Beyond TED: Understanding Boron Shallow Junction Formation

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Abstract

As implant energies are reduced with the aim of forming shallower junctions, transient enhanced diffusion (TED) effects are greatly reduced. With TED less pronounced, other effects emerge to dominate the diffusion of dopants such as boron. In particular, coupled dopant/defect diffusion injects interstitials leading to enhanced tail diffusion, while oxidation and the diffusion of silicon through thin oxides affects the surface point defect concentrations. This paper shows that by careful consideration of models developed for much deeper junctions, the dependence of junction depth on processing conditions can be understood for shallow junctions as well.

Introduction

Transient enhanced diffusion (TED) has been the dominant effect in determining junction depths for the past decade and will continue to be important. However, the use of ultra-low energy implants and short, high temperature RTP annealing has greatly diminished the importance of TED in ultra-shallow boron junctions. Reducing the implant energy is particularly effective as it puts the damage closer to the surface where it can be more readily annihilated, thus reducing the time period over which TED is present. Recent work [1–3] shows that TED can be nearly eliminated for implant energies below about 1keV. However, the reduction in TED has revealed other effects controlling boron diffusivity (and thus junction depth) for ultrashallow profiles. This paper focuses on understanding and modeling of these effects.

Coupled Diffusion Effects

Agarwal *et al.* [1–3] found that although silicon implants at 1keV and below resulted in normal marker layer diffusion, boron implants with similar doses and ranges led to significantly ($\sim 4\times$) enhanced diffusion. They termed this effect BED (boron enhanced diffusion). To investigate the source of this phenomena, we simulated their experimental conditions using fully coupled diffusion processes [4] plus a moment-based model for {311} defect evolution [5] and a simple boron clustering model:

$$\frac{\partial C_\mathrm{B}}{\partial t} = \bigtriangledown \cdot D_\mathrm{B}\left(\frac{C_\mathrm{I}}{C_\mathrm{I}^*}\bigtriangledown C_\mathrm{B} + C_\mathrm{B}\bigtriangledown\frac{C_\mathrm{I}}{C_\mathrm{I}^*}\right) - R_\mathrm{cluster} \quad (1)$$

$$\frac{\partial C_\mathrm{I}}{\partial t} = \bigtriangledown \cdot D_\mathrm{B}\left(\frac{C_\mathrm{I}}{C_\mathrm{I}^*}\bigtriangledown C_\mathrm{B} + C_\mathrm{B}\bigtriangledown\frac{C_\mathrm{I}}{C_\mathrm{I}^*}\right) + \bigtriangledown \cdot D_\mathrm{I}C_\mathrm{I}^*\bigtriangledown\frac{C_\mathrm{I}}{C_\mathrm{I}^*} - k_{I/V}\left(C_\mathrm{I}C_\mathrm{V} - C_\mathrm{I}^*C_\mathrm{V}^*\right) - R_{311} \quad (2)$$

$$\frac{\partial C_\mathrm{V}}{\partial t} = \bigtriangledown \cdot D_\mathrm{V}C_\mathrm{V}^*\bigtriangledown\frac{C_\mathrm{V}}{C_\mathrm{V}^*} - k_{I/V}\left(C_\mathrm{I}C_\mathrm{V} - C_\mathrm{I}^*C_\mathrm{V}^*\right) \quad (3)$$

$$\frac{\partial C_\mathrm{I}^{311}}{\partial t} = R_{311} \quad (4)$$

$$\frac{\partial C_\mathrm{B}^\mathrm{cluster}}{\partial t} = R_\mathrm{cluster} \quad (5)$$

Note that the diffusion coefficients and equilibrium defect concentrations are Fermi level dependent to include the range of charge states.

The parameters for the models were based on our previous work [4, 5, 6] limited to consideration of much deeper junctions [7]. The results of those simulations are shown in Figs. 1–3. As is evident, the simulations accurately predict the observed boron junction depths and/or marker layer broadening, not only for implants, but also for boron deposited on the surface via MBE. There is indeed significantly enhanced diffusion in this system, driven by the same pair injection process which leads to enhanced phosphorus tail diffusion, although the effects are less pronounced for boron due to the lower solubility and the asymmetry in the charge states of the interstitial [4].

