MODELLING OF THE DEPENDENCE OF SHEET RESISTANCE OF BORON DOPED LAYERS ON MASKING OXIDE GEOMETRY

S A Abbasi, M.Sc.Engr. Ph.D.,MIEEE, MIETE
Department of Electrical Engr.,
Aligarh Muslim University, Aligarh-202001 (INDIA)

SUMMARY

It has been reported earlier that in the case of deposition from a vapour source of boron, the sheet resistance produced on a large boron diffused check slice is, almost always, considerably smaller than the sheet resistance determined from the fabricated resistors. The actual value of the discrepancy depends upon the size of the window, the surrounding masking oxide geometry and the process parameters. The spreading resistance and the infra-red free carrier emission measurements made on a large sample, with respect to an oxide edge,suggest a long range nature of the effect. Further investigations have therefore been made in an attempt to present a theoretical model to explain the experimental observations.

The results of a careful series of experiments using multi-layered mask structures consisting of thermal oxide, silicon nitride and silox have been presented. On the basis of these experiments, it is suggested that most of the experimental observations may be explained with the help of a theoretical model based on 'surface-diffusion' of boron over silicon and silicon dioxide. The model assumes a high solubility of boron in oxide and a high surface diffusion coefficient. Numerical calculations are made, initially, with a very simple steady-state model. The model after a few successive improvements, is found to be capable of quantitatively explaining most of the experimental observations.

* Work performed at Southampton University, England.

1. INTRODUCTION

It has earlier been established (1,2) that in the case of diffusion from a vapour source of boron, there is a discrepancy between the values of sheet resistance produced on a large boron diffused unmasked plain check slice and sheet resistance determined from actual fabricated resistors. The latter has been found to be about 25% greater than the former in the case of a typical boron base diffusion. The discrepancy has been shown to be due to the presence of the masking oxide surrounding the windows of the diffused resistors, which is absent in the case of the plain check slices. The actual value of the discrepancy depends upon the geometry of the window and that of the surrounding masking oxide. It has been found to occur at the deposition stage and reduces with an increase in the total amount of doping per unit surface area (1). The effect is independent of background concentration, surface orientation, oxide thickness and oxide growth conditions. It disappears however, if the boron is ion implanted or if a 'spin-on' source is used (1). The spreading resistance and infra-red free carrier emission measurements made on a large diffused sample, with respect to an oxide edge show a variation of sheet resistance extending to several hundred microns from the edge and thus suggest a long range nature of the effect (3).

The observations seem to be important in:

(i) the design of resistors in conventional processing
(ii) the device modelling since the practical devices are oxide masked but the profiles are measured on large check slices and
(iii) the design of large devices of 1 mm size or over

2. POSSIBLE EXPLANATIONS FOR THE DISCREPANCY

It has been conclusively shown (1) that during predeposition of boron the presence of masking oxide tends to reduce the amount of boron going into the windows. The following explanations are therefore considered.

2.1 Two Dimensional Diffusion

No explanation on the basis of two dimensional diffusion (lateral diffusion) may be accepted because that would in fact reduce (4) the value of sheet resistance calculated from resistors which is opposite to experimental observations.

2.2 The Tendency of Boron to deposit over oxide

Due to a greater affinity of boron towards oxide compared to silicon, it may be argued that a disturbance of boron distribution in the gas phase close to the oxide edge may take place. This causes less boron to deposit on silicon near the oxide. However, any such disturbance of boron distribution in the gas phase is very unlikely to stay because of a very large amount of boron present and a very high diffusion rate in the gas phase. Therefore, this explanation is not physically possible.

2.3 The Mismatch Stress in the Window

There is a known mismatch between linear coefficients of thermal expansion of silicon and silicon dioxide (5). This is likely to produce stress in the silicon under the edge of the oxide window thus changing the diffusion kinetics. However, the stress is known to cause enhanced diffusion (6) & (7) which should increase the amount of boron going into the windows. This will increase the doping in the window which is once again opposite to the experimental observations. Some of the boron may, however, become electrically inactive under the influence of stress. A possible cause may be precipitation. If this is so, an increase in the oxide thickness should increase stress and hence cause an increase in the value of sheet resistance in the window. Experimentally, no effect of oxide thickness is observed. Also, the effect of stress is not expected to influence the dopant at a distance of several hundred microns as observed from the spreading resistance and infra-red free carrier emission measurements (3). Although these results do suggest that the above explanation is less likely to be acceptable, some more direct evidence to negate, is required.

