

a) The mean free path of the sputtering molecules is greater than the source to substrate distance r.

b) r is very much greater than the height of any step in the substrate.

c) The rate of growth is proportional to a function of the angle of incidence θ and inversely proportional to r squared.

d) The film grows towards the source and no roughening due to a large θ is allowed.

e) The sticking coefficient is unity.

f) A hemispherical vapour source is used.

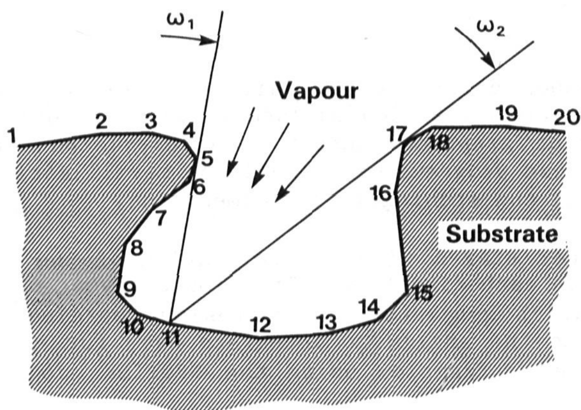

Fig.1. Section through substrate showing data points.

The profile to be sputtered over is defined by a set of data points which are numbered sequentially from left to right (Figure 1). The angles ω_1 and ω_2 are found using the logic described by the flow diagram (Figure 6).

The equations defining the growth in the X and Y directions, using the notation in Figure 2 are:-

$$\Delta x = \int_{\omega_1}^{\omega_2} \frac{K}{r^2} \left(\int_{-\frac{\Pi}{2}}^{\frac{\Pi}{2}} r \cos \alpha . F(\theta) r \, d\alpha \right) \sin \omega . d\omega \qquad (1)$$

$$\Delta y = \int_{\omega_2}^{\omega_2} \frac{K}{r^2} \left(\int_{-\frac{\Pi}{2}}^{\frac{\Pi}{2}} r \cos \alpha . F(\theta) r \, d\alpha \right) \cos \omega . d\omega \qquad (2)$$

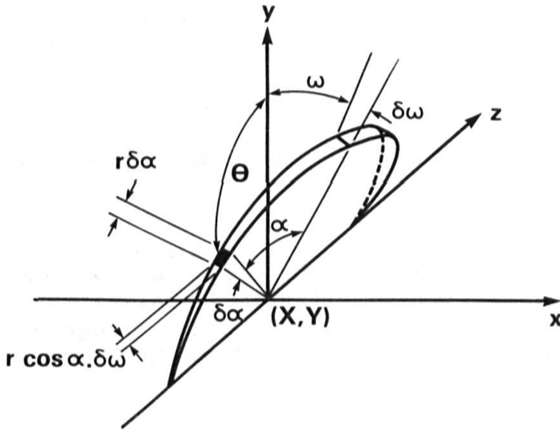

Fig.2. Three-dimensional view of data point

where F(θ) is a function of θ depending on the type of distribution of the sputtering or etching media.

$F(\theta) = 1$ for isotropic distribution

$= \cos\theta$ for cosine distribution

$= \cos^2\theta$ for cosine squared distribution

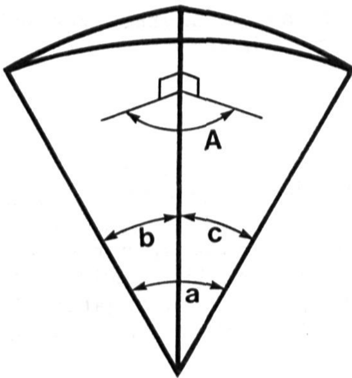

Fig.3.
Angles used in equation (3)

