

PROFILES OF BORON DIFFUSED INTO
SILICON THROUGH NARROW WINDOWS

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SUMMARY

It has been reported earlier that the diffusion of boron into silicon is affected by the presence of surrounding masking oxide. The effect is significant in a typical boron base diffusion used in bipolar IC fabrication. The results of a thorough investigation reported earlier suggest that the effect occurs at the predeposition stage of boron diffusion and it is independent of background concentration, surface orientation of the material and the oxide growth conditions. It is of long range nature and depends upon the size of the windows and that of the surrounding oxide. The diffusion through windows, thus, becomes geometry dependent. It has been concluded on the basis of a careful series of experiments involving multi-layered masking structures consisting of silox, thermal oxide and nitride, that the effect can be explained on the basis of 'surface diffusion' of boron ad-atoms over the silicon surface assuming a high solubility of boron in the surrounding oxide. A simple model has demonstrated the capability of the surface diffusion phenomenon to explain the experimental observations. The model is further updated. After a number of successive improvements, it is found that the developed computer simulation program is capable of giving boron profiles in silicon windows after taking into account the effects of the surrounding masking oxide on diffusion.

1. INTRODUCTION

It has been reported earlier (1,2) that in the case of predeposition from a solid planar boron source, there is a discrepancy between the values of sheet resistance produced on a large boron diffused check slice, $\rho_s(\text{plane})$ and the sheet resistance determined from actual fabricated resistors, $\rho_s(\text{res})$. It has been concluded that the amount of boron diffused into the windows opened in oxide is always less than the amount of boron diffused in the check slices. The actual discrepancy depends upon the size of the window and the surrounding masking oxide width. It has been shown (1,2) to occur at the deposition stage and reduces with an increase in the total amount of doping per unit surface area. The effect is independent of background concentration and surface orientation of the starting material, 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 the 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 for several hundred microns from the edge and thus suggest a long nature of the effect.

The use of silicon nitride as the mask shows none of the effects observed with oxide masking. The results of a careful series of experiments using multi-layered composite masking structures involving thermal oxide, silicon nitride and silox are summarised below:

- a) The use of silicon nitride as the masking material in place of SiO_2 does not produce any discrepancy between $\rho_s(\text{plane})$ and $\rho_s(\text{res})$.
- b) A film of oxide on nitride as a mask does produce a discrepancy between $\rho_s(\text{plane})$ and $\rho_s(\text{res})$ of the same order as with the oxide alone.
- c) If the surface of masking oxide is covered by silicon nitride, the discrepancy reduces to a small value of about 5%.
- d) A small width of oxide left uncovered by nitride is enough to cause a discrepancy of about 14% between $\rho_s(\text{plane})$ and $\rho_s(\text{res})$.
- e) If the masking oxide is doped with boron prior to deposition, the discrepancy between $\rho_s(\text{plane})$

and $P_s(\text{res})$ disappears altogether.

- f) The spreading resistance measurements confirm that the use of silicon nitride as the masking material shows none of the effects observed with oxide masking.

The experimental results may qualitatively be explained on the basis of a surface diffusion model, assuming a very high dissolution rate of boron in the oxide surrounding the window. Thus the surface concentration near the oxide edge may be reduced drastically due to dissolution in the oxide. A significant amount of boron at the surface may thus be removed towards oxide due to surface diffusion (3) under the influence of concentration gradient across the surface. This results in a higher value of sheet resistance in the windows. An attempt is therefore made to develop a theoretical model which would predict diffusion profiles in the windows taking into account the masking oxide effects.

2. THE STEADY STATE MODEL

A steady state surface diffusion model under various simplifying assumptions has already been discussed (4). It has been found that this model does not explain most of the experimental observations and is therefore not considered further.

