International Journal of Electronics Engineering, 4 (2), 2012, pp. 163– 166 © Serials Publications, ISSN : 0973-7383

Three Dimensional Modeling of Boron Diffusion Into Silicon

F. Rahman[1]

[1]*Department of Physics, A.M.U., Aligarh–202 002 (U.P.), Indian, (E-mail: faiziphys@gmail.com)*

Abstract: In the case of diffusion of boron into silicon, the sheet resistance values observed in narrow diffusion windows differ significantly from the values obtained on plain un-masked check slices with the former always being greater than the latter. The actual value of this discrepancy depends upon several factors such as the size of the window, the surrounding masking oxide geometry and the process parameters. These observations add another important factor in 2-D simulation for diffusion processes. An attempt has been made to present a theoretical model to explain the experimental observations. The results of few experiments with oxide masking 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 is based upon the phenomenon of surface diffusion over silicon and silicon dioxide with a high solubility of boron in oxide. Numerical calculations demonstrate the capability of the model to explain most of the experimental observations.

Keywords: Boron, Diffusion, Masking, Oxide, Profile.

1. INTRODUCTION

It has been reported earlier (1) that in the case of diffusion of boron and phosphorous in silicon, the sheet resistance obtained on patterned resistors depends upon the surrounding masking oxide frame width. The results of a more careful investigation have also been reported (2, 3). It has been observed that the sheet resistance measured on a large area plain check slice, using the four point probe method (3). The actual value of the discrepancy depends upon the size of the window, the surrounding masking oxide geometry and the process parameters. It has been concluded (2,3) that the effect occurs only with boron and is due to the presence of the masking oxide surrounding the window which is absent in the check slice. It has been shown (3) that the effect occurs at the deposition stage and is independent of background concentration, surface orientation, oxide thickness and oxide growth conditions and decreases with an increase in the total amount of doping per unit surface area. The effect disappears in boron is ion-implanted. The spreading resistance and the infra-red free carrier emission measurements shows (4) that the effect is of long range nature and extends to a distance of several hundred microns from the oxide edge on an open slice.

These observations are important in: (i) the design of resistors in conventional processing and (ii) the process/ device modeling since the practical devices are oxide masked but the profiles are measured on large check slices.

Thus it is concluded that the diffusion of boron through patterned silicon is three dimensional in nature and the presence of masking oxide and its geometry plays an important role in the diffusion kinetics. Further investigations have therefore been made in order to develop a satisfactory model for the observed results.

2. POSSIBLE EXPLANATION FOR THE OBSERVED DISCREPANCY

2.1. 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.

2.2. The influence of Si-SiO_2 Interface

One may argue that some phenomenon associated with the Si-SiO_2 interface may cause the effect. Gibbon *et al.* (4) have demonstrated enhanced diffusion at the window edge. This would in fact result in higher doping in the window and hence a lower value of ρ_s (res) compared to ρ_s (4 pt). Other possibilities may include the stress caused by the mismatch between the coefficient of thermal expansion of silicon and silicon dioxide (5), the intrinsic stress or precipitation resulting in electrical inactivity of some of the boron atoms. Although none of these possibilities are likely to explain the long range nature of the observed masking oxide effects as seen from the spreading resistance and the

free carrier emission measurements (6), some more direct evidence to negate is necessary.

2.3. The Surface Diffusion Over Silicon

A more likely explanation based on the surface diffusion of boron over silicon and silicon dioxide is now considered. It is suggested that due to the high solubility of boron in silicon dioxide (7), the concentration of boron over the oxide surface is reduced and the boron ad-atoms (atoms adsorbed at the silicon surface) near the oxide edge move towards it. This results in a concentration gradient of boron ad-atoms over the silicon surface in the window. The surface diffusion of these atoms then takes place under the influence of this concentration gradient, thereby removing some of the boron laterally from the silicon window into the oxide. This reduces the surface concentration at different points in the window, resulting in lesser amount of boron diffused and hence causing a higher value of sheet resistance in the windows. The surface diffusion, seems to be the most plausible mechanism to explain the effects of masking oxide on boron diffusion.