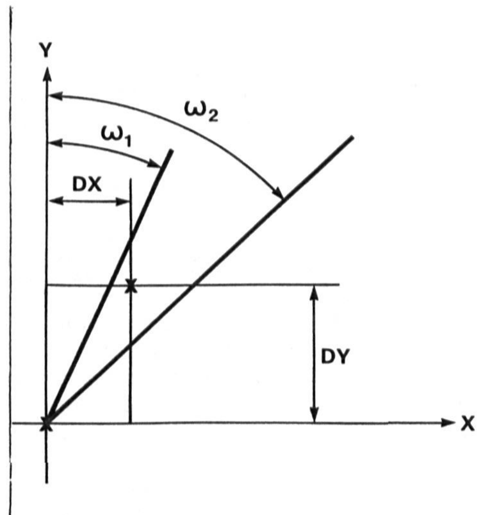

Fig.4.
Growth in two-dimensions

From the solid geometry of Figure 3 it is true that:-

$$\cos a = \cos b \cos c + \sin b \sin c \cos A \tag{3}$$

From equation (3), with $A = 90°$, $a = \theta$, $b = \omega$, $c = \alpha$

$$\cos\theta = \cos\omega \cos\alpha \tag{4}$$

Hence $F(\theta)$ can be put in terms of $\cos\omega \cos\alpha$, and equations (1) and (2) can be integrated analytically, to give the following equations to be used in the program, to give the growth in the X and Y directions shown in Figure 4.

g) Isotropic distribution

$$DX = K*(\cos\omega_1 - \cos\omega_2) \tag{5}$$

$$DY = K*(\sin\omega_2 = \sin\omega_1) \tag{6}$$

h) Cosine distribution

$$DX = K*(\cos^2 \omega_1 - \cos^2 \omega_2) \tag{7}$$

$$DY = K*(\sin\omega_2 \cos\omega_2 - \sin\omega_1 \cos\omega_1 + \omega_2 - \omega_1) \tag{8}$$

i) Cosine^2 distribution

$$DX = K*(\cos^3 \omega_1 - \cos^3 \omega_2)/3 \tag{9}$$

$$DY = K*(\sin\omega_2(1 - \sin^2 \omega_{2/3}) - \sin\omega_1(1 - \sin^2 \omega_{1/3})) \tag{10}$$

The growth factor K is read in and adjusted in the program to equal the growth in the Y direction at each step.

$$DY = K \text{ and } DX = 0 \text{ if } \omega_1 = -\frac{\pi}{2} \text{ and } \omega_2 = \frac{\pi}{2}$$

3. LAYOUT OF DATA AND LOGIC TO FIND ANGLES

The data for both programs consists of a list of cartesian coordinates X(I), Y(I) which are separated by the number of equal divisions between consecutive data points. A negative X coordinate ends this list. The program linearly interpolates the intermediate points.

A radius at the corners is entered with its number of divisions. All upward pointing corners in the SPUTTER data are

then rounded with these parameters, whereas in the ETCH data all downward pointing corners are rounded. The total number of data points is then worked out by the program.

The ETCH program also asks for the range of etch, which can be limited to act between two Y coordinates only, and four further parameters which tell the program how much of each type of distribution is to be used.

Both programs then ask for the growth factor and number of steps of growth. A simple example of a SPUTTER data set is given in Figure 5.

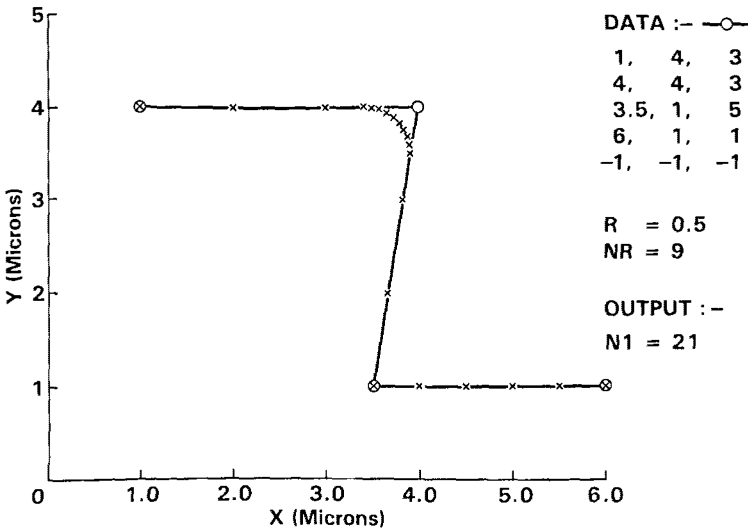

Fig.5. Example of how initial SPUTTER data is set up

The logic to find the angles to be integrated over is shown in Figure 6. This flow chart just finds ω_1, known as W1, and evaluates $S3 = \sin(\omega_1)$ and $C3 = \cos(\omega_1)$.