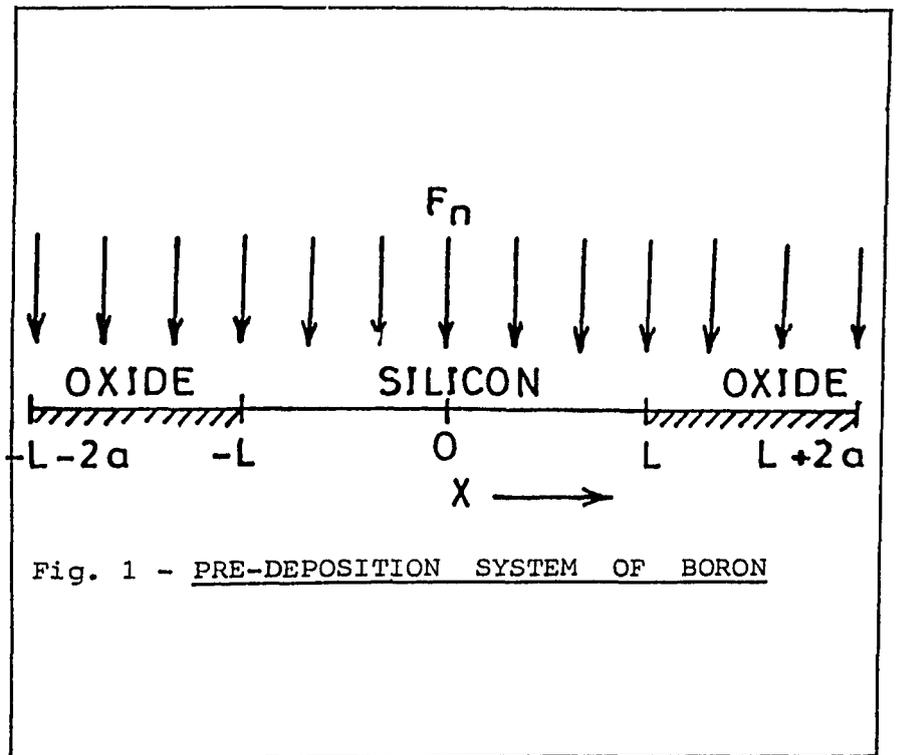
3. THE TIME VARYING SURFACE DIFFUSION MODEL

The experimental results suggest that the masking oxide effects tend to decrease with an increase in time or the doping level. This clearly suggests a time dependent model. Following assumptions are therefore made:

- a) The length of the window is infinitely large and the flux of boron going into the silicon bulk at any point of the surface is negligible compared to the lateral flux due to surface diffusion. This reduces the problem to one dimension.
- b) In the absence of complete understanding of boron deposition kinetics, the flux F_n of boron atoms arriving at the surface of the wafer, from the source per unit area per unit time is considered to be constant.
- c) The surface diffusion is considered to take place both over the silicon window as well as

the surrounding oxide, with the same surface diffusion coefficient.

- d) The boron is dissolved uniformly all over the oxide width upto a maximum concentration of C Atoms/Sq.Cms.
- e) The rate at which the boron may be dissolved in oxide is proportional to the difference between C_1 and the actual concentration of boron in the oxide. Thus, if the concentration of boron in the oxide at any instant of time 't' is $C_{ox}(t)$, the rate at which boron may be dissolved in the oxide is equal to $G(C_1 - C_{ox})$; where G is the constant of proportionality. In the beginning of diffusion, however, the boron surface concentration at the oxide will be zero until the above value becomes less than the total rate of arrival of boron atoms at the oxide.
- f) The ideal one-dimensional diffusion corresponding to a single diffusion coefficient in the silicon bulk is assumed.



Referring to fig.1, the equations to be solved are:

On silicon surface,

$$D_s \frac{\partial^2 c(x,t)}{\partial x^2} - \frac{\partial c(x,t)}{\partial t} = -F_n \quad -L < x < L$$

On Oxide surface,

$$D_{ox} \frac{\partial^2 c(x,t)}{\partial x^2} - \frac{\partial c(x,t)}{\partial t} = -F_n + G [C_1 - C_{ox}(t)] \quad L < x < (L+2a)$$

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

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

where, $C(x,t)$ is the concentration per unit surface area.

D_s is the surface diffusion coefficient over silicon.

D_{ox} is the surface diffusion coefficient over oxide.

x is the distance from the centre of the window.

$2L$ is the width of the window.

$2a$ is the width of the oxide.

The above equations are solved numerically using the Crank Nicholson method on our VAX 11/780 Computing system. The interval $0 < x < L+a$ only is considered because of symmetry with respect to $x=0$. The variation of C with respect to time at any point in the window may be calculated. Using the variation of C , the profile of boron in the silicon bulk and hence the sheet resistance may be obtained with the help of the ideal one dimensional diffusion theory. The concentration of boron in the silicon bulk is assumed to be limited by the solid solubility limit.

