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# Modeling and simulation of spatial dependent transient diffusion after $BF_2$ implantation

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The quest for understanding boron redistribution after $BF_2$ implantation has triggered considerable experimental [1] and modeling [2] efforts. The use of $BF_2$ molecular ions as a replacement of B-alone implants is done frequently for meeting scaling issues of submicron Metal Oxide Semiconductor devices. The influence of fluorine on transient and equilibrium dopant redistribution remains a critical issue, since final device characteristics are directly affected. It is generally agreed that the diffusion of boron in fluorine-containing samples is retarded. This phenomena has been attributed to an increased trapping of silicon interstitials in fluorine containing species. Trap models have been proposed and applied with success to account for the reduced redistribution without changing the boron parameters themselves [3].

In this paper, we study the effect of high-dose $BF_2$ implantation/annealing sequences on the redistribution of dopant atoms already present in the crystal. Transient diffusion and activation effects are investigated using numerical simulation and experimental data obtained from silicon samples containing a buried layer of boron.

In-situ doped low temperature epitaxial layers have been deposited on silicon wafers to produce 300nm thick buried layers of boron, sandwiched in between a nominally intrinsic, 7$\mu$m thick buffer and a 700nm thick, lightly p-doped capping layer. As-grown samples received a 5s RTA step at 1000°C to homogeneize possible residual defect configurations remaining from the growth process. SIMS analysis did not detect a significant redistribution of the buried layers during the RTA. Moreover, the oxygen content was below the SIMS detection limit everywhere in the EPI-layer, confirming suitability of the samples for point defect studies. One split of the wafers received a $2\text{x}10^{15}\text{cm}^{-2}$ $BF_2$ implant at 60 keV. After deposition of a low temperature oxide, samples received another split into four different time/temperature schedules for inert thermal processing. Wafers were thermally treated at, alternatively, 850°C or 950°C. Duration of the anneals was 30 min or 2 hours. An example of the experimental result of the 850°C, 30 min anneal is shown in Figure 1. In the sample which received no implant, there was much less redistribution of the buried layer, indicating that the epi-layer region has experienced considerable transient diffusion in the implanted wafers.

Transient diffusion effects can easily be modeled using empirical relations for a time dependent diffusivity enhancement [4]. Generally, this approach fails for nonlocal diffusion effects as they are studied in this paper. To account for the redistribution of the buried layer, we use the point defect assisted diffusion model implemented in TESIM [5], a one-dimensional multilayer process simulator. In this study, we solve coupled balance equations of dopant-point defect pairs, isolated point defects and point defect clusters. To account for the trapping effect of fluorine, we include an inhomogeneous, Gaussian trap distribution, located at the end-of-range of the as-implanted $BF_2$-profile. The location of the amorphous/crystalline ($\alpha/c$) interface was determined using the binary collision code Crystal-TRIM [6]. We do not simulate the solid phase epitaxial regrowth (SPE) and assume instead that the point defect concentrations are at their equilibrium level in the former amorphized layer as initial conditions. Beyond the $\alpha/c$ interface we use a modified "+1 model" [7], i.e. the initial interstitial concentration is proportional to the dopant concentration. Dopants within the regrown layer are assumed to be incorporated substitutionally during the regrowth process, up to a threshold concentration of $3 \times 10^{20}\text{cm}^{-3}$. Dopants beyond this region are assumed to be entirely clustered, i.e. the treatment corresponds to the case of a nonamorphizing B-only implant. The activation of the tail region was modeled with the same parameters as used in previous work on boron. Initial conditions are illustrated in Figure 2.

Figure 3 shows the diffusion front displacements of the buried boron layer and the tail of the implant after the thermal treatments. Also shown is the result of the point defect model, both with and without trapping. One can observe that the experimentally determined redistribution of the buried layer is much stronger than that of the tail region of the implanted profile. It is also illustrated in Figure 3 that this result is not reproduced by the stationary point defect model alone. In the latter case, the displacement of the diffusion tail is overestimated, indicating that there is not only a (partial) suppression of the transient effect, but even a reduction of the stationary interstitial concentration after the transient has vanished. Both initial point defect supersaturation and the trapping model have to be included to give the correct trend of the spatial dependence of the redistribution effects and an accurate description of the transient behavior.

The numerical value of the trapping rate had to be assumed as very high, thus leading to a strong reduction of the interstitial supersaturation in the region immediately below the $\alpha/c$ interface. It turns out that the trapping mechanism in this region is very efficient in the case of high-dose $BF_2$ implants.

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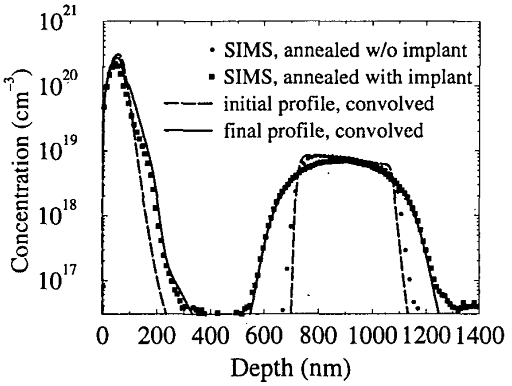

Figure 1: Comparison of experimental and calculated results for the 30min, 850°C annealing step.

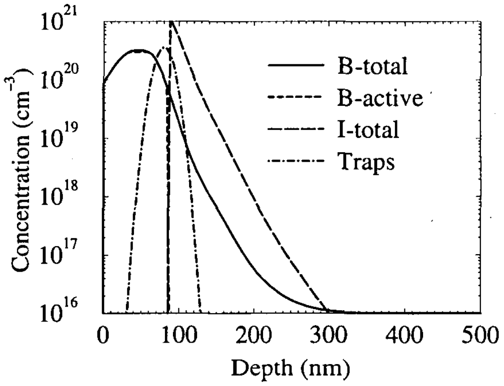

Figure 2: Initial conditions used for the calculation of the anneals after amorphizing $BF_2$ implants.

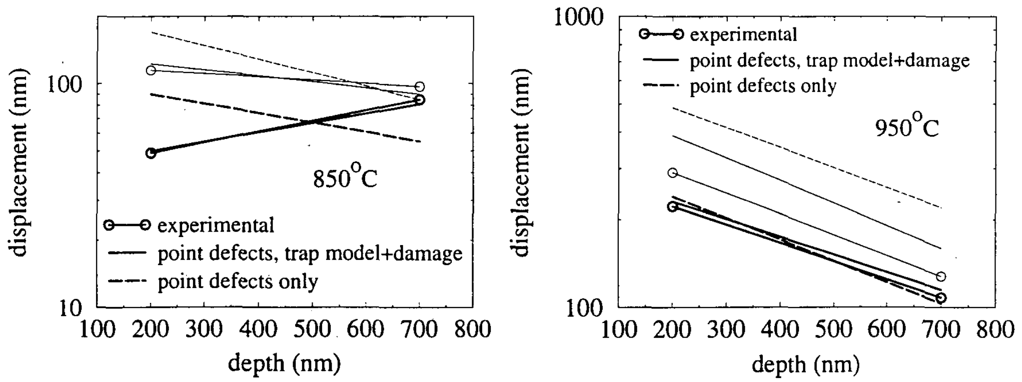

Figure 3: Displacement of the boron diffusion front at a concentration of $1 \times 10^{18} cm^{-3}$ for the 850°C and 950°C thermal treatments. The value at a depth of 200nm is related to the tail of the implanted profile, the value at 700nm shows the displacement at the leading edge of the buried layer. Normal lines correspond to the 30min thermal treatments, bold lines to the 120 min anneals.