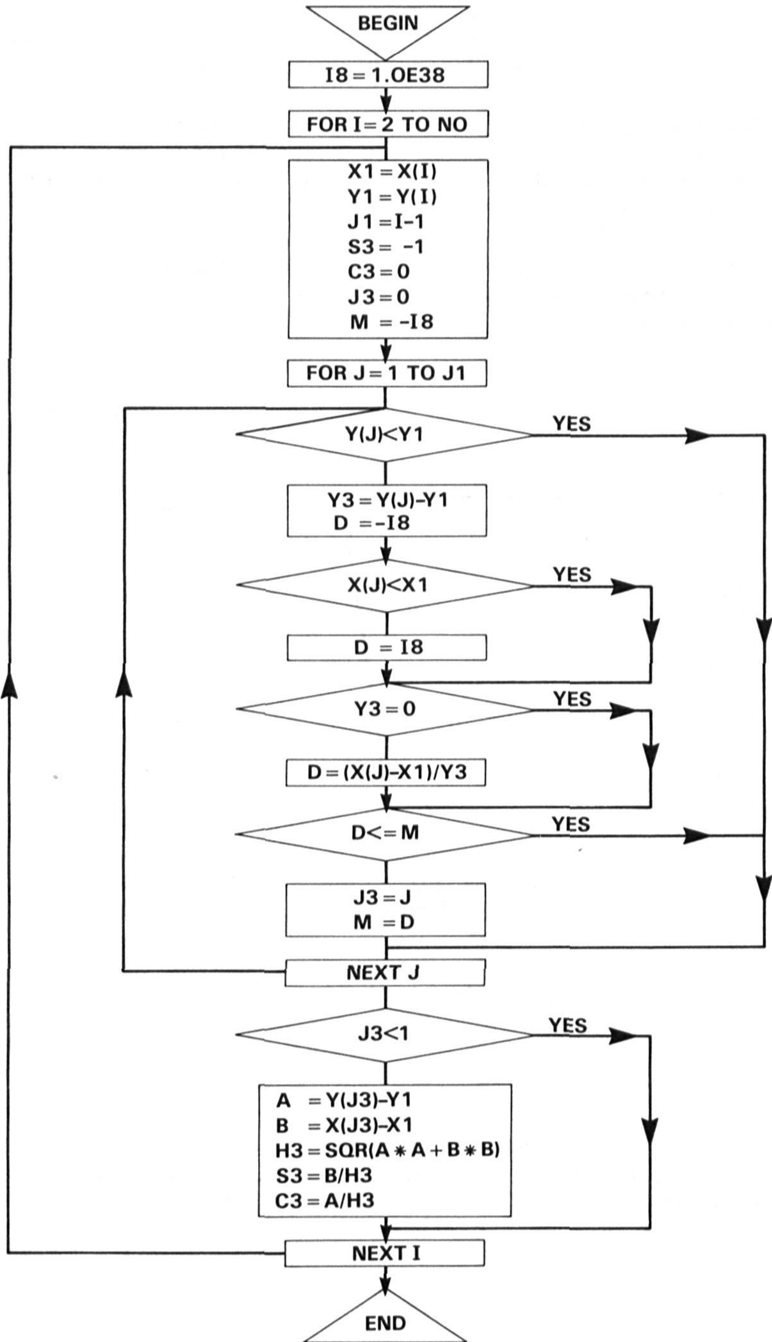

Fig.6. Flow chart showing search for W1 angle

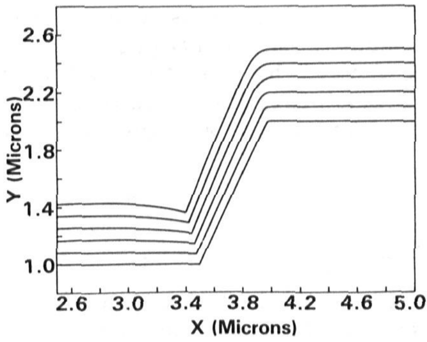

Fig.7.
Computer output of sputtering over a 65° step

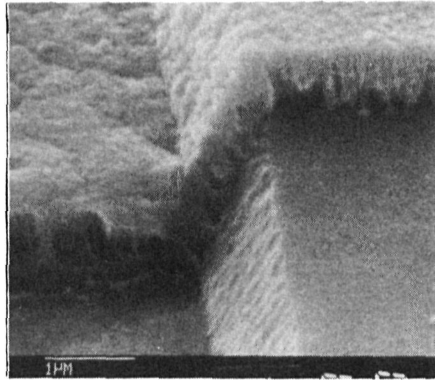

Fig.8.
S.E.M. photograph of sputtering over a 65° step

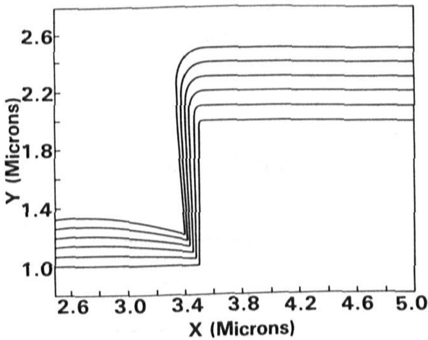

Fig.9.
Computer output of sputtering over a 90° step

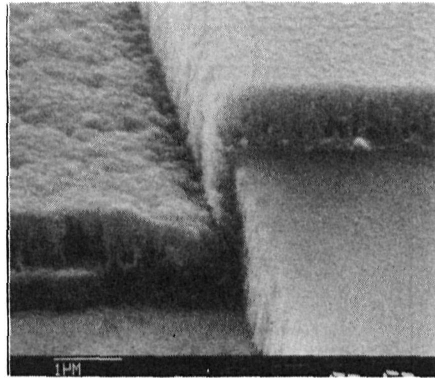

Fig.10.
S.E.M. photograph of sputtering over a 90° step

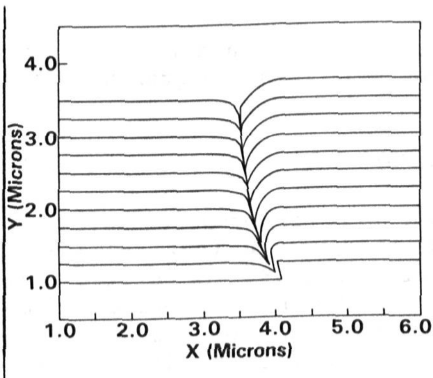

Fig.11.
Computer output showing crack formed

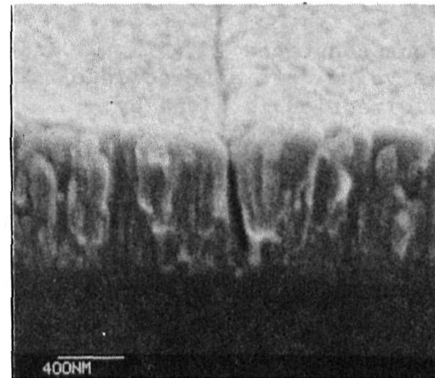

Fig.12.
S.E.M. photograph showing crack formed

The example in Figures 11 and 12 illustrates one of the practical difficulties which can occur when sputtering over a small re-entrant step. The crack formed by the fast growing areas shielding the bottom of the crack presents a problem when a further etch is needed. A fault known as wicking occurs.

4. ETCH PROGRAM

4.1. Description of the ETCH Program

The ETCH program allows up to four types of distribution of the etching medium. The effect of each one is shown in Figure 13.

