A MODEL FOR THE OXIDATION ENHANCED DIFFUSION OF BORON IN EXTRINSIC SILICON

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ABSTRACT

It has been reported earlier that 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-marked 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 a careful series of experiments using multilayered mask structures 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. Further details of the modeling and calculations will be presented.

Keywords: Boron, Diffusion, Silicon, Oxide, Masking

I. INTRODUCTION

It has been reported earlier (1) that in the case of diffusion of boron, the sheet resistance obtained on diffused resistors depends upon the surrounding masking oxide frame width. The results of a more careful investigation have been reported (2,3). It has been observed that the sheet resistance on boron diffused resistors is always greater than the sheet resistance measured on a large area check slice, using the four point probe method (3). These values are referred as ρ_s (res) and ρ_s (4 pt) respectively, and the normalized value of ρ_s (res) expressed as a percentage of ρ_s (4 pt) is denoted by ρ_{sn}. It has been concluded on the basis of a thorough study that the discrepancy between the values of the sheet resistance is observed only with boron and is due to the presence of masking oxide surrounding the window, which is absent in the case of a plain check slice. The experimental results (3) that the effect occurs at the predeposition stage and is independent of background concentration in silicon, oxide thickness, oxide growth condition and decreases in the total amount of doping per unit surface area. The discrepancy disappears if boron is ion-implanted. A significant reduction in free carrier concentration (increase in sheet resistance) has been observed even at distances of several hundred microns from an oxide edge on an open slice. This indicates that the effect of masking oxide on boron diffusion is of long-range nature. Further investigations have therefore been made in order to find a satisfactory explanation of the observed results. An attempt to present a theoretical model has been made.

II. 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, there by 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.

III. QUALITATIVE MODEL

The predisposition system of boron through patterned silicon is shown in Fig. 1. The following simplifying assumptions are made:

(i) The flux of boron going in to the silicon bulk at any point of the surface is negligible compared to the lateral flux due to the surface diffusion.

(ii) In the absence of complete understanding of boron deposition kinetics, the flux F_n of boron atoms arriving at the surface of the water, from the source per unit area per unit time is considered to be constant.

(iii) 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.

(iv) The boron is dissolved uniformly all over the oxide width up to a maximum concentration of C_L atoms/sq.cms.

(v) The rate at which the boron may be dissolved in oxide is proportional to the difference between C_L and actual concentration of boron in the oxide. Thus, if the concentration of boron in the oxide at any instant of time 't' is Cox(t), the rate at which boron may be dissolved in the oxide is equal to $G(C_L\text{-}Cox)$; 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.

(vi) Because of much greater solubility of boron in oxide the rate of boron reflected back from the oxide surface may be much smaller compare to that over silicon.

(vii) The ideal one-dimensional diffusion corresponding to a single diffusion coefficient in the silicon bulk is assumed (8).

Referring to Fig. 2 the equations to be solved are as follows using the well established concepts (8):

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

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

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

$$\frac{\partial C(x,t)}{\partial t} = D_s \frac{\partial^2 C(x,t)}{\partial x^2} + Fn - G[CL - Cox(x,t)] \; ; \qquad -L < x < L+a$$

Where, C (x,t) is the concentration per unit surface area.
D_s is the surface diffusion coefficient.
x is the distance from the center of the window.
2L is the width of the window.
2a is the width of the oxide.

The above equations are solved using the Crank Nicholson method. 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 ideal one dimensional diffusion theory. The concentration of boron in the silicon bulk is assumed to be limited by the solid solubility limit.

IV. VALUES OF DIFFERENT PARAMETERS

For surface diffused studies, it is important to know that adsorption kinetics of B_2O_3 over silicon and silicon dioxide. In particular, it is necessary to know that proportion of B_2O_3 is actually adsorbed. Unfortunately, nothing is known about this 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 values of these flux at 890^oC has been calculated to be $2.2x10^4$ molecules/sq.cm. which is a very high value. The other possibility may therefore be assumed that the adsorption kinetics is such that the effective constant rate of arrival of B_2O_3 over silicon is much less. Similarly, nothing is known about Ds, G and CL 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^{o}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 $2x10^{20}$ atoms sq.cms and $2.9x10^{-15}$ sq.cms./sec. respectively.