4. VALUES OF DIFFERENT PARAMETERS

For surface diffusion studies, it is important to know the adsorption kinetics of B_2O_3 over silicon and silicon dioxide. In particular, it is

necessary to know what proportion of B_2O_3 is actually adsorbed and what is the residence time. Unfortunately, nothing is known about these parameters. It may be assumed that the whole flux of B_2O_3 molecules sticks to the surface of silicon and is adsorbed there permanently. However, the value of this flux at $890^\circ C$ has been calculated to be 2.2×10^{14} molecules/Sq.cm., which is a very high value. The other possibility may therefore be to assume that the adsorption kinetics is such that the effective constant rate of arrival of B_2O_3 over silicon is much less than the value of flux obtained from the vacuum pressure data. For sample calculations, a value of 3×10^{11} atoms/Sq.cm./sec. is assumed.

Similarly, nothing is known about Ds, G and C1 and thus the values for these parameters are selected to provide a suitable fit to the experimentally observed results. The calculations have been done, assuming a temperature of $890^\circ C$. The values of solid solubility limit of boron in silicon at this temperature and the diffusion coefficient in silicon bulk are extracted from experimental data and are 2×10^{20} atoms/Sq.Cms. and 2.9×10^{-15} Sq.Cms./Sec. respectively.

5. RESULTS OF CALCULATIONS

To study the window frame width effect, calculations are done with a window width of $40 \mu m$ and the frame widths of 4, 8, 24, 60 and $100 \mu m$. For window width effect, the resistor widths have been taken to be 12, 20, 40 and $80 \mu m$ with a $100 \mu m$ wide window frame. The values of $\rho_s(\text{res})$ have been normalized and expressed as a percentage of $\rho_s(\text{plane})$ and are denoted by ρ_{sn} .

The results are shown in fig.2. It has been found that as the window frame width is increased, the value of ρ_{sn} increases continuously at a much faster rate compared to experimental results. Also, the increase shows no sign of saturation as observed in experimental results. Similarly, in the window width effect, there is a continuous decrease in the value of ρ_{sn} with an increase in the window width with no signs of saturation. It was not found possible to find a reasonable fit to the experimental data in spite of a large number of trials with different parameters.

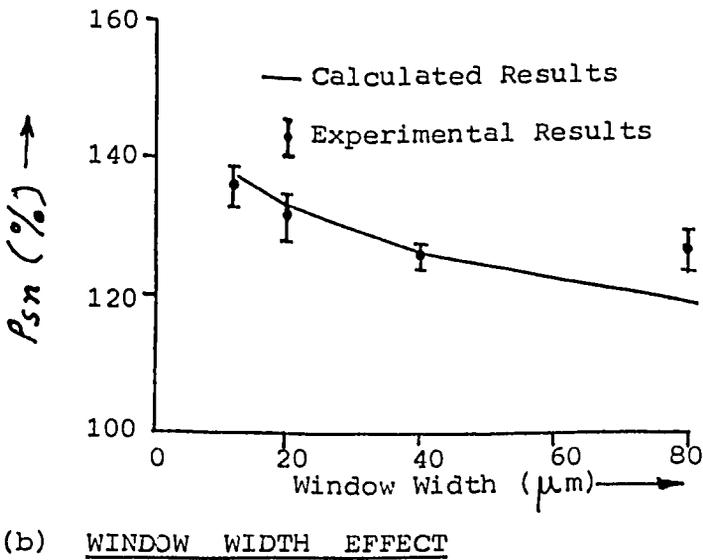
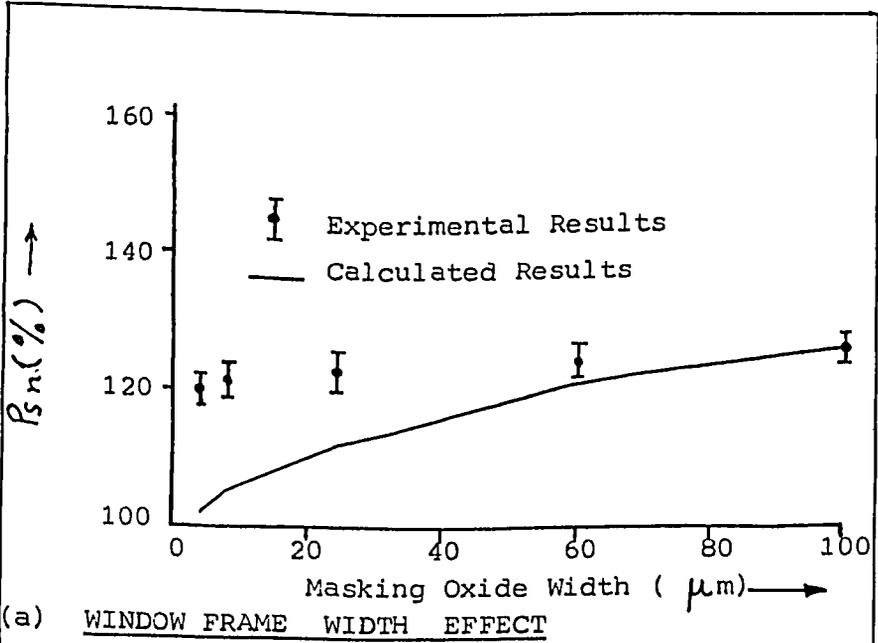