3. EXPERIMENTAL RESULTS WITH OXIDE MASKING

Results of few experiments are given below:

(i) Resistors were fabricated by etching off silicon in selected areas of a boron doped layer. The measurement of these resistors showed that the sheet resistance values on the resistors and on the plain the regions were equal. These rules out any effect of the presence of masking oxide on electrical measurements or on the mobility of the charge carriers.

(ii) Wafer were annealed in nitrogen before and after opening windows in oxide to relieve stresses or strains, if, any. The results were same as before.

(iii) Boron was diffused through a thin uniform layer of poly silicon deposited over the wafer after opening windows in oxide. No effects of masking oxide were seen which indicates that the oxide surface and not the Si-SiO_2 interface is responsible for the influence of oxide on diffusion.

(iv) The effects of masking oxide were found to decrease with increase in total concentration suggesting a limitation to the effect. To confirm this, oxide was carefully doped with boron prior to diffusion through the windows. The effects of masking oxide were found to decrease.

3.1. The Surface Diffusion Model

On the basis of a careful analysis and consideration of experimental results described earlier, it is concluded that the effects of masking oxide on boron diffusion may be explained with the help of a 'surface diffusion model, described below:

During pre deposition of boron, the atoms arriving at the silicon surface (ad-atoms), are loosely bound. The ad-atoms close to the masking oxide surface are absorbed by the oxide due to high solubility of boron in silicon dioxide, resulting in a depletion of boron near the oxide edge. This causes a concentration gradient across the window. Surface diffusion of ad-atoms of boron then takes place under the influence of this concentration gradient. The amount available at the surface of silicon for diffusion into the bulk is thus reduced causing an increase in the actual sheet resistance values in the windows. The model is quantitatively developed in the following sections.

3.2. The Quantitative Model

(a) The pre deposition system of boron through patterned silicon is shown in Figure 1. The following simplifying assumptions are made:

(b) It is assumed that an average value of flux F_n per unit area per unit time of boron atoms arriving at the surface of silicon from the source is constant.

(c) The surface diffusion takes place, both over the silicon window as well as the surrounding oxide with surface diffusion coefficients of Ds and Dox respectively.

(d) The boron is dissolved uniformly all over the oxide width up to a maximum concentration of Cl atoms/ sq.cm.

(e) The maximum rate at which boron may be dissolved in oxide is proportional to the difference between Cl and the actual concentration of boron in the oxide, Cox(t), with G as the constant of proportionality. In the beginning of diffusion, the rate of arrival of boron at the oxide is smaller than the above and hence all the boron is dissolved in the oxide. Thus the boron surface concentration at the oxide surface continues to remain zero until the maximum dissolution rate of boron becomes less than the rate of its arrival.

(f) Because of a much greater solubility of boron in oxide (7) and a higher value of sticking coefficient 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.

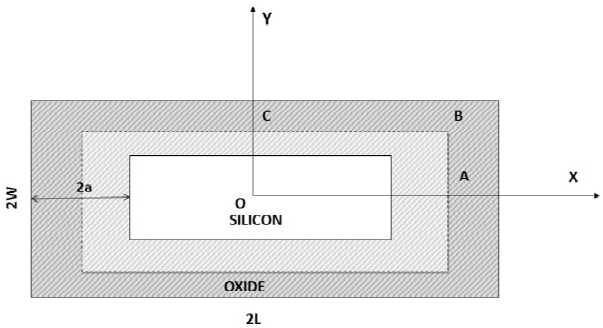
Referring to Figure 1 the equations to be solved are as follows using the well established concepts (8):

3.3. On Silicon Surface

Rate of change of concentration at any point = Rate of change of surface diffusion flux + Effective rate of arrival of boron from the source. This leads to

$$\frac{\partial c}{\partial t} = D_s \frac{\partial^2 c}{\partial x^2} + D_s \frac{\partial^2 c}{\partial y^2} + F_n \qquad (1)$$