V. RESULTS OF CALCULATIONS

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 µm. For window width effect, the resistor width have been taken to be 12, 20, 40 and 80 µm with a 100 µm 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}.

The experimental and calculated results are shown in Fig. 3. 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 trails with different parameters.

VI. THE RESULTS OF WINDOW FRAME EFFECT

The calculated variation of normalized ρ_s (res) with window frame width may be adjusted to give a close agreement with the 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 are shown in Fig. 4.

VII. CONCLUSIONS

A careful and accurate investigation of the effects of masking oxide on the diffusion of boron into silicon has been made. A quantitative difference in the results compared to the previously published ones has been observed. An attempt to explain the observed effects has been made and a theoretical model has been developed. The capability of the theoretical model proposed to explain experimental observations quantitatively. Further work is being done to improve the model by developing efficient algorithms. An attempt is also being made to perform experiments to extract the values of the parameters used in the model, once this is done, the model may be incorporated in a 2-D process simulator.

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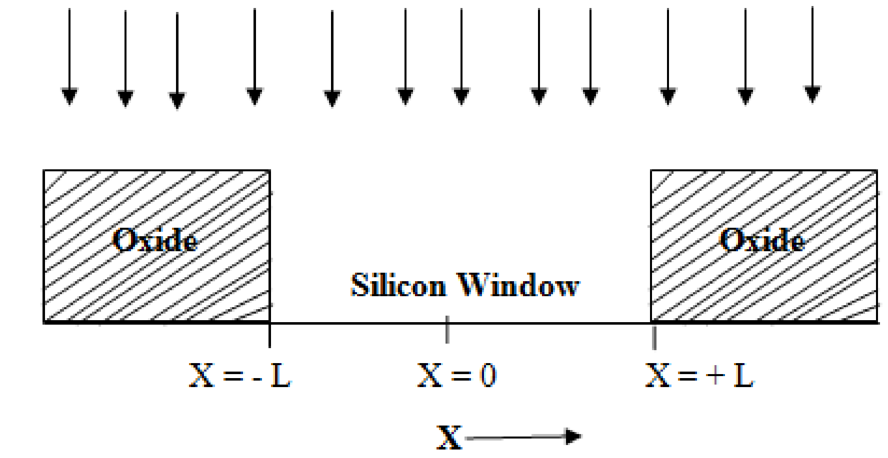