Fig. 2 - COMPARISON OF EXPERIMENTAL AND CALCULATED RESULTS

6. MODIFIED SURFACE DIFFUSION MODEL.

Considering the results of section 5, the reason for a much larger and ever increasing value of calculated window frame width effect needs to be studied. In fact, in the beginning, before the surrounding oxide is sufficiently doped, the concentration at the oxide edge remains zero and most of the boron goes into the oxide. The oxide thus receives boron in the following two ways:

- (i) direct from the gas phase at the rate of F_n atoms/Sq.Cms./Sec.
- (ii) from the silicon window through surface diffusion.

The rate of boron atoms crossing the oxide edge per unit length is equal to $D_s \frac{\partial C}{\partial x} \Big|_{x=L}$. Since it has been assumed that this boron is absorbed uniformly all over the oxide width, the rate of arrival of boron into oxide from the window would be $\frac{D_s}{a} \cdot \frac{\partial C}{\partial x} \Big|_{x=L}$. Thus the total rate of boron, F_t , arriving at the oxide is given by,

$$F_t = F_n + \frac{D_s}{a} \frac{\partial C}{\partial x} \Big|_{x=L}$$

Thus, the surface concentration at the oxide edge will start building up after a time ' T_c ' at which the following condition is obtained.

$$F_t \gg G [C_L - C_{ox}(t)]$$

The value of ' T_c ' will obviously depend upon the values of ' a ' and $D_s \frac{\partial C}{\partial x}$ and would largely govern the value of $P_s(\text{res})$. In the case of window frame width variation, the value of ' a ' changes while in the case of window width variation the value of $D_s \frac{\partial C}{\partial x}$ varies. It may be seen that the value of $D_s \frac{\partial C}{\partial x}$ is in fact proportional to the width of the window ($D_s \frac{\partial C}{\partial x} = 1.135 F_n L$) and the value of the term $\frac{D_s \partial C}{a \partial x}$ is comparable to the value of F_n . Thus,