2.4 The Surface Diffusion Over Silicon

A more likely explanation based on the surface diffusion of boron over silicon and silicon dioxide assuming a high solubility of boron in oxide is now considered. It is suggested that due to the high solubility of boron in oxide, the concentration over oxide surface is reduced which results in a concentration gradient of boron ad-atoms (atoms adsorbed at the silicon surface) near the oxide edge. The surface diffusion of boron ad-atoms then takes place under the influence of this concentration gradient, thereby removing some of the boron laterally from the silicon window. This will result in a higher value of sheet resistance in the windows.

The surface diffusion phenomenon has been extensively studied by surface chemists. Most of the studies reported however, deal with metals like Ni,Co, Cu, Mo, Fe and W etc., in entirely different contexts. The adsorbed atoms or molecules are usually loosely bound to the surface and are therefore highly mobile at temperatures usually encountered in solid state diffusion processes. After acquiring sufficient energy these atoms break bonds with their neighbours and move along the surface. Because of the high surface mobility, the value of surface diffusion coefficient Ds on various metals has been found to be many orders of magnitude greater than the corresponding bulk diffusion coefficient at a given temperature (8). Such high values of Ds are also capable of explaining the observed long range nature of the effect. The surface diffusion model, therefore, seems to be the most plausible mechanism to explain the effects of masking oxide on boron diffusion and experiments have therefore been made to confirm it.

3. THE TEST MASK AND THE MEASUREMENT PROCEDURE

The test mask used, described elsewhere (1) consists of nine resistors. Four of them are 40 μm wide and surrounded by oxide widths of 4, 8, 24 and 60 μm. The masking oxide is surrounded by at least 100 μm of bare silicon receiving the same diffusion. The remaining resistors are 12, 20, 40, 80 and 80 μm wide and surrounded by at least 100 μm of masking oxide.

The actual resistor widths were found to differ slightly from the designed values but all these widths were accurately measured before calculating any sheet resistances. The 80 μm wide resistor was found to have the least variation (around 2%) in measured width and was primarily used in subsequent measurements unless mentioned otherwise.

Only about half of the slice had resistor pattern, with the remaining portion used to make four-point probe measurements. Several slices were processed in each experiment and the experiments were repeated to check consistency. When resistor measurements were required after deposition without drive-in, spin-on oxide densified at 420°C for 15 min in N_2 was used as insulation under metallisation.

Four point probe measurements were made in the dark with usual precautions. From now on, these values will be referred to as ρs(4pt) while the sheet resistance calculated from actual fabricated resistor measurements will be called as ρs(res). The normalized value of ρs(res), expressed as a percentage of ρs(4pt) is represented as ρsn, which is a

measure of discrepancy between ρs(res) and ρs(4pt). In most of the cases, the average of a large number of readings followed by the standard deviation is given.

The starting material used was n-type,<111>, czochralski pulled (CZ), 6-9 ohms cms, 2 inch dia. silicon wafers. The thickness of thermal oxide was 0.3 μm and of silox 0.2 μm (wherever used). The silicon nitride (Si_3N_4) films were 700Å thick and were deposited by the low pressure CVD techniques.

These films were etched in orthophosphoric acid at 160 ± 5°C for about 40 minutes. Silox was used for defining pattern in silicon nitride. The standard RCA clean process was used for cleaning the wafers.

Unless mentioned otherwise all measurements are made after a boron predeposition at 890°C for 20 minutes in 1 lit./m N_2 ambient using the 'Boron plus' (B_2O_3) solid planar diffusion source supplied by electro-oxide corporation.

4. EXPERIMENTAL RESULTS

4.1 Silicon Dioxide Masking

The results of diffusion with standard SiO_2 masking are as follows:

ρs (4pt)	:	130.5	ohms/Square
ρs (res)	:	166.3 ± 3.8	-do-
ρs n	:	127.4 ± 2.9	%

4.2 Silicon Nitride Masking

The results of diffusion with silicon nitride masking are as follows:

ρs (4pt)	:	130.0	ohms/Square
ρs (res)	:	132.7 ± 1.5	-do-
ρsn	:	102.1 ± 1.2	%

It is clearly seen that there is no significant discrepancy between ρs (res) and ρs (4pt).