It was noted by Agarwal *et al.* [1–3] that there was a slightly greater diffusion enhancement for higher temperatures (e.g., factor of 3 at 950°C versus 4 at 1050°C), while coupled diffusion effects give smaller enhancements at higher temperatures. For coupled diffusion effects, the interstitial supersaturation (and thus diffusion enhancement) in the tail region depends on the balance between interstitial injection, which is proportional to boron diffusion, and interstitial diffusion back to the surface, which is

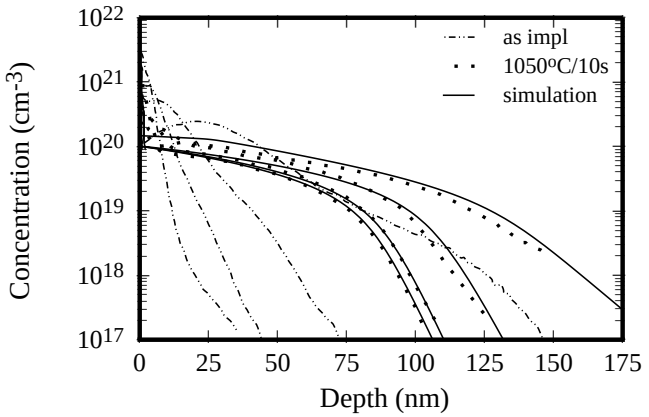

Figure 1: Comparison between simulated and measured boron profiles following 10^{15}cm^{-3} boron implants at 0.5 to 5keV and annealing at 1050°C for 10s. Also included are the measured as-implanted profiles which were used as starting conditions for the simulations. Data from Agarwal *et al.* [1].

proportional to the self-diffusion coefficient. Since boron diffusion has a smaller activation energy (and thus smaller increase with temperature) than the self-diffusion, smaller supersaturations are expected at higher temperatures for the same boron surface concentration. However, for the high boron concentrations in these experiments, the surface concentration is not constant due to the changes in the solubility with temperature. We find from our simulations that the increased solubility at higher temperatures approximately compensates for the changes in the boron diffusion to self-diffusion ratio, leading to very little change in enhancement with temperature. As can be seen from Figs 1–3, our simulations accurately predict the experimental behavior.

Figure 3 shows the change in diffusion enhancement versus implant dose. Agarwal *et al.* [1–3] suggested that the rather abrupt increase in diffusion enhancement with dose might be due to the formation of a boride phase. However, it can be seen that the dose dependence is accurately predicted simply based on coupled diffusion as the increased boron concentration with dose leads to larger fluxes of BI pairs into the substrate.

Oxidation Enhanced and Retarded Diffusion

Another recent observation is that for annealing of nominally bare silicon wafers, changes in oxygen concentration in the 0–10000 ppm range in an otherwise inert N_2 ambient have a strong effect on junction depth [8, 9]. Comparing these results to our simulations, it appears that for oxygen partial pressures below about 1000 ppm at

