Simulation of Plasma Immersion Ion Implantation

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***Abstract*—Ion implantation profiles of boron after a BF_3 plasma immersion ion implantation in a plasma implanter with a pulsed voltage ion extraction were investigated both experimentally and by means of numerical simulation. Boron profiles for different ion implantation doses in the range 10^{15} to 10^{17} cm^{-2} were measured using the SIMS method. Simulations were performed using a Monte-Carlo based binary-collision approach for ion implantation. A good reproduction of the measured boron profiles was obtained using a double-exponential energetic spectrum of the boron ions.**

Keywords: Plasma immersion, Ion implantation, Simulation

I. INTRODUCTION

Plasma immersion ion implantation (PIII) has several advantageous features which make this method of semiconductor doping important in leading edge semiconductor technology: In PIII much higher mean ion current density can be achieved for low energies than in beam-line implantation, allowing for short processing time and moreover for a significant reduction of the implantation energies. Currently used in semiconductor manufacturing for DRAM polysilicon counter-doping and contact doping, it is also a candidate for conformal doping (FinFET, trench doping) and for ultra-shallow junction formation. In this work, the PULSION plasma doping tool developed by IBS was applied. The tool enables an efficient customer control of the dominant physical phenomena – deposition, implantation, or etching. The PULSION chamber and wafer electrode are shown schematically in Figure 1.

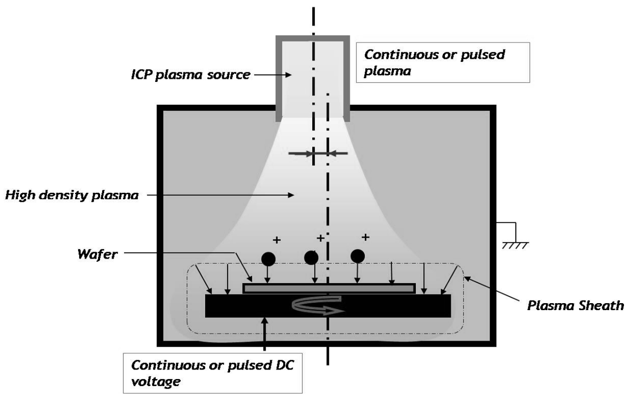

Fig. 1: Schematic illustration of PULSION plasma source and process chamber

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The key features of this tool are a proprietary, remote RF plasma source that enables a high density plasma with low chamber pressure, resulting in a wide process space, and special chamber and wafer electrode designs that optimize doping uniformity and minimize contamination [1]. Positively charged ions are extracted from the plasma by negative voltage pulses. The magnitude of the negative, pulsed dc voltage applied to the wafer electrode can be varied from 30 V to 10 kV. The voltage pulse width is typically varied in the range 1 µs to 100 µs with a rise time of less than 500 ns. For the specific process described here, typical BF_3 decomposition after ion extraction is 90% BF_2^+, 8% BF^+, remainder 2% being mainly composed by B^+ and F^+. Process parameters were optimized in order to limit etching/deposition.

II. SIMULATION APPROACH

Currently, no specialized simulation tools for PIII modeling are available in leading edge commercial TCAD simulation packages. Therefore, trying to fill the gap, we investigate here the possibilities to apply the well established theory of binary inter-atomic collisions [2] for the simulation of PIII. As a starting point we use the Monte-Carlo code MCSIM [3] developed initially for the simulation of conventional ion implantation, sputtering, etc. To adapt the MCSIM code for the simulation of PIII, the program was modified so that instead of a fixed energy and ion beam direction, statistical distributions for the energy and direction of motion of the ions from the plasma were implemented.

Two models for the energy distributions were tested, the Maxwell-Boltzmann distribution [4] and a two-exponent-approximation that describes the energy spectrum of the ions extracted from the plasma as follows:

$$F(E) = Ae^{-aE} + Be^{-bE}, \qquad (1)$$

where E is the energy of boron atoms to be implanted from the plasma, A, B, a, and b are the model parameters. Normalization of the distribution yields the condition $A/a+B/b=1$. This normalization conditions can also be interpreted as the sum of the probabilities A/a and B/b for the boron ions to belong to the energy spectrum represented by the first or by the second term of Eq. (1). Without the loss of generality, we assume that $a > b$. Then a, the larger of the two coefficients, is responsible for the near-surface part of the implantation profile, while the other term is used to describe the tail part of the implantation profile. The second term in (1) is also responsible for the reproduction of the channeling part of the boron profile that can appear at the initial stage of ion implantation, before the silicon amorphization dose is achieved. It should be noted that ion doses in the range of 10^{15} to 10^{17} cm^{-2} considered here during BF3 plasma implantation all exceed the critical dose needed for silicon amorphization. In conventional ion implantation of BF_2 a dose of $1 \cdot 10^{15}$ cm^{-2} already leads to silicon amorphization [5].