4.3 Silox/Nitride Masking

A composite structure as shown in fig. 1 below is used as the mask. The results of diffusion are as follows:

ρs (4pt)	:	125.3	ohms/Square
ρs (res)	:	148.7 ± 3.0	-do-
ρs n	:	118.7 ± 2.4	%

It is clearly seen that in this case a discrepancy of about 19% is present between ρs(res) and ρs(4pt). This discrepancy is somewhat less than the one observed with the usual oxide masking. It is conceivable that whatever property is responsible for the effect, is different quantitatively in the cases of silox and thermal oxide. The experiment that follows was made to confirm it.

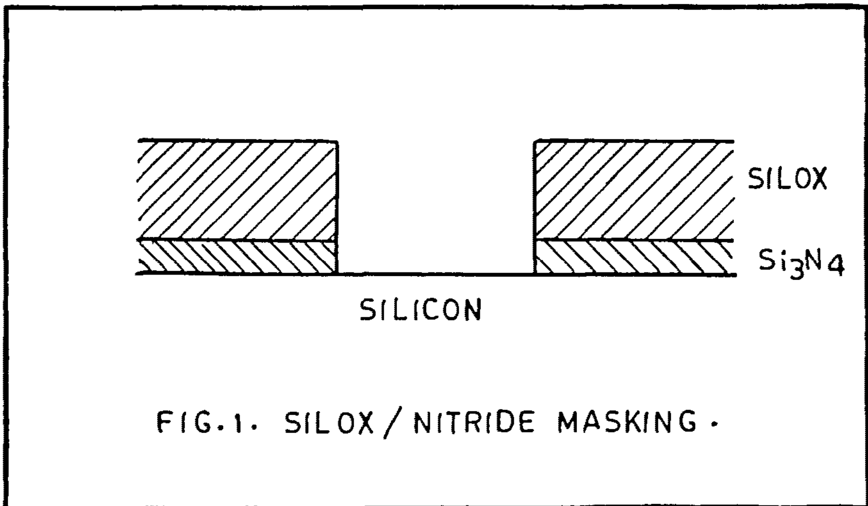

FIG.1. SILOX/NITRIDE MASKING.

4.4 Thermal Oxide/Nitride Masking

A thickness of 100Å of thermal oxide was produced by heating the nitride coated wafers at a temperature of 950°C in 1 lit/min. wet O_2 for 120 minutes. This oxide was used to cover nitride in fig. 1. The results of diffusion are as follows:-

ρs (4pt)	:	121.8	ohms/Square
ρs (res)	:	154.4 ± 3.1	ohms/Square
ρsn	:	126.8 ± 2.5	%

It may be seen clearly that thermal oxide over nitride gives the same order of discrepancy as seen with the thermal oxide masking thus supporting the argument of the preceding section.

4.5 Thermal Oxide Covered by Nitride

A composite mask structure using thermal oxide covered by nitride as shown in fig. 2 was used.

The results of diffusion are:

ρs	:	122.0	Ohms/Square
ρs(res)	:	129.9 ± 2.0	Ohms/Square
ρsn	:	106.5 ± 1.6	%

A small discrepancy of 6.5% is observed.

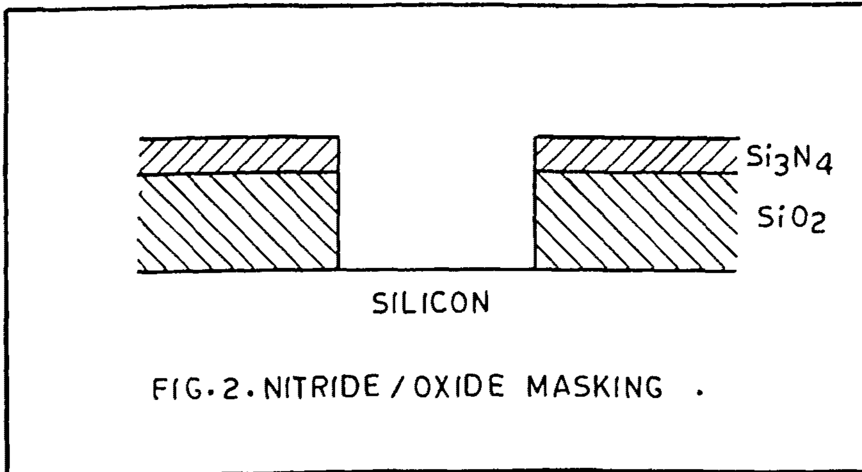

FIG.2. NITRIDE / OXIDE MASKING .