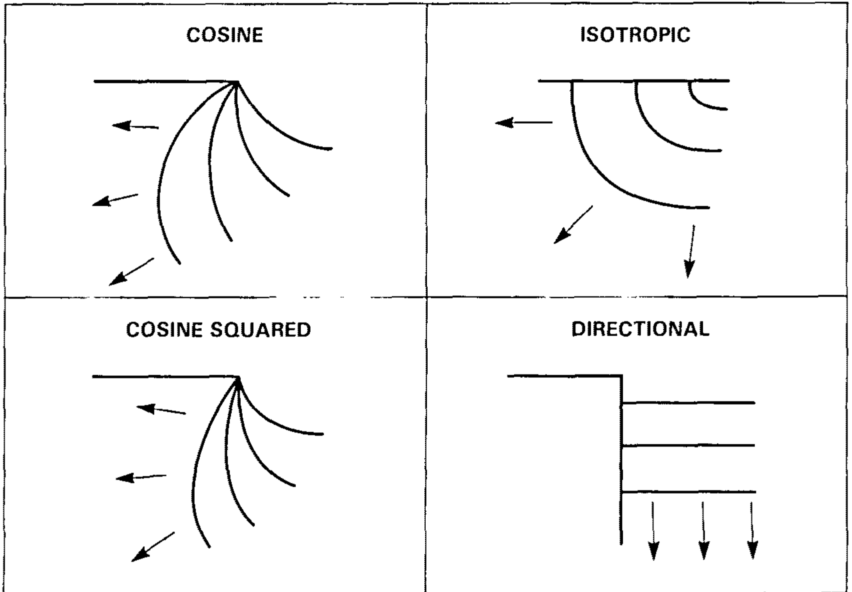

Fig.13. Sketches showing the effect of each type of distribution

Four constants E1, E2, E3 and E4, each between zero and unity in value, are entered into the program. Then the growth in the Y direction is given by:-

$$DY = E1*DY1 + E2*DY2 + E3*DY3 + E4*DY4 \quad (11)$$

The cosine distribution component, DY1, is proportional to a function of ω_1, ω_2 and $\cos(\theta)$, as in equation (8). Similarly the cosine squared distribution component, DY2, is derived from equation (10). For an isotropic distribution the values of ω_1 and $\omega 2$ used in equation (6) are replaced by two new values $\omega 3$, ω_4 which are the angles at a point subtended by its adjacent neighbours.

$$\text{Hence } DY3 = K*(\sin \omega_4 - \sin \omega_3) \quad (12)$$

The directional etching component DY4 is a constant equal to the growth factor K as defined in Section 2. The growth in the X direction DX is evaluated similarly from equations (7), (9) and (5) with DX4 = 0 by definition.

It is of course possible to vary the four constants, E1, E2, E3 and E4, to give different shapes of the etched profile. To model the plasma etch of a one and a half micron polyimide layer, between a mask and a base plate, we used E1 = 0 E2 = .7 E3 = .3 E4 = 0, but maybe a better combination could be used.

4.2. Use of a Discriminant to Find Points to be Removed

If the paths moved by two data points cross, the effect shown in Figure 14 occurs.

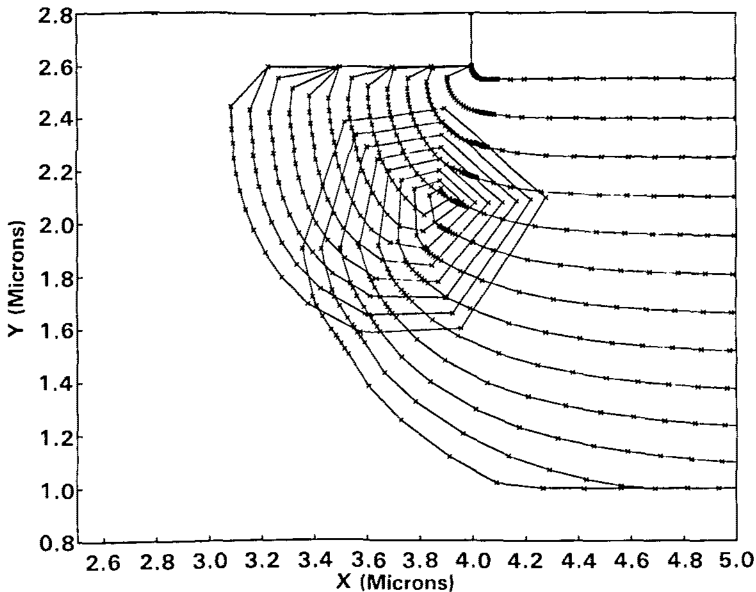

Fig.14. Graph showing effect of paths crossing

This bad effect can be prevented by the program checking at each growth step whether paths cross and then eliminating both the points.

With the notation in Figure 15, let the lines AB, CD cross at the point (x, y)

Let

$$
\begin{aligned}
A1 &= x_2 - x_1 & \quad B1 &= y_2 - y_1 \\
A2 &= x_3 - x_1 & \quad B2 &= y_3 - y_1 \\
A3 &= x_4 - x_3 & \quad B3 &= y_4 - y_3 \\
A4 &= x_4 - x_1 & \quad B4 &= y_4 - y_1 \\
A5 &= x_2 - x_3 & \quad B5 &= y_2 - y_3
\end{aligned}
\tag{13}
$$