Fig.1 Pre-Deposition System of Boron

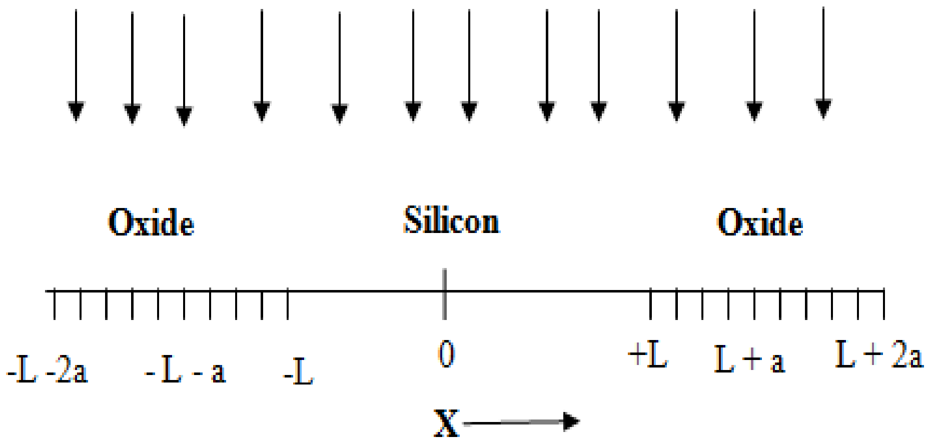


Fig.2 Pre-Deposition System of Boron

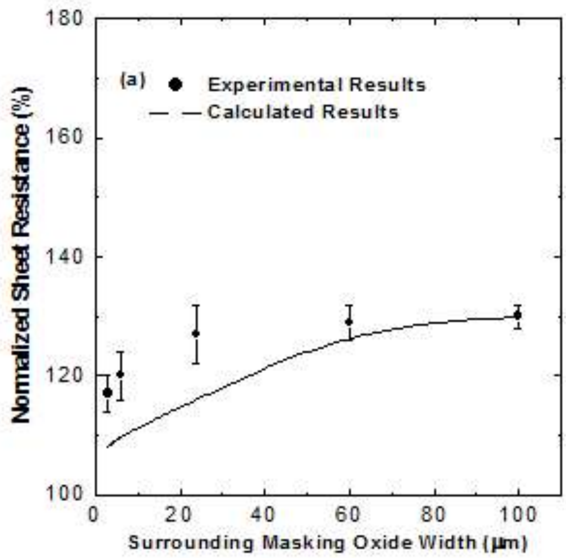


Fig. 3 Experimentally Measured and Theoretically Calculated Normalized Sheet Resistance As A Function of (A) Surrounding Masking Oxide Width (µM) and (B) Window Width (µM)

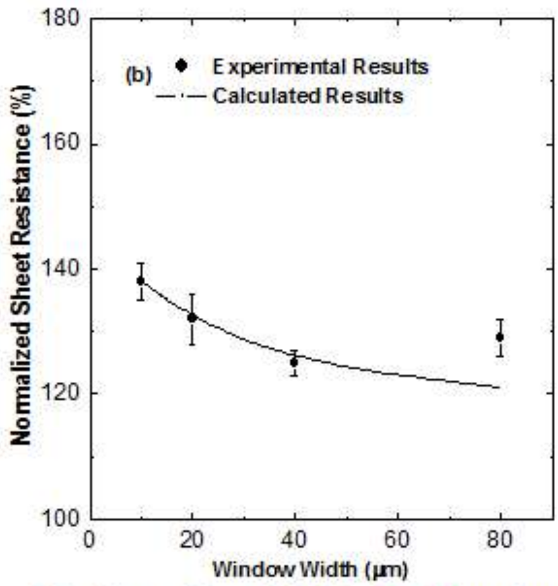
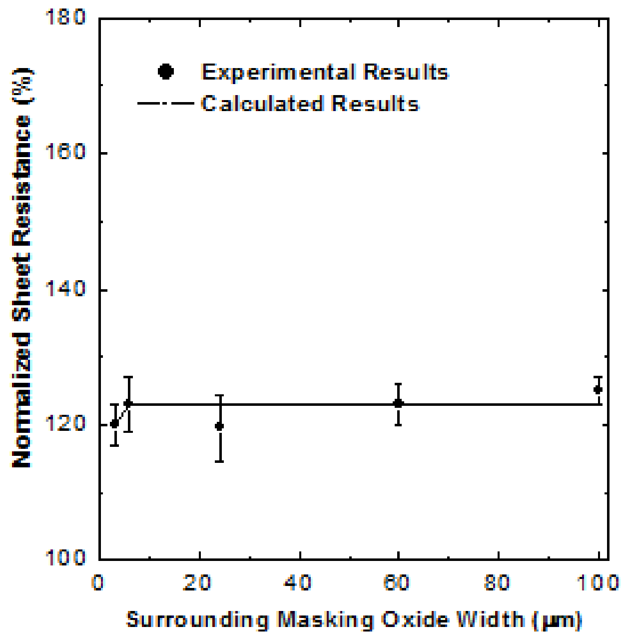


Fig. 4 Comparison of Calculated and Experimental Results of Window Frame Width Effect



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