4.6 Thermal Oxide Partially Covered by Nitride

A structure, leaving about 2 μm oxide uncovered, as shown in fig.3 was used. The results of diffusion are:

ρ (4pt)	:	120.0	Ohms/Square
ρ (res)	:	135.0 ± 2.5	Ohms/Square
ρsn	:	112.5 ± 2.1	%

It is seen that the small width of about 2 μm left uncovered is sufficient to cause a discrepancy of 12.5%.

5. DISCUSSION

It may now be seen that the experimental observation strongly support the surface diffusion model. It is, however, know that the linear coefficient of thermal expansion of Si_3N_4 is close to that of silicon, thus causing no mismatch. This may explain the absence of discrepancy between ρs (4pt) and ρs (res) in the case of nitride masking.

Similarly, it may be argued that the oxide/nitride masking may still be causing stress in the window and hence the discrepancy. However, in the experiment of section 4.5 the presence of oxide underneath the nitride should still produce the same stresses and hence should give the same discrepancy. A drastic reduction in the discrepancy experimentally observed in this case therefore, suggests that the effects of masking oxide are not due to the stress generated by it. Also, in section 4.6, the appearance of the discrepancy with an exposure of only 2 μm of oxide with the rest covered by nitride again rejects this model. Further support of this rejection comes from the following results reported earlier:

a) no discrepancy in the case of ion-implantation followed by annealing(1).

b) no effect of oxide thickness on the discrepancy (1) and

c) the long range nature of the effect shown by the spreading resistance and infra-red free carrier emission measurement (3).

Thus, it may be concluded that the phenomenon of mismatch stresses cannot be accepted as a possible explanation. However, all the experiments described clearly indicate that the presence of exposed oxide surface and not the Si/SiO_2 interface is responsible for the observed discrepancy and therefore suggest the surface diffusion model.

The absence of discrepancy in the case of silicon nitride masking may be explained if a low solubility of boron in silicon nitride is assumed. Further, in oxide/nitride masking, since the oxide surface is available for the suckout of boron and hence surface diffusion, effects similar to standard oxide masking may clearly be expected.

The surface diffusion would also be expected to take place over the surrounding masking oxide. An increase in the masking oxide width would therefore increase the effective area over which boron is dissolved and hence cause more boron suck out which would increase the discrepancy. This might explain the effect of surrounding oxide frame width.

In the case of nitride/oxide masking, the presence of small exposed oxide edge (the window wall) would explain the discrepancy observed in section 4.5 and 4.6. Similarly if a limit to dissolution of boron in SiO_2 is assumed, the reduction of ρsn with a reduction in ρs (4pt) may also be

explained. Because of a high surface diffusion coefficient the long range nature of effect may also be explained.

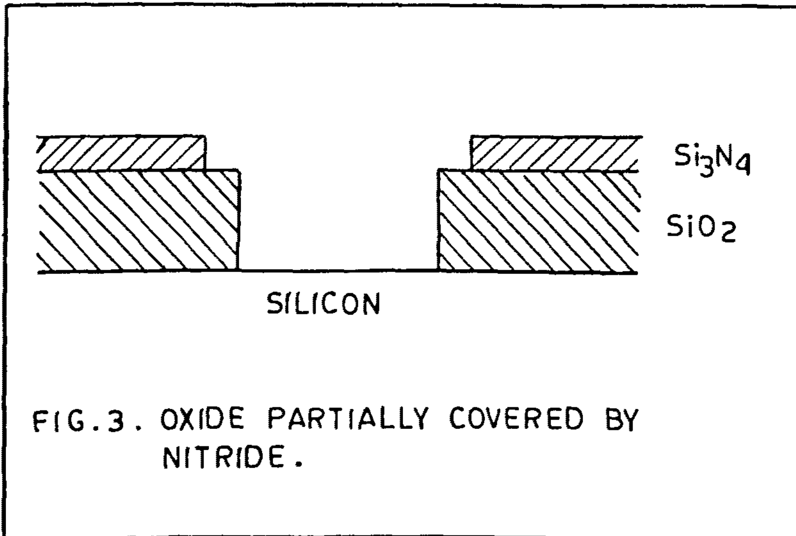

FIG.3. OXIDE PARTIALLY COVERED BY NITRIDE.