Equation (1) for the energetic spectrum of the boron ions simplifies the actual rather complicated physics of the ion extraction from the plasma. From BF3 plasma, different positive ions containing boron, namely BF_2, BF, and B are extracted. For the time being, interactions of different species in BF3 plasma are not well quantified and, therefore, we assume a simplified energetic profile described by Eq. (1). The energy distribution (1) has a peak at zero energy and continuously decreases with energy. Such a distribution with the peak of the energy distribution at zero energy qualitatively corresponds to the results of Linder et al. [6] obtained by means of numerical plasma simulation for the case of pulsed ion extraction.

III. EXPERIMENTAL RESULTS, COMPARISON WITH SIMULATION

In this work, we investigate boron profiles in silicon obtained for the same extraction voltage but for different implantation fluxes. The ion extraction was done using pulses of a negative voltage of 6.5 keV applied to the implantation target. The ion dose in a PIII machine with a periodically pulsed extraction is proportional to the total implantation time, if other parameters of the plasma and of the plasma reactor remain unchanged. Although the silicon target changes significantly on a microscopic scale due to ion implantation, essential properties of the target as a part of the PIII reactor remain unchanged. For low ion implantation doses, a proportionality of doping concentration to the dose is typical. Here, due to higher doses and a very high doping concentration at the surface, deviations from such proportionality can appear.

To check if the boron concentration increases proportional of the implantation dose, we compare the boron profile obtained at lowest implantation flux of $1 \cdot 10^{15}$ cm^{-2} with the profiles obtained at $1 \cdot 10^{16}$ cm^{-2} and $1 \cdot 10^{17}$ cm^{-2}. Boron implantation profiles after PIII were measured using the SIMS method. For a better comparability, we divide the concentration in the $1 \cdot 10^{16}$ cm^{-2} profile by 10 and in the $1 \cdot 10^{17}$ cm^{-2} profile by 100 and overlay the profiles in one figure. If all three profiles normalized in this manner coincide, then the assumption of proportionality to the implantation flux is justified. Figure 1 shows that the normalized profiles do not completely coincide. For the two lower doses of $1 \cdot 10^{15}$ cm^{-2} and $1 \cdot 10^{16}$ cm^{-2} the normalized distributions coincide at smaller depths below 15 nm, but differ at larger depths. For the highest implantation dose of $1 \cdot 10^{17}$ cm^{-2}, the maximum of the profile near the surface is wider and lower in comparison to lower doses. These deviations from the proportionality to the dose can be explained by three physical effects: swelling, sputtering and ion beam mixing. The simulation approach presented in Section II takes into account all these effects in terms of the theory of binary atomic collisions. To account for the swelling, sputtering and ion beam mixing, not only the trajectories of the primary ions have to be simulated, but also the movement of the recoils in the target including the recoils of implanted impurities.

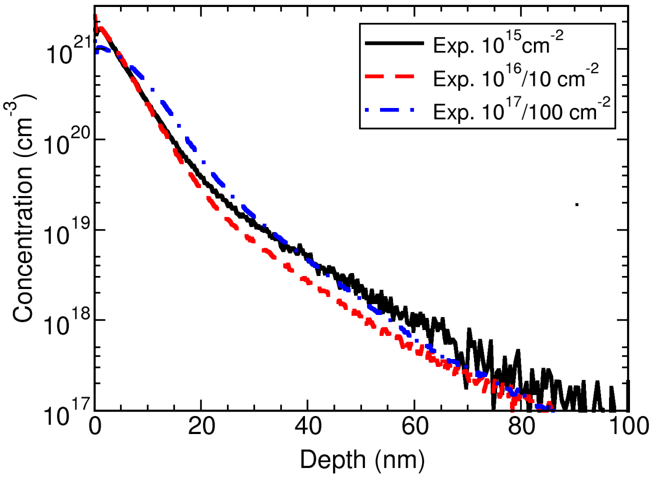

Fig. 2: BF3 plasma implantation: Comparison of the boron profiles measured for three different doses but normalized for a dose of $1 \cdot 10^{15}$ cm^{-2}

In Figure 2, the Maxwell-Boltzmann energy distribution with a mean energy of boron atoms of 6.5 keV in a combination with a uniform angular distribution was used. Such distribution is typical for high temperature plasmas. However, for the plasma implantation conditions used here, agreement is limited.