Figure 1: The Pre Deposition System



3.4. On Oxide Surface

Rate of change of concentration at any point = Rate of change of surface diffusion flux + Effective rate of arrival of boron from the source – Rate of dissolution of boron in oxide. This leads to

$$\frac{\partial c}{\partial t} = D_{ox}\frac{\partial^2 c}{\partial x^2} + D_{ox}\frac{\partial^2 c}{\partial y^2} + F_n - G\,[Cl - Cox\,(t)] \qquad (2)$$

Where, $c = c(x, y, t)$ is the concentration per sq.cm. of the surface.

F_n is the effective constant rate of arrival of boron.

D_s is surface diffusion coefficient at the silicon surface.

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

The initial and boundary conditions are:

$$c(x, y, 0) = 0 \qquad (3)$$

$$\left.\frac{\partial c}{\partial x}\right|_{x=0} = \left.\frac{\partial c}{\partial x}\right|_{x=L+a} \qquad (4)$$

$$\left.\frac{\partial c}{\partial y}\right|_{y=0} = \left.\frac{\partial c}{\partial y}\right|_{y=W+a} \qquad (5)$$

The solution will give the variation of concentration with respect to time at different points in the window. This variation may then be used to determine the profiles of boron in the silicon bulk. The concentration in the silicon bulk is limited by the solid solubility limit.

3.5. Solution of Equations

Considering equation (1), the use of Crank-Nicholsan method will give:

$$\frac{C_{l,m}^{n+1} - C_{l,m}^{n}}{k} = D_s\left\{\frac{\delta^2 x}{h^2} + \frac{\delta^2 y}{h^2}\right\} C_{l,m}^{n+1} + F_n \qquad (6)$$

Where, l, m and n are number of steps along x, y and t.

k is the size of time step and h is the step size in x and y direction.

Substituting these values for $\delta^2 x$ and $\delta^2 y$ and re-arranging will give:

$$C_{l,m}^{n+1} = \left\{r\,(C_{l+1,m}^{n+1} + C_{l-1,m}^{n+1} + C_{l,m+1}^{n+1} + C_{l,m-1}^{n+1}) + C_{l,m}^{n} + F_n\,k\right\}/(1+4r) \qquad (7)$$

Similar treatment is given to equation (2) and the following result is obtained;

$$C_{l,m}^{n+1} = \left\{r_1(C_{l+1,m}^{n+1} + C_{l-1,m}^{n+1} + C_{l,m+1}^{n+1} + C_{l,m-1}^{n+1}) + C_{l,m}^{n} + F_n\,k + G\,(Cl - Cox)\right\}/(1+4r_1) \qquad (8)$$

Where; $r = D_s.k/h^2$ and $r_1 = Dox.k/h^2$

Gaus Seidel method is now used taking initial values from explicit scheme.

4. RESULTS AND ANALYSIS

To study window frame width effect, calculations are done with a window width of 40 μm and the frame width of 4, 8, 24, 60 and 100 mm. For window width effect, the resistor width has been taken to be 12, 20, 40 and 80 mm with a 100 mm wide window frame. The value of ρ_s (res) have been normalized and expressed as a percentage of ρ_s (plane) and are denoted by ρ_{sn}.

Table 1
Comparison of Calculated and Experimental Results

Oxide Frame Width Effect *Window Width = 40 μm*			*Window Width Effect* *Oxide Width = 100 μ*		
	ρ_{sn} *(%)*			ρ_{sn} *(%)*	
Oxide Width	*Experi-mental*	*Calcu-lated*	*Window Width*	*Experi-mental*	*Calcu-lated*
4 μm	119.8±2.2	102.6	12 μm	136.0±2.3	137.5
8 μm	121.6±2.6	104.8	20 μm	131.5±3.5	133.5
28 μm	122.7±2.8	111.7	40 μm	126.2±2.1	126.5
60 μm	124.5±2.5	120.9	80 μm	126.8±2.9	118.3
100 μm	126.2±2.1	126.5			

A comprehensive simulation program is developed and profiles are obtained under widely different conditions. The results of numerical calculations with suitable values of different parameters are presented in Table 1 A good agreement between the experimental and calculated results are shown in Figure 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.