6. THE SURFACE DIFFUSION MODEL

6.1 The Steady - State Model

Refering to fig 4, the following simplifying assumptions are made:

i) The length of the window is infinitely large.

ii) In the absence of complete understanding of boron deposition kinetics, the flux Fn of boron atoms arriving at the surface of the wafer from the source per unit area per unit time is considered constant.

iii) The flux going into the silicon bulk at any point of the surface is negligible compared to the lateral flux due to surface diffusion.

iv) A steady state condition in which the surface diffusion flux at any point is equal to Fn, is assumed.

v) A boron concentration of Co is maintained at the oxide edge.

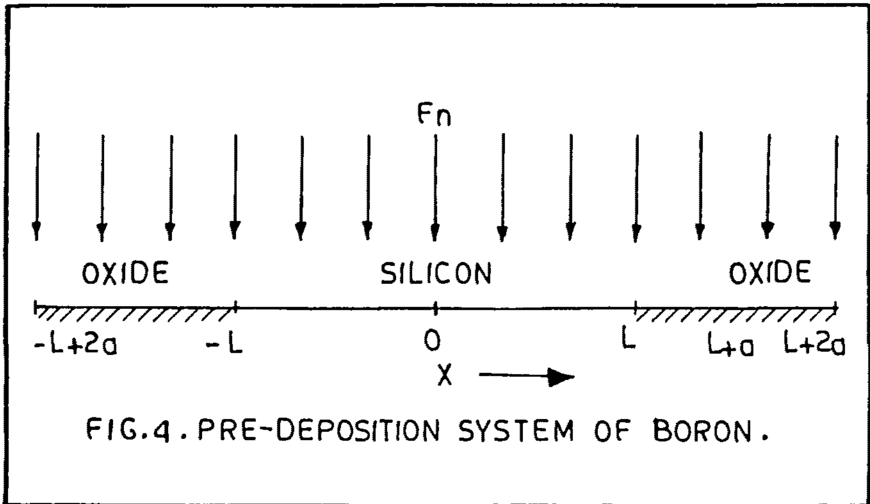

FIG.4. PRE-DEPOSITION SYSTEM OF BORON.

The equations to be solved are:

$$Ds \frac{d^2C(x)}{dx^2} = - Fn$$

$$C(\pm L) = Co$$

Where,

C(x) is the concentration per unit surface area
Ds is the surface diffusion coefficient
x is the distance from the centre of the window
2L is the window width

The solution is:

$$C(x) = \frac{Fn}{2Ds} (L^2 - x^2) + Co$$

It may easily be seen that although the discrepancy between ρs (4pt) and ρs(res) may be explained with a proper selection of Co and Ds, many other effects like the masking oxide frame width effect, the reduction of discrepancy with an increase in the total doping etc. may not be explained by this simple model. Also, the assumption of steady state conditions does not look physically justifiable. A modification of the model therefore follows.

6.2 Time Dependent Surface Diffusion Model

The following modifications are made to the assumptions of the preceeding, section.

i) A time varying condition instead of the steady state condition is assumed.

ii) The surface diffusion takes place at the silicon as well as the oxide surface with the same value of Ds.

iii) The boron is dissolved uniformly all over the oxide width up to a maximum concentration of Gm atoms/cm^2.

iv) The rate at which boron may be dissolved in oxide is proportional to the difference between Cm and the actual concentration of boron in the oxide, Cox (t) at that instant of time; the constant of proportionality being G. In the beginning of diffusion, however, the rate of arrival of boron at the oxide will be smaller than the above rate and hence all the boron will be dissolved in the oxide. Thus the boron concentration at the oxide surface will continue to remain zero until the maximum dissolution rate of boron becomes less than the rate of its arrival.

v) Because of a much greater solubility of boron in oxide the rate of boron reflected back from the oxide surface may be much smaller compared to that over silicon. Hence the effective flux over the oxide is assumed to be a factor H times greater than that over silicon.

vi) The ideal one-dimensional diffusion corresponding to a single diffusion coefficient, in the silicon bulk is assumed.