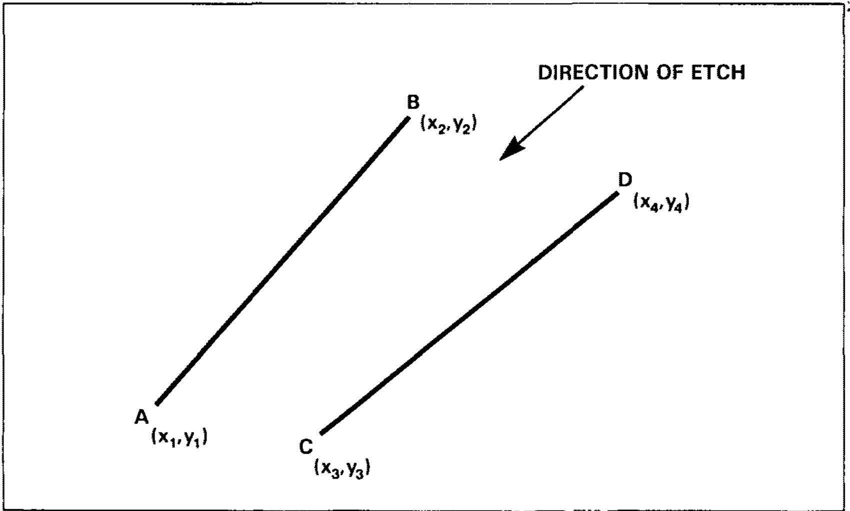

Fig.15. Notation used for two points B, D, etching to positions A, C

The equation of line AB is:-

$$y = y_1 + (x - x_1)\frac{B1}{A1} \tag{14}$$

The equation of line CD is:-

$$y = y_3 + (x - x_3)\frac{B3}{A3} \tag{15}$$

These lines cross where:-

$$x = \frac{B2 + \frac{B1}{A1}x_1 - \frac{B3}{A3}x_3}{\frac{B1}{A1} - \frac{B3}{A3}} \tag{16}$$

x lies between A and B if:-

$$(x_2 - x)(x - x_1) > o \tag{17}$$

x lies between C and D if:-

$$(x_4 - x)(x - x_3) > o \tag{18}$$

Substituting from equations (13) and (16) into the inequalities (17) and (18), eliminating squared factors and simplifying leads us to the two discrimant definitions:-

$$D1 = (A1.B4 - A4.B1)(A2.B1 - A1.B2) \quad (19)$$

$$D2 = (A5.B3 - A3.B5)(A2.B_3 - A3.B2) \quad (20)$$

Then lines do not cross if $D1 < 0$ and $D2 < 0$

Using the above method the same data which produced Figure 14 gives Figure 16 which is quite acceptable.

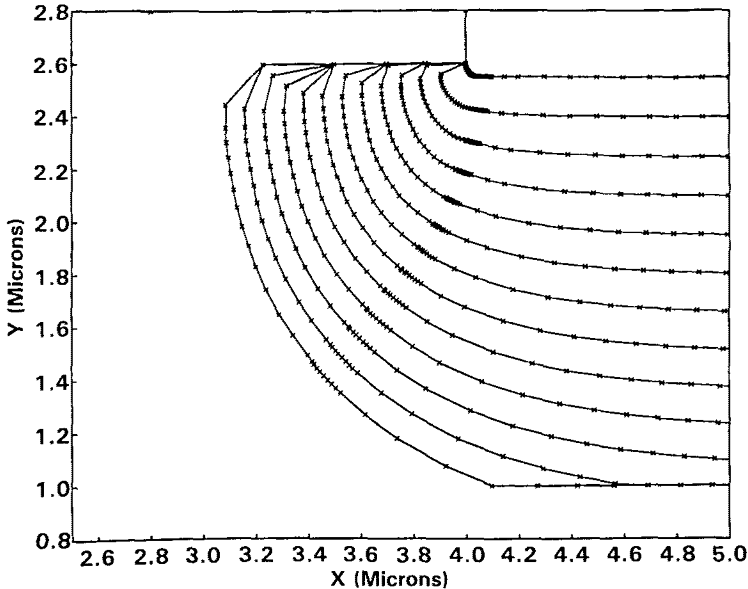

Fig.16. Example of output from ETCH program with E1=0, E2=.5, E3=.5, E4=0

6. CONCLUSIONS

Two dimensional simulations compare favourably with S.E.M. photographs, and it is easier to model on a micro computer than in a laboratory.

