# Monte Carlo Simulation of Multiple-Species Ion Implantation and its Application to the Modeling of 0.1µ PMOS Devices

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#### Abstract

New process concepts require multiple implantations into the same volume of Si with only one annealing step after all implantations have been performed. Moreover, there is a trend towards BF2 implantation for shallow p-doping. We have extended the Monte Carlo simulator IMSIL to consider for each implantation the accumulated lattice damage of all previous implantation steps, and we have determined the parameters of the stopping power and damage accumulation models for BF2 ions. The influence of the cumulative damage on the implantation profiles and on the threshold voltage behavior is discussed for a specific PMOS device.

## 1. Introduction

The fabrication of ultra-small devices by ion implantation and subsequent annealing requires minimization of implantation energy and thermal budget. BF2 is an attractive implant species for p-doping, since the B atom carries only 11/49 of the energy of the BF2 molecule. Moreover, the additional damage generated by the F atoms reduces the channeling tail of the B profile. Low thermal budgets, on the other hand, result in a trend to perform an annealing step only after the last implantation. Modeling of ion implantation is challenged by these considerations in two ways: (1) Simulation of BF2 implantation in crystalline Si requires to keep track of the damage generated by both the B and the F atoms. (2) Multiple implantations into the same volume of Si require for each implantation to consider the accumulated damage of all previous implantation steps. In this paper we present for the first time Monte Carlo simulations which take into account both effects. As an application, we investigate the influence of the additional damage produced by F during the BF2 implantation on the electrical behavior of an ultra-short PMOS transistor [1] by coupled process and device simulation.

### 2. Implantation modeling

For implantation modeling we use our Monte Carlo simulator IMSIL [2]. IMSIL has been demonstrated to successfully predict impurity profiles not only after tilted implantations but also after implantations in all major channeling directions for different doses, in a wide energy range, and for light (B, P) as well as for heavy (As) ions [2-5]. This has been achieved primarily by appropriate models for electronic stopping and damage accumulation. Damage is taken into account using the modified Kinchin-Pease model and multiplying the amount of generated damage with a factor *frec*, modeling defect recombination [4,5]. Moreover, damage saturation is considered for B implantations. Employing the modified Kinchin-Pease model is justified since it has been shown [5] that neglecting the recoil range has only a minor effect on the dose dependence of implantation profiles due to damage accumulation, even for the heavy ion species As. The influence of damage on subsequent trajectories is considered by performing amorphous collisions with a probability proportional to the local number of displaced atoms. The recombination factor *frec* has been determined for B, P, and As as 0.125, 1, 2, respectively [2,4,5]. In this work we determine the recombination factor frec to be 1.2 for BF2. This value is obtained by calibrating the model with the 65 keV,  $5 \cdot 10^{15}$  cm<sup>-2</sup> dose implantation profile shown in Fig. 1. This result is verified by simulating the other BF2 implantations from Fig. 1 and additional low-energy channeling implantations from the literature [6,7], providing very good agreement between our simulations and the experimental data. Notice, that frec = 1.2 for BF2 is considerably larger than for B and even larger than for P, which is heavier than both B and F. This may be explained by damage multiplication due to the overlapping of recoil cascades generated by simultaneously implanted B and F. BF2 implantation is simulated by calculating alternatively one B and two F trajectories and recording the damage generated by each of the ions. Moreover, IMSIL has been extended for the simulation of successive implantations. The damage produced by previous implantations is regarded in the simulation of the following implantation steps. The simulator also allows the computation of implantation into arbitrarily shaped 2-D structures [2]. It was found, however, that consideration of the ions scattered out of mask sidewalls is not significant in the process considered here.

Fig. 1: B concentration distribution after 65 keV, 7° tilted BF2 implantation into (100) Si. Continuous lines: experiments [6], histograms: simulations.





Fig.2: B profile resulting from B and BF2 S/D implantations for the 0.2µ PMOS transistor.



Fig. 3: Net doping of the 0.2µ PMOS transistor after all implantation steps have been performed. S/D implantations carried out with B B (full line) or BF2 (dotted line).



Fig. 4: Resulting threshold voltage over the gate length for the 0.1, 0.15, 0.2, and the 0.25µ PMOS transistors.



Fig. 5: Damage distribution for the 0.2µ PMOS transistor after all implantation steps have been performed. S/D implantation carried out with BF2.

## 3. Application to the Modeling of a 0.1µ PMOS Device

The implantation steps of the investigated process [1] have been simulated with the extended version of IMSIL. Fig. 2 shows the shape of the as-implanted B profile after the two S/D BF2 implantation steps (shallow junction: 0° tilt,  $1 \cdot 10^{15}$  cm<sup>-2</sup> dose, 10 keV energy, deep junction: 0° tilt,  $5 \cdot 10^{15}$  cm<sup>-2</sup> dose, 20 keV energy). For comparison, the B profile resulting from the similar B implantation steps with the energy reduced proportional to the mass ratio 11/49 is also shown. Notice that the B profile resulting from the BF2 implantation is shallower because of the increase in lattice damage induced by the F. Both implantation profiles show lateral channeling leading far below the gate. When looking at the net doping (Fig. 3), however, we observe that the As channel implantation  $(1 \cdot 10^{13} \text{ cm}^{-2} \text{ at})$ 100 keV) and the P anti-punch implantation  $(4 \cdot 10^{12} \text{ cm}^{-2} \text{ at } 120 \text{ keV})$  are chosen as to adjust the threshold voltage (Vth) of the 4 nm gate oxide device and to cover the B lateral channeling "nose". Regarding diffusion modeling, we mention that there is no widely accepted and confirmed model for diffusion of implanted boron at high concentrations. We obtained the information about the subdiffusion from Vth as a function of the gate length (L<sub>gate</sub>) as measured in [1]. The time averaged boron motion during the RTA step at  $1050^{\circ}$ C for 10 sec was calibrated by a coupled process/device simulation (TSUPREM-4 [8], MINIMOS [9]) to give the same threshold roll-of as in [1] (Fig. 4). In addition these measurements show a delayed onset of the threshold roll-of. This reverse short channel effect (RSCE) was taken into account by fixed surface charges [10]. Fig. 4 shows the results for the V<sub>th</sub> vs. L<sub>gate</sub>. A difference of about 0.1 V can be observed for the 0.1  $\mu$ PMOS device depending on whether B or BF2 is used for the implantation. The difference is explained by the different amount of damage generated during the implantation. The damage distribution after all implantation steps (S/D implantation performed with BF2) is shown in Fig. 5.

## 4. Conclusions

BF2 implantations in crystalline silicon have been studied and the parameters for BF2 of the stopping power and damage accumulation models have been determined. The influence of the additional damage produced by F on the doping distribution and on the threshold behavior is discussed for a specific device. The simulation of BF2 implantation with the equivalent energy underestimates damage and therefore overestimates channeling.

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