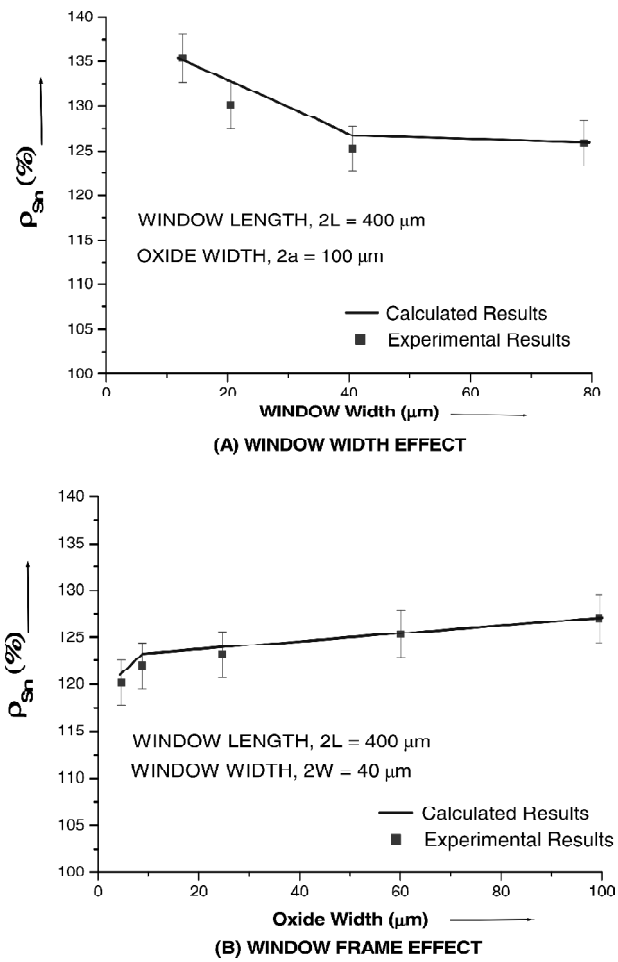


Figure 2: Experimental and Computational Results

5. CONCLUSIONS

A careful and accurate investigation of the effects of masking oxide on the diffusion of boron into silicon has been made. 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 model is capable of explaining the dependence of sheet resistance of boron doped layers on the patterning geometry. Thus it is concluded that the model is capable of explaining the effect of masking oxide on the diffusion of boron in silicon. A more accurate estimation of various parameters is however desired.

REFERENCES

[1] J.P. Decosterd, D. Chauvey and K. Hubner (1968), *J. Electrochem. Soc.,* 115, 291.

[2] S.A. Abbasi and A. Brunchweiller (1981), *IEEE Proc.,* Vol. 128, Pt. I, No. 5, 185.

[3] S.A. Abbasi and A.A. Khan 1986, The Electrochemical Society Extended Abstracts, Vol. 86-2, San Diego, CA, Oct. 19-24.

[4] C.F. Gibbon, E.I. Porilonis and D.R. Ketchew (1972), *Journal of Electrochemical Society,* 49, 769.

[5] H.H Lee (1990), Fundamental of Microelectronics Processing, McGraw Hill Pub. Co., New York.

[6] S.A. Abbasi, O. Takleh, A. Brunchweiller and J.G. Smith (1980), *Electron Letter,* 17, 578.

[7] T. T. Rocket and W.R. Foster (1965), *J. Amer. Ceram. Soc.,* 48, 76.

[8] A.S. Grove (1967), Physics and Technology of Semiconductor Devices, John Wiley & Sons, Inc., New York.