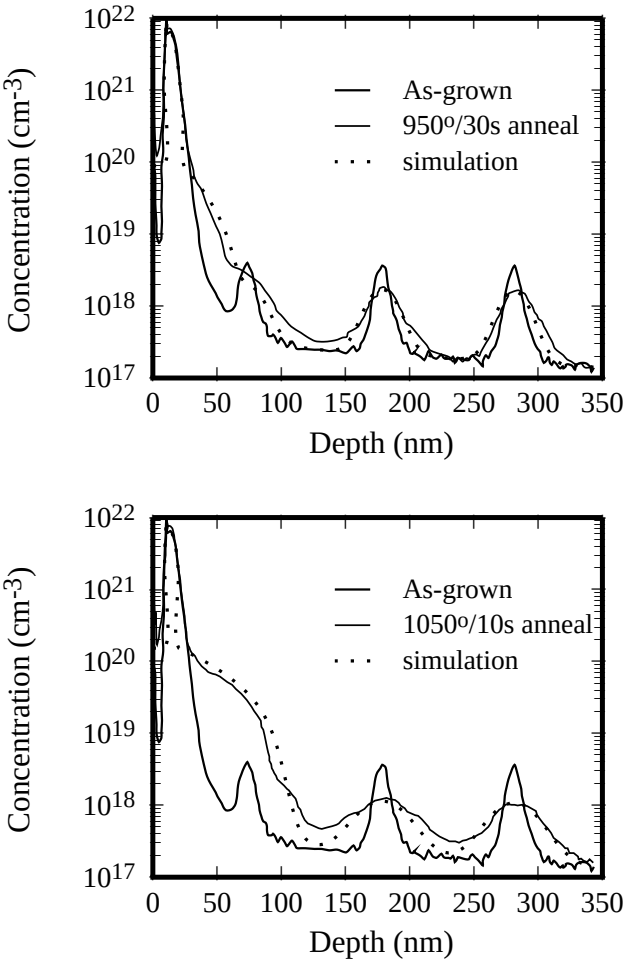

Figure 2: Comparison between simulated and measured broadening of boron delta-doped superlattices in the presence of an MBE-deposited boron layer and annealing at (a) 950°C and (b) 1050°C for 10s. Data from Agarwal *et al.* [1].

1050°C, the diffusion is actually retarded rather than enhanced (Figs. 4 and 5). This is consistent with our previous work on point defect interactions at the Si/SiO_2 interface, which predicts that very low O_2 partial pressures should lead to retarded diffusion [11]. This behavior has also been previously observed experimentally for slow oxidation of ⟨111⟩ silicon at high temperature (1160°C) [10].

Our models for retarded diffusion in Si/SiO_2 structures are based on the segregation of interstitials between silicon and SiO_2 under both oxidizing and nonoxidizing conditions [11]. During oxidation, the interstitial concentration near the interface is determined by a balance between two processes: generation of interstitials at the interface to accommodate the volume needed for oxide growth,

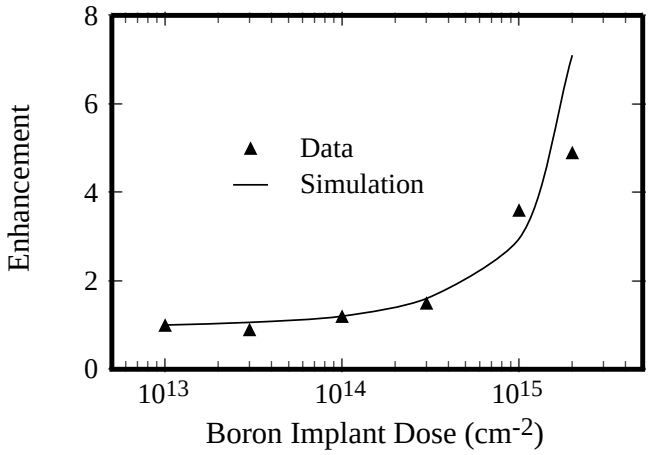

Figure 3: Predicted and measured diffusivity enhancement of boron marker layers for various 0.5 keV boron implant doses and annealing at 1050° C for 10s. Data from Agarwal *et al.* [2].

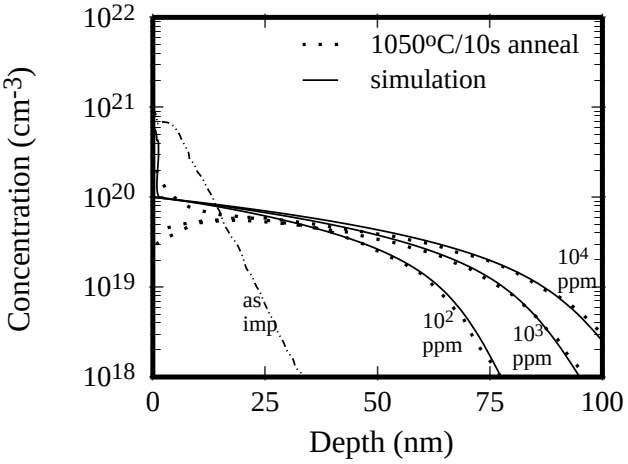

Figure 4: Boron profiles versus oxygen partial pressure for 1keV, 10^{15}cm^{-2} boron implants annealed 10s at 1050° C (Lerch *et al.* [8]) are shown along with simulations including coupled diffusion effects matched to these profiles by varying the surface interstitial concentration.

