Normal and Transient-Enhanced Diffusion of Boron as a Function of Background Doping Level

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Semiconductor device structures include multiple dopant species, which diffuse simultaneously during the fabrication process. In order to accurately model the resulting doping profiles, it is necessary to be able to separate out effects due to the doping level from those due to non-equilibrium point defect concentrations. In this work, the diffusivity of boron is measured in silicon with nearly uniform arsenic, phosphorus, or boron background doping under both transient-enhanced diffusion (TED) as well as normal conditions. We find the the resulting behavior is well-modeled by considered the effect of donor-acceptor pairing, which is commonly ignored in process simulators.

Floatzone wafers were implanted with arsenic, boron 11, or phosphorus and furnace annealed (FA) at temperatures of 1100°C to 1150°C to remove implant damage. Multiple doses and energies were chosen to keep peak concentrations below $1 \times 10^{20}/\text{cm}^3$ at all times during the processing, avoiding dopant precipitation and the formation of stable end of range damage. The implant/anneal cycle was repeated to obtain a range of background doping levels for each dopant (Figure 1). Boron 10 was implanted into each of the prepared wafers and rapid thermally annealed (RTA) for 40s at 1000°C (Figure 2). Each wafer was then diffused by FA. SIMS was used to obtain dopant concentrations before and after each step. Diffusivities were obtained by matching profiles to simulations starting from measured initial profiles and assuming constant diffusivity (Figures 3 and 4).

It is well-known that boron diffusivity is enhanced in p-type backgrounds and retarded in n-type backgrounds. Process simulation models generally attribute this to diffusion being dominated by positively charged point defects with diffusivity via neutral defects negligible even in n-type silicon, so that

$$D_B = D_B^0 + D_B^+(n/n_i) \cong D_B^+(n/n_i). \tag{1}$$

However, this explanation is found insufficient to explain the data obtained in this study. Accurately matching diffusion in p-type material requires a significant contribution from neutral defects, greatly overestimating diffusion in n-type material. Ignoring neutral defects overestimates the diffusion in both n and p-type material (Figure 3).

The formation of immobile pairs between oppositely charged donors and acceptors is suggested as an explanation for the reduced diffusivity and also for the decrease in transient enhanced diffusivity which follows ion implantation. The phenomena has previously been shown to account for the dependence of phosphorus diffusion on doping level [Wittel and Dunham]. In the donor-acceptor pairing model, the reaction $\text{P}^+ + \text{B}^- \Leftrightarrow \text{PB}$, with equilibrium constant K, leads to a diffusivity D_{eff} reduced from Eq. (1) by a factor

$$\alpha = \frac{1}{2} + \frac{1}{2}\left(C_\text{P} - C_\text{B} + 1/K\right)\left[\left(C_\text{P} + C_\text{B} + 1/K\right)^2 - 4C_\text{P}C_\text{B}\right]^{-1/2}, \tag{2}$$

which accurately accounts for the experimental results (Figure 3).

Dopants experience TED during ion implant annealing due to the excess in point defects resulting from implant damage. The enhancement stops when the defect concentration returns to equilibrium values. In this study, we found that the amount of TED is nearly independent of p-type background, but is greatly reduced in n-type backgrounds (Figures 2 and 4). This result is in contrast to previous work which found enhanced TED in a p-type background [Giles]. However, that work used FA rather than RTA, which may have led to substantial normal diffusion (which is enhanced in p-type material). The observed dependence of TED on background doping is accurately predicted by a very simple model. In contrast to normal diffusion, in which the number of *neutral* defects is fixed through surface and bulk recombination processes, the number of *total* defects is fixed during TED. Thus changes in Fermi level only redistributes those defects among the charge states, with little effect on diffusion while in n-type material, donor-acceptor pairing still acts to reduce the effective diffusivity (by factor α).

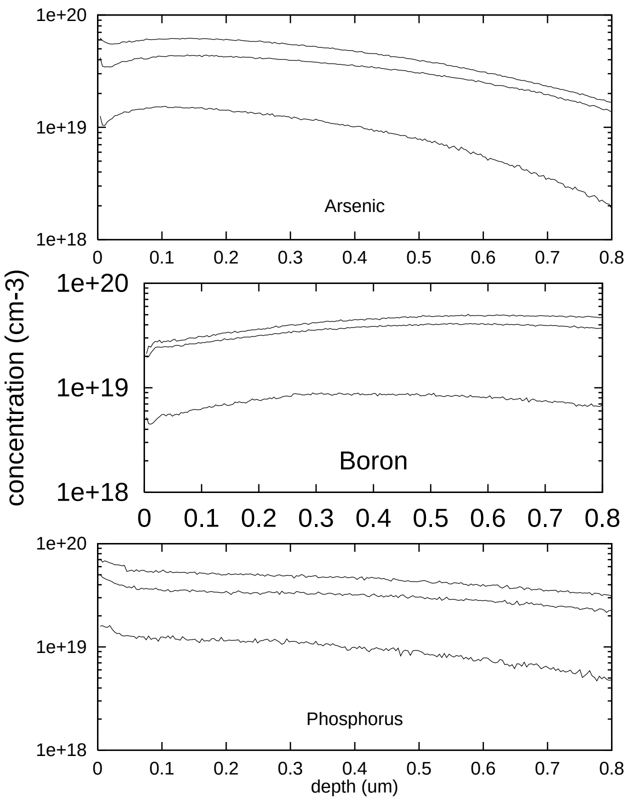

Figure 1: Nearly-uniform background doping profiles.