Refering to fig. 4 the equations to be solved are as follows:

On Silicon Surface,

$$Ds \frac{\partial^2 C(x,t)}{\partial x^2} - \frac{\partial C(x,t)}{\partial t} = - Fn \qquad -L<x<L$$

On Oxide Surface,

$$D_s \frac{\partial^2 C(x,t)}{\partial x^2} - \frac{\partial C(x,t)}{\partial t} = -Fn + G(Cm - Cox)$$

$$L<x<L+2a$$

$$C(L+,t) = C(L-,t)$$

$$\left.\frac{\partial C}{\partial x}\right|_{(L+,t)} = \left.\frac{\partial C}{\partial x}\right|_{(L-,t)}$$

6.3 The Results of Calculations

Since no data for Ds, Cm, G and H etc., are available, suitable values are chosen to give a close agreement with the experimental results. It is found that reasonable values of these parameters may give the desired discrepancy between ρs (4pt) and ρs(res). The effect of Ds over a very wide range is found to be negligibly small. For any value of G ranging from 0.001 to 1.0 per sec., it is possible to find a value of Cm to give a discrepancy of 27%. Almost all experimental observations may be confirmed quatitatively. The results of calculations with a few sets of assumed parameters along with the experimental data are given. Figure 5 gives the results of sheet resistance variation with respect to the oxide window frame width variation. Figures 6 shows the variation with respect to an oxide masked edge over a large sample.

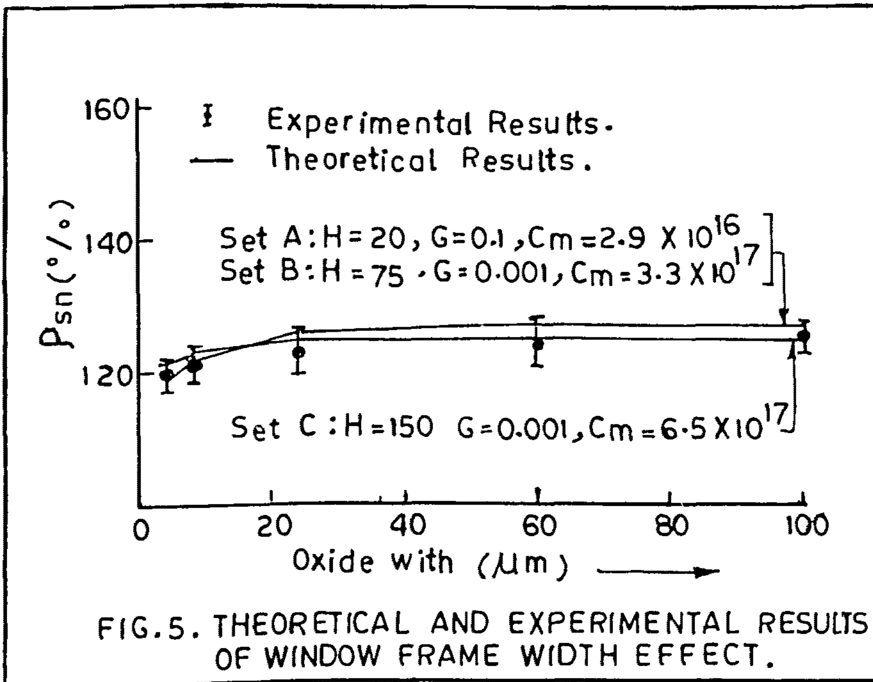

FIG. 5. THEORETICAL AND EXPERIMENTAL RESULTS OF WINDOW FRAME WIDTH EFFECT.