and diffusion of interstitials (excess silicon) into the oxide and subsequent reaction with incoming oxidant species (molecular or atomic). For normal oxidation rates, the first process dominates leading to oxidation enhanced diffusion (OED), but as the oxidation rate drops (due to low ambient pressures or very thick oxides) the flux into the oxide comes to dominate, dropping the interstitial concentration below its equilibrium value [16]. This changeover arises because the flux into the oxide depends inversely on the diffusion length which in turn depends inversely on the *square root* of the oxidant concentration (rather than linearly as in the case of the interface generation). Including the role of both molecular and atomic oxidant species, the resulting interstitial super/undersaturation is of the form [12, 13]

$$\frac{C_{\rm I}}{C_{\rm I}^*} = \frac{K_1\left(\frac{dx_{ox}}{dt}\right)}{\sqrt{(\rho-1)*(\rho-1+K_3)}}, \qquad (6)$$

where $\rho = \sqrt{1.0 + K_2(dx_{ox}/dt)}$. Figure 5 shows a comparison of the predicted interstitial under/supersaturation versus partial pressure to the values extracted by comparison to the data of Downey *et al.* [9] and Lerch *et al.* [8] (Fig. 4). Parameters from our previous work [12, 13] were used, including the dependence of oxidation rate on partial pressure. Although this model does predict slightly retarded diffusion for very low partial pressures, the effect observed experimentally is much more pronounced. We attribute this to an additional phenomena arising from the presence of extremely thin oxides (∼18 Å): Interstitials diffuse through the film to the gas/oxide interface where they react to form volatile SiO, resulting in etching. Argon annealing of samples with thin oxides has previously been observed to cause retarded diffusion of phosphorus [11, 14]. When we also include this effect, which leads to an interstitial flux through the oxide of

$$F_{\rm I} = D_{\rm I}^{\rm SiO_2} m_{\rm I} C_{\rm I}^{\rm Si}(0)/x_{ox}, \qquad (7)$$

and use parameters from our previous analysis of the spatial extent of oxidation enhanced diffusion [15], we predict quite accurately the experimentally observed results, including the crossover from oxidation enhanced to retarded diffusion at about 1000 ppm (Fig. 5).

Conclusions

In summary, we have investigated the phenomena which control junction depth for ultra-low energy boron implants. As TED is reduced, coupled diffusion effects and oxidation enhanced and retarded diffusion become dominant. Understanding these effects is a critical step along the way to optimizing ultra-shallow junction processes for future generations of VLSI devices.

Acknowledgments

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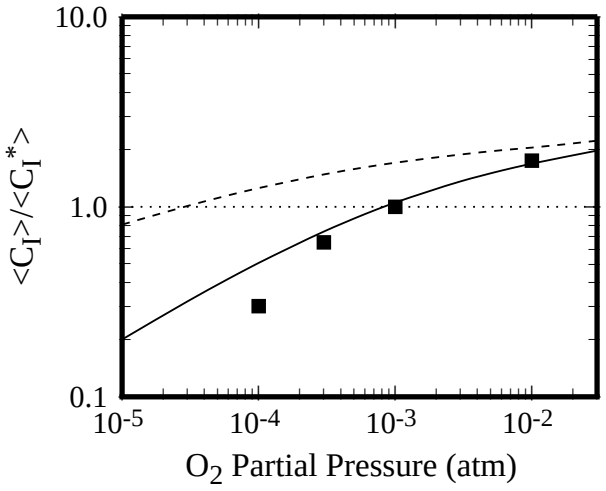

Figure 5: Comparison of interstitial under/supersaturation versus oxygen partial pressure at 1050°C based on experimental results to model predictions using parameters from previous work. The experimental points are based on diffusivity enhancements/retardations during 10s rapid thermal anneals of shallow boron junctions extracted by comparing simulated to measured profiles as in Fig. 4 [8]. The dashed line shows the interstitial concentration predicted by models and parameters of Dunham and Plummer [12, 13], while the solid line shows the same model modified to account for the loss of silicon to the ambient as expected for thin oxides.

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