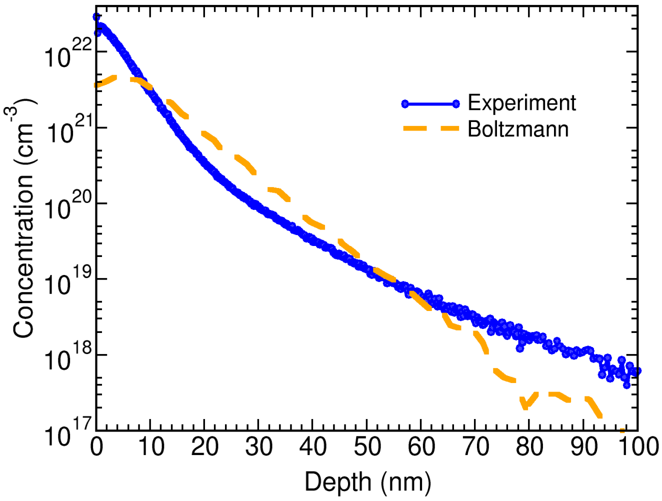

Fig. 3: BF3 plasma implantation: Comparison of simulation assuming a Maxwell-Boltzmann energy distribution for boron ions (dashed line) and measurement (continous line) for a dose of $1 \cdot 10^{16}$ cm^{-2}

The measured PIII profile has a much higher maximum and the location of the maximum is much closer to the surface in comparison to the result of the simulation based on the Maxwell-Boltzmann distribution of the boron ions. This means that the energetic spectrum of the boron ions from a

PIII machine differs essentially from the Boltzmann distribution and that this model is not adequate for our goal.

Finally, the results with the energy distribution described by Eq. (1) are compared with the measurements performed at different PIII doses. The parameters of the energetic distribution (1) were first fitted to reproduce the boron implantation profile at the lowest implantation dose of $1\bullet10^{15}$ cm^{-2}. Simulations using the Monte-Carlo based program MCSIM show that at this low dose the effects of ion beam induced swelling, sputtering and ion beam mixing can be neglected. Therefore, the shape of the implantation profile is in the first line determined by the energetic distribution of the boron ions bombarding the silicon surface. The coefficients *a* and *b* determine the slope of the concentration profile in logarithmic scale. The coefficients were chosen so that *a* was responsible for the profile slope at depths below 20 nm and the coefficient *b* for the slope at larger depths.

Further, the value of *A/a* regulates the relative height of the profiles at small depths and the value of *B/b* determines the profile height at larger depths. The higher is the corresponding value of *A/a* or *B/b* the higher is the boron concentration at smaller depths or at larger depths, respectively. The result of the parameter fitting for the energetic spectrum of the boron ions obtained from the comparison with the boron profile at the lowest implantation dose of $1\bullet10^{15}$ cm^{-2} is shown in Table I.

TABLE I. PARAMETERS OF THE ENERGY DISTRIBUTION OF BORON IONS PRESENTED BY EQUATION (1)

Parameter	*a*	*b*	*A/a*	*B/b*
Normal	$1.8/E_0$	$0.45/E_0$	0.88	0.12
Uniform	$2.0/E_0$	$0.5/E_0$	0.85	0.15

E_0 in the table means the energy of a boron atom which results from an acceleration of the single charged BF_3 ion by a voltage equal to the amplitude of the extraction voltage pulse. The model parameter extraction was done for two limiting cases of the angular distributions of boron ions: for the fixed implantation direction normal to the sample surface (table row marked *Normal*) and for a three-dimensionally uniform distribution of the directions of ion implantation (table row marked *Uniform*). Both model variants well reproduce the measured profiles at the lowest implantation dose of $1\bullet10^{15}$ cm^{-2}. Figures 4 and 7 show the comparison of the simulated and measured boron profiles obtained using the model parameters from Table I for the cases of a normal ion impact and for a uniform angular distribution, respectively. In both cases, approximation (1) with parameters presented in Table I shows a good agreement to the experimental results. On the other hand, if we assume a normal impact of the ions, the simulation predicts a slightly lower surface concentration at the dose of $1\bullet10^{16}$ cm^{-2} as shown in Figure 5 and too much profile widening at the dose of $1\bullet10^{17}$ cm^{-2}, Figure 6. This indicates that the effect of ion beam mixing is too strong in the simulation, if a normal ion impact is assumed.