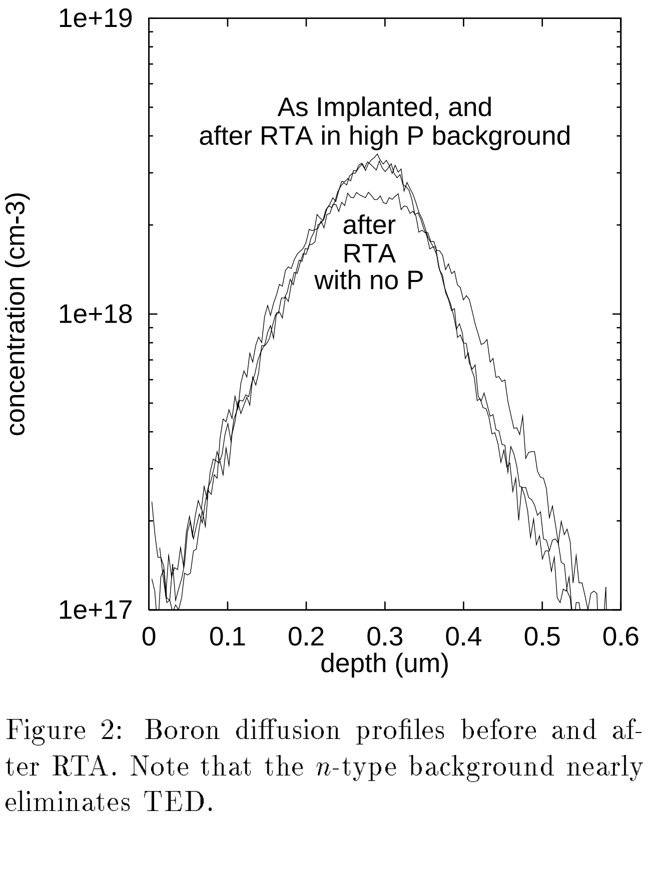

Figure 2: Boron diffusion profiles before and after RTA. Note that the n-type background nearly eliminates TED.

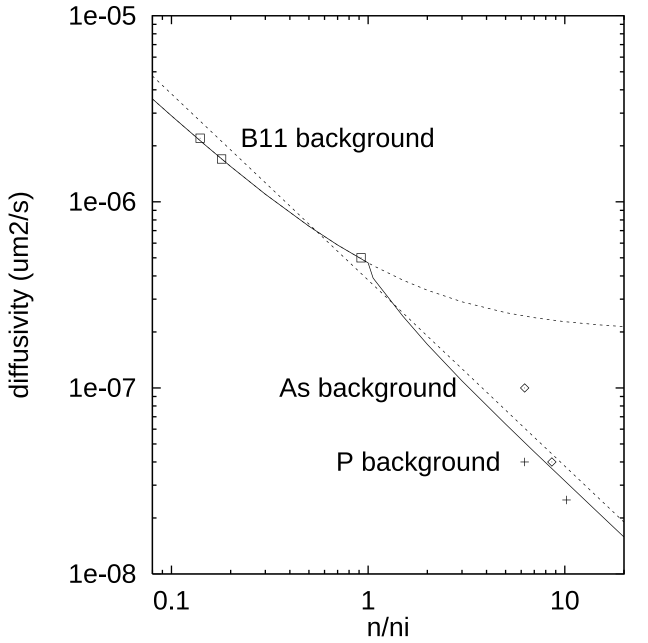

Figure 3: Boron diffusivity at 900°C as a function of doping (Fermi level). The solid line shows the model including pairing (Eq. (2)), while the dashed lines indicate the standard model (Eq. (1)) matched to the p-type data and the full date set (no contribution from neutral pairs). Since the effect of arsenic and phosphorus backgrounds are approximately the same, a single pairing coefficient is used for both.

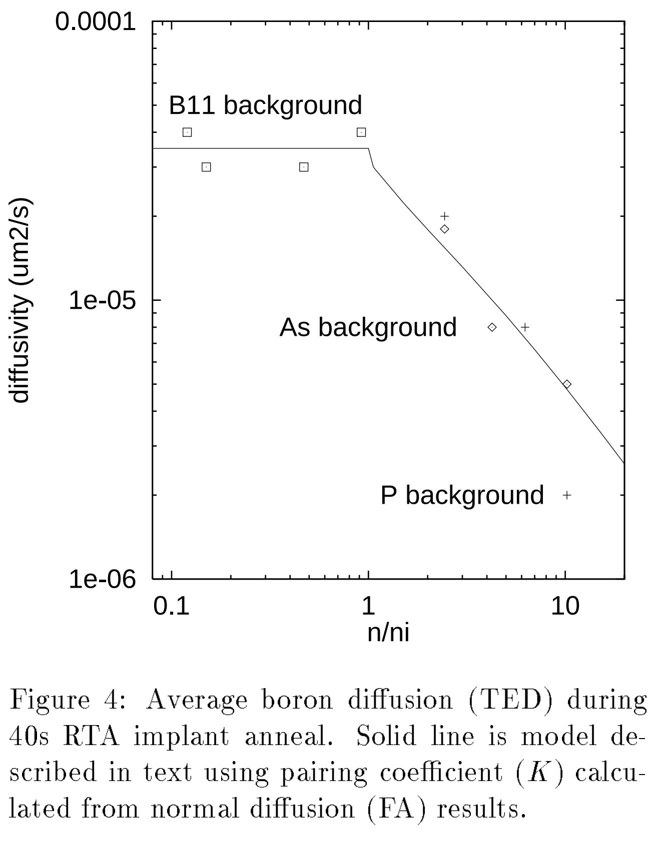

Figure 4: Average boron diffusion (TED) during 40s RTA implant anneal. Solid line is model described in text using pairing coefficient (K) calculated from normal diffusion (FA) results.