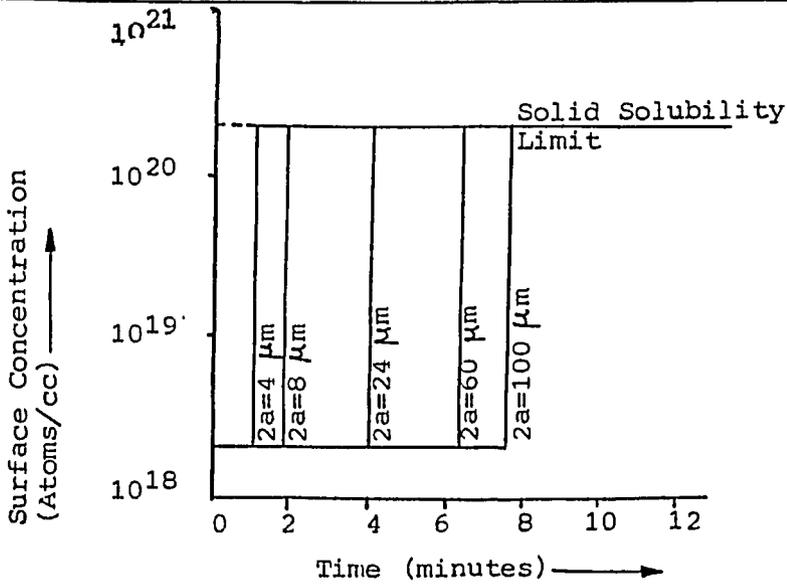
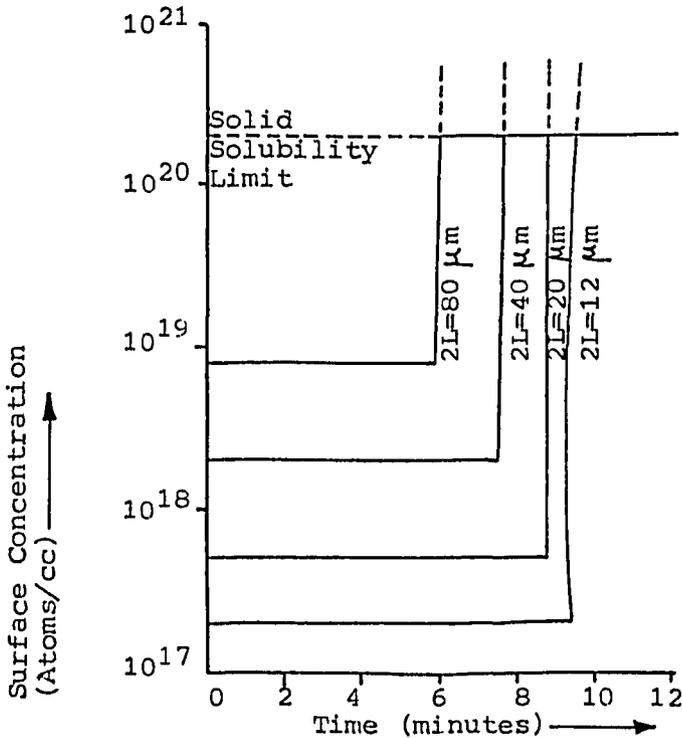
(a) FOR A CONSTANT WINDOW WIDTH OF $40 \mu\text{m}$ (b) FOR A CONSTANT WINDOW FRAME WIDTH OF $100 \mu\text{m}$

Fig. 3 - SURFACE CONCENTRATION VS TIME

with a variation of 'a' or 'L' or both, there is a considerably large variation in the value of F_t , resulting in a large variation of T_c and hence $P_s(\text{res})$ and P_{sn} . Figures 3(a) and (b) demonstrate it on the 'surface concentration versus time' plot, in the case of window frame width and window width effects respectively.

One of the possible solutions to reduce the drastic variation of $P_s(\text{res})$ with L and a may be

to make the term $\frac{D_s}{a} \cdot \frac{\partial C}{\partial x}$ less significant in

comparison with F_n so that the effects of L and a over F_t are reduced. This may be achieved by assuming that the effective rate of arrival of boron from the gas phase over SiO_2 is greater than over silicon. This assumption may be physically justifiable. 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 rate of arrival of boron over SiO_2 may be assumed to be greater than over Si. It has thus been assumed that the effective flux over SiO_2 is a factor HP times greater than over Si. Calculations have now been made with this modification.