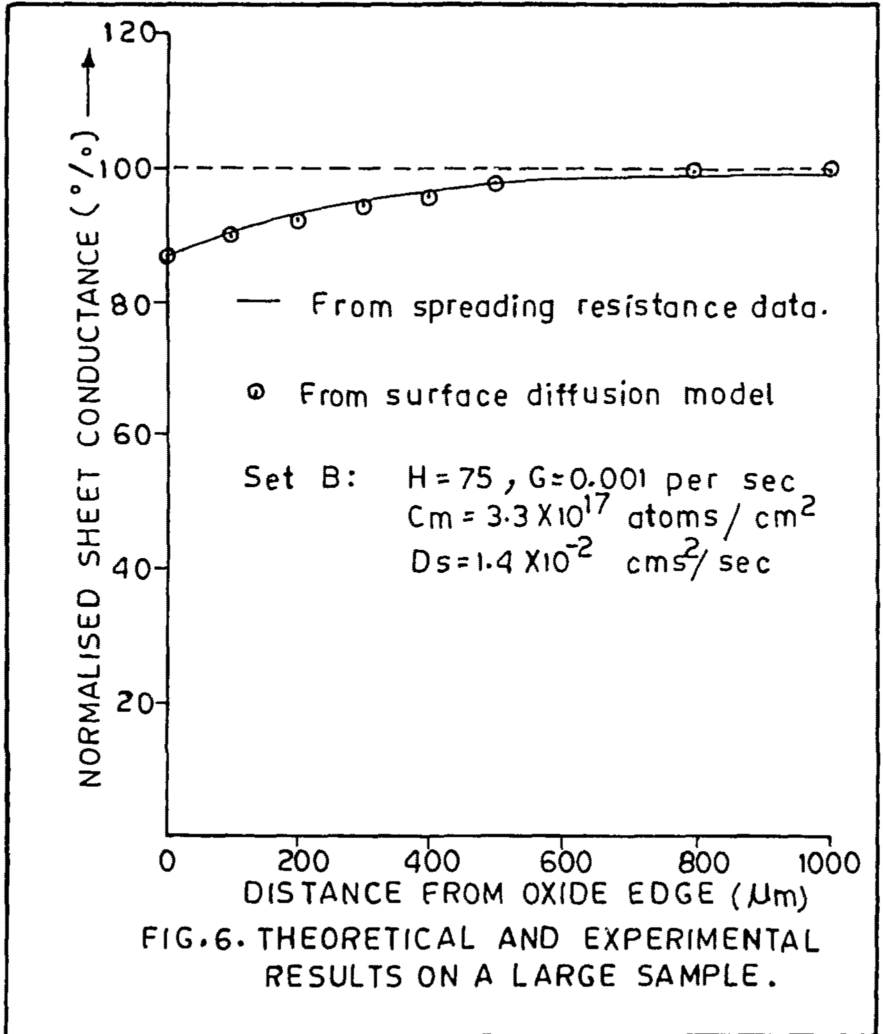

FIG. 6. THEORETICAL AND EXPERIMENTAL RESULTS ON A LARGE SAMPLE.

7. CONCLUSIONS

A further investigation of the earlier reported effects of masking oxide on the diffusion of boron into silicon has been made. A series of experiments using various forms of multi-layered masking structures consisting of thermal oxide, silicon nitride and silox etc. lead to the development of a theoretical model. The model is based on the surface diffusion of boron over silicon assuming a high solubility of boron in the surrounding oxide. The calculations made, suggest that the model is capable of explaining the dependence of sheet resistance of boron doped layers on the masking oxide geometry.

8. ACKNOWLEDGEMENTS

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9. REFERENCES

1. ABBASI, S A and BRUNNSCHWEILER, A
"Effect of Masking Oxide on Diffusion Into Silicon".
IEE Proc. Vol. 128, Pt. I, No. 5, p.185, 1981.

2. ABBASI, S A and BRUNNSCHWEILER, A
"The Effects of Oxide Masking on Boron Deposition",
In: Europhysics Conf. Abs., 10th ESSDERC York, England, p. 180, 1980.

3. ABBASI, S A., TAKLEH, O. BRUNNSCHWEILER A. and SMITH, J G. "Variation of Diffused Boron Concentration in the Neighbourhood of Oxide Masked edge".
Electronics Letters, Vol. 17, No.6, p.578, 1980.

4. YANAGAWA, T
"Resistance of Narrow Diffused Layers"
IEE Trans. on Electron Devices, Vol. ED-19, No.11, p.1166 1972.

5. GROVE, A S
"Physics and Technology of Semiconductor Devices"
John Wiley and Sons, Inc., London, 1967.

6. PRUSSIN, S
"Generation and Distribution of Dislocations by Solute Diffusions".
Jl. of Appl Phy. Vol. 32, No. 10, p.1276, 1961.

7. LAWRENCE, J E
"Behaviour of Dislocations in Silicon Semiconductor Devices: Diffusion, Electrical".
Jl. of Electrochem. Soc. Vol. 115, p.860, 1968.

8. SOMORJAI, G A
Principles of Surface Chemistry".
Prentice Hall, Inc., New-Jersey, 1972.