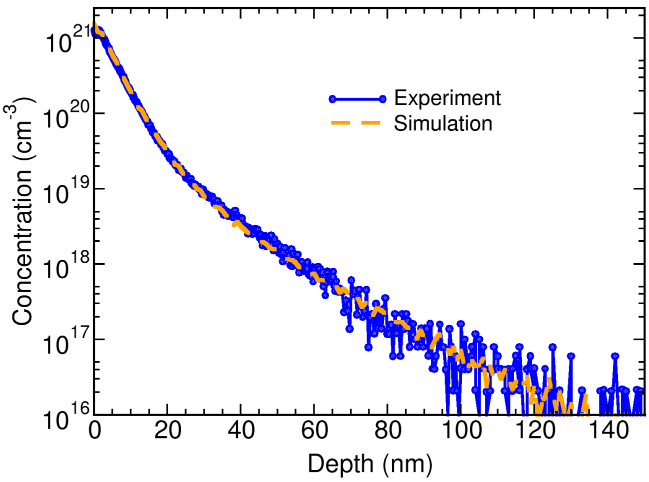

Fig. 4: BF3 plasma implantation: Comparison of simulation assuming the normal impact of boron ions and energy distribution of Eq. (1) (dashed line) and measurement (continuous line) for a dose of $1\cdot10^{15}$ cm^{-2}

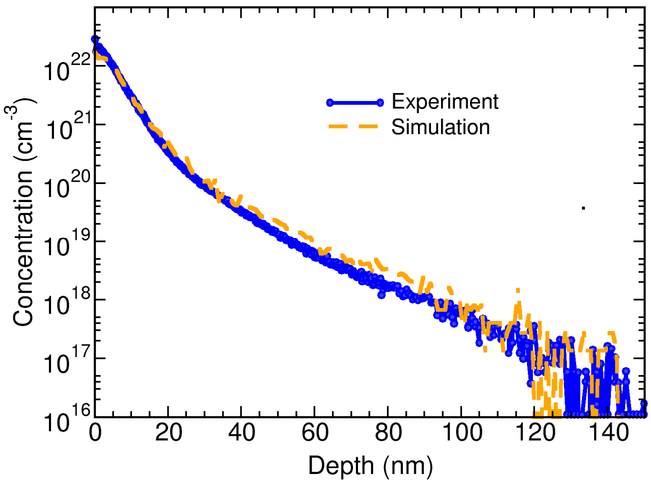

Fig. 5: The same as Fig. 4, but for a dose of $1\cdot10^{16}$ cm^{-2}

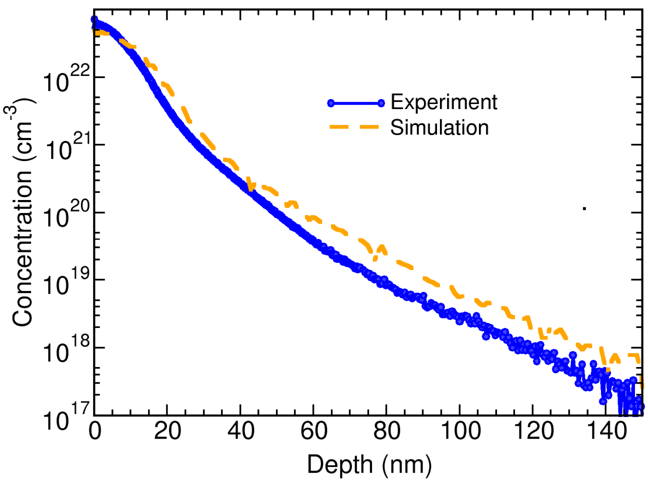

Fig. 6: The same as Fig. 4, but for a dose of $1\cdot10^{17}$ cm^{-2}

A very good agreement of the simulation results with the measurements for all doses considered, as shown in Figures 7 to 9, was achieved if a uniform angular distribution for boron atoms was assumed in the simulations. In this case, the simulation predicts properly the dynamics of the widening of the boron profile with increasing implantation dose. Possible physical reasons for a wide angular distribution of the boron atoms could be inter-atomic collisions in the plasma, which should not be the predominant phenomenon for the plasma condition used in this experiment, as well as interactions between the boron and fluorine atoms during the dissociation of BF_2^+ ions at the target surface.