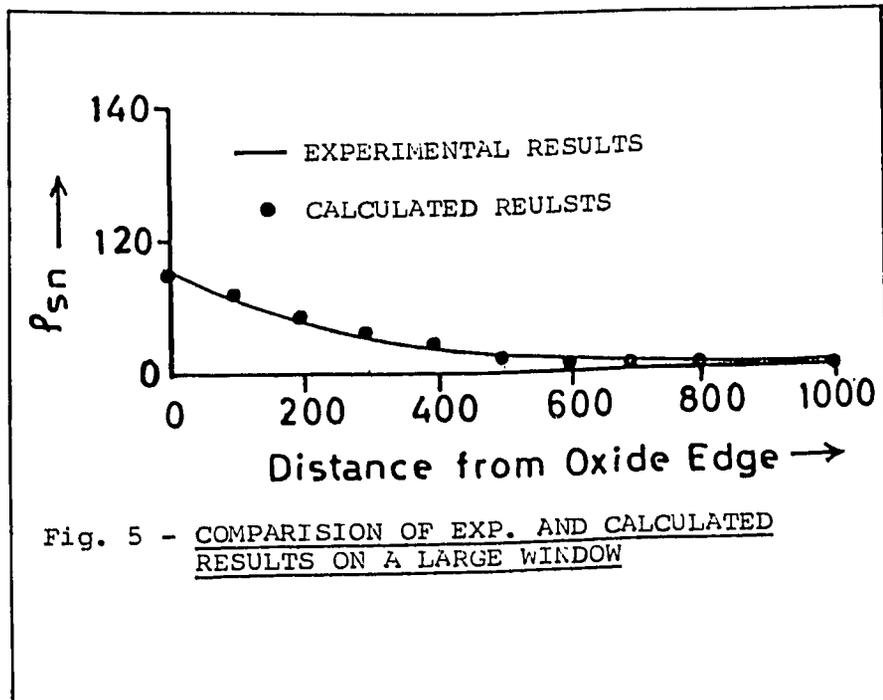
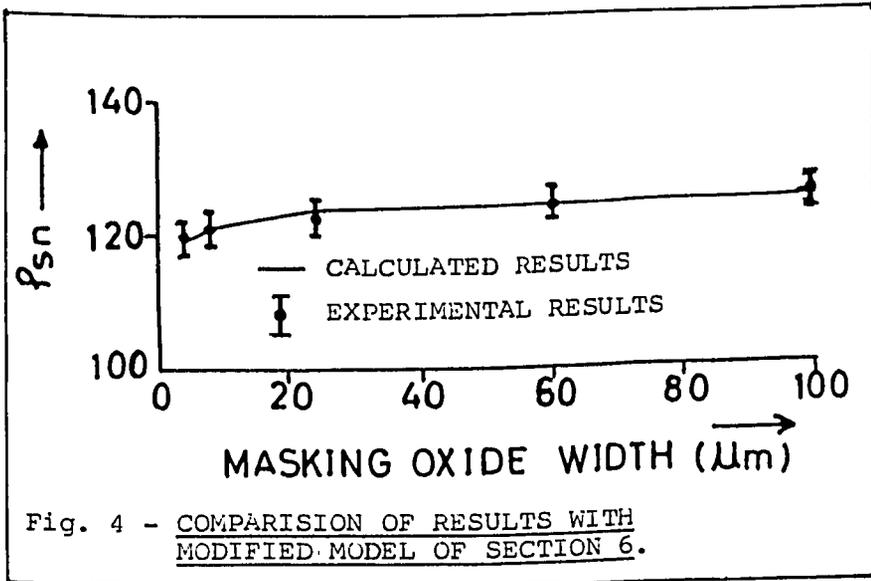
6.1 The Results of the window Frame Effect

The calculated variation of normalized $P_s(\text{res})$ with window frame width may be adjusted to give a close agreement with experimental results by choosing suitable values of HP, G and Cl. Many sets of values of these parameters may be used to provide agreement with experimental data. The results with the following set of parameters are shown in fig.4.

$$\begin{aligned} D_s &= 10^{-4} \text{ Sq.Cms./sec.}, & Cl &= 0.53 \times 10^{16} \\ & & & \text{atoms/Sq.Cm.} \\ HP &= 40, & G &= 0.09 \end{aligned}$$

6.2 The Results of the large sheet

The calculations were done for the case of a very wide window (10mm wide) to determine the variation of boron concentration with respect to the oxide edge. It is observed that in this case, the effect of D_s over the calculated results is quite significant. A value of 10^{-4} Sq.cms./sec. gives only a very small variation of concentration



with respect to the oxide edge. Higher values are therefore tried. The results with D_s equal to 1.4×10^{-2} Sq.cms./sec. and other parameters same as in section 6.1 are shown in fig.5. The agreement with the experimental results obtained from the spreading resistance data is good.

6.3 The Other Results

Calculations have been made for the experimental conditions of section 1. It has been observed that most of the results of calculation are in agreement with the experimental data.

7. CONCLUSIONS

The model proposed to explain the effects of masking oxide on the diffusion of boron into silicon has further been updated. The model assumes a high rate of diffusion of boron over silicon along with a high solubility of the same in oxide. It has been observed that the effects may be adequately modelled if a higher effective rate of arrival of boron ad-atoms over silicon dioxide is assumed. The numerical calculations give results which are in agreement with most of the experimental data.

8. REFERENCES

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