With the rapid growth of the micro computer, one can foresee greater storage capacity and ever faster computation times. In view of this, I would say it would be easy to combine both of these programs to make a version which would carry out all sequences of operations on a particular structure, i.e. sputter, etch, sputter and then further etch, etc. The data points could be kept stored throughout and pictures at each stage could be generated. Figures 17 and 18 show the final picture with S.E.M. photograph after modelling a similar sequence on a larger computer.

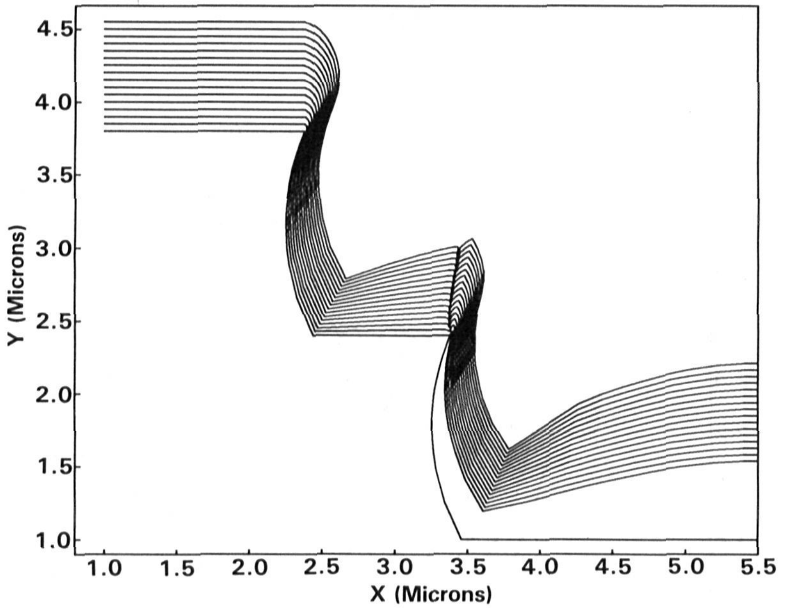

Fig.17. Computer graph after two etching and two sputtering stages

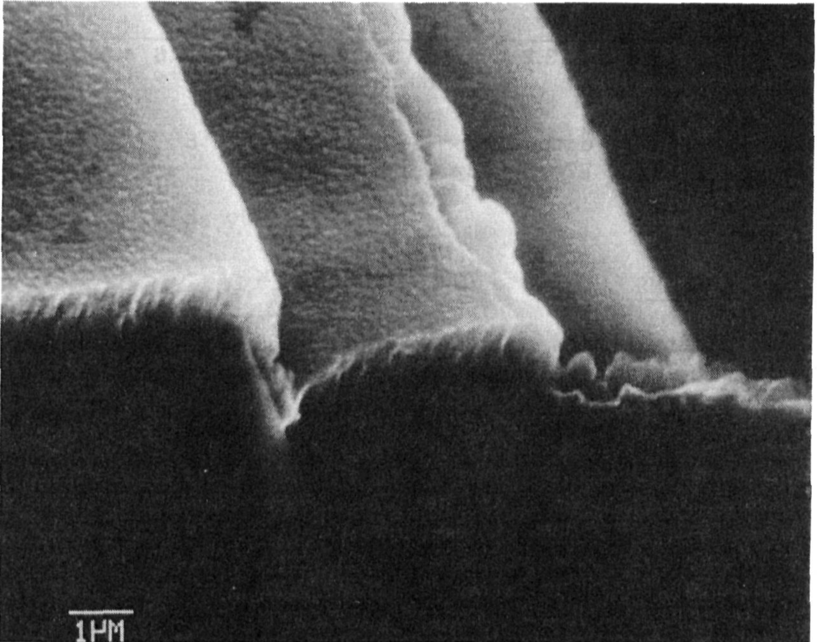

Fig.18. S.E.M. photograph of similar build up

Although written to model sputtering and etching processes, these programs could be used to model other things like evaporation, paint spraying, build up of snow or even corrosion. The original integrals may have to be modified to suit the defined conditions, but it is almost certainly possible. These integrals and the program might also be modified to model in three dimensions.

7. REFERENCE

a) Paper

1. BLECH, I.A.
"Evaporated Film Profiles over Steps in Substrates"
Thin Solid Films, Vol.6, p113-8, 1970