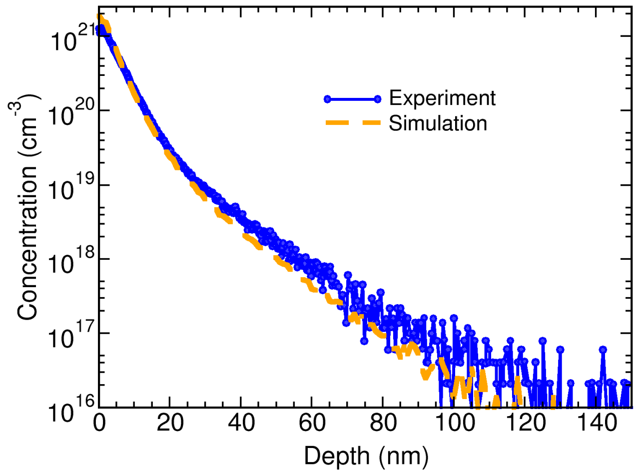

Fig. 7: BF3 plasma implantation: Comparison of simulation assuming the uniform angular distribution and energy distribution of Eq. (1) for boron ions (dashed line) and measurement (continous line) for a dose of $1\cdot10^{15}$ cm^{-2}

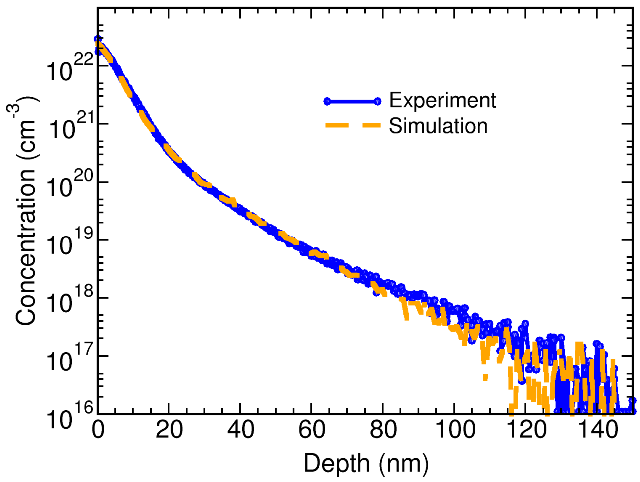

Fig. 8: The same as in Fig. 7, but for a dose of $1\cdot10^{16}$ cm^{-2}

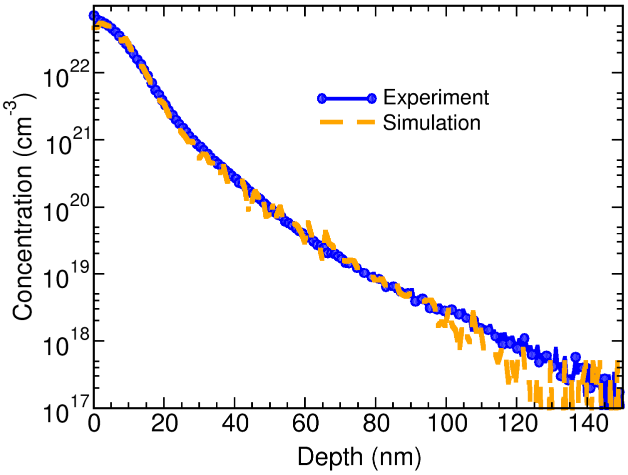

Fig. 9: The same as in Fig. 7, but for an implantation dose of $1\bullet10^{17}$ cm^{2}

IV. Conclusion

This paper shows that the use of a Monte-Carlo code based on the binary collision theory with a proper choice of the angular and energetic distribution of the bombarding ions allows to correctly describe the evolution of the implantation profiles with the increasing dose during plasma ion implantation.

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