Simulation of BF₃ Plasma Immersion Ion Implantation into Silicon

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Abstract. Plasma immersion ion implantation from a BF₃ plasma into crystalline (100) silicon was performed using the PULSION plasma doping tool. Implanted boron profiles were measured with the SIMS method and simulated using models with different levels of sophistication. The physical implantation model is based on an analytical energy distribution for ions from the plasma and uses a Monte-Carlo simulation code. An analytical model of plasma immersion ion implantation that assumes a uniform and isotropic implantation was implemented in a software module called IMP3D. The functionality of this module which was initially envisaged for the three-dimensional simulation of conventional ion implantation was extended to plasma immersion ion implantation and examples of 2D and 3D simulations from this are presented.

Keywords: Plasma immersion ion implantation; BF₃; Silicon; Simulation.
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INTRODUCTION

Plasma immersion ion implantation (PIII) has several advantages which make this method of semiconductor doping important for leading-edge semiconductor technology. In this work, the PULSION plasma doping tool developed by Ion Beam Services was applied to investigate PIII and based on the results of experimental investigations different models for numerical simulation of PIII were tested. Conventional software tools for process simulation have only a limited suitability to the simulation of PIII, because the physical effects and parameters that determine the final doping profiles after plasma implantation are not captured by the models implemented. In this work, we began by performing a PIII of boron into crystalline (100) silicon from a BF₃ plasma using different extraction voltages. Next we measured the resulting implantation profiles of boron, then we tried to characterize the main parameters that are relevant for the doping profiles, and after that we simulated the observed plasma implanted boron profiles using models with different levels of sophistication. First, we considered a physically motivated model that is based on an assumption of a certain energetic distribution of the extracted ions. This plasma specific energy distribution, applied for separate ion species of BF₃ plasma, was then used in the Monte-Carlo simulation code that is implemented in the Sentaurus Process simulator of Synopsys [1]. Although the Monte-Carlo approach requires long simulation times if applied for complicated two or three-dimensional (2D and 3D) device structures, it nevertheless allows relatively fast calculations, if only one-dimensional ion implantation profiles have to be calculated. Further we show that the suggested physical model is able to properly describe the dependence of the boron doping profiles after PIII from a BF₃ plasma on extraction voltage. In case of complicated non-planar 2D and 3D device structures, efficient analytical PIII models are needed. In Section 4 of this paper we consider an analytical model and show the results of analytical simulations using an implementation in the Fraunhofer proprietary version of the IMP3D software module for 3D simulation of ion implantation.

PHYSICAL MODEL

The energetic distribution of different molecular and atomic ions after extraction from the plasma is known to cover the range from zero to the maximum energy $E_{\text{max}}$ which is equal to the product of the ion charge times the extraction voltage. In this work, we use the analytical model for the energy distribution of Tian et al. [2] based on the analysis of the plasma behavior at the onset of the extraction pulses. The energy distribution presented by Tian et al. as an integral number of particles having their energy in a given interval can be rewritten in a differential form as follows:
The energy distribution $f(E)$ presented by Eq. (1) is normalized, i.e. the integral over all possible energies of the extracted ions ranging from 0 to $E_{\text{max}}$ is equal to one. The implantation direction of the ions perpendicular to the silicon surface was used in Monte-Carlo simulations. Assuming the energy distribution described by Eq. (1) for the extracted ions of different masses, the implantation velocity of the boron species is the lower the higher the mass of the molecular ion is. Therefore, different boron implantation profiles result for different ions. This is shown in Figure 1, where boron profiles simulated separately for singly charged ions of BF$_3^+$, BF$_2^+$, BF$^+$, and B$^+$ are presented.

![Figure 1](image_url)

**FIGURE 1.** Boron implantation profiles from single ionized ions of BF$_3^+$, BF$_2^+$, BF$^+$, and B$^+$ for extraction voltages of 1 keV (a) and 4 keV (b).

These profiles were calculated for each ion type extracted from BF$_3$ plasma for an implantation dose of 1×10$^{15}$ cm$^{-2}$ and the energies up to $E_{\text{max}}$ used in Eq. (1). The profiles exhibit a maximum near the surface and channeling tails with different penetration depths. The shallowest boron profile is observed for the heaviest ions, BF$_3$, and the lighter the ion containing boron is, the deeper the boron penetration. The deepest boron penetration is seen for the B$^+$ ions.

At larger depths, more than 50 nm for an extraction voltage of 1 keV and more than 170 nm at an extraction voltage of 4 keV, implantation of pure boron ions dominate in the doping profile. Generally, the higher the extraction voltage, the deeper the implantation profiles are for all ions considered. The final profile of boron doping is formed as a mixture of separate contributions from different ion types. Hereby we assume that the composition of the plasma, in a first approximation, is independent of the extraction voltage. This assumption is increasingly valid with decreasing duration of the extraction pulse and with longer durations of time without voltage for plasma relaxation.

**BORON DEPTH PROFILES**

For the simulation of boron doping profiles at different extraction voltages we have to make certain assumptions about the abundance of different ion types extracted from the plasma. Assuming that the final boron doping profile is a weighted sum of the profiles for separate ion species, we performed an optimization of the weights for different ion types to obtain a good agreement with the measured profiles. It appeared that the assumption about the independence of the abundance of the separate ion species on the extraction voltage is a good approximation. The result of the ion abundance optimization is presented in Table 1.

**TABLE 1.** Relative abundance of different ions extracted from BF$_3$ plasma.

<table>
<thead>
<tr>
<th>Ion</th>
<th>Abundance(%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>BF$_3^+$</td>
<td>0</td>
</tr>
<tr>
<td>BF$_2^+$</td>
<td>50</td>
</tr>
<tr>
<td>BF$^+$</td>
<td>40</td>
</tr>
<tr>
<td>B$^+$</td>
<td>10</td>
</tr>
</tbody>
</table>

The values of the abundance for different ions influence the final profile differently. For example, profiles at larger depths are dominated by the B$^+$ ions of atomic boron. The shape of the profile at medium depths is formed by the contributions from BF$_2^+$ and BF$^+$. Since the fraction of BF$_3^+$ was not observed in a significant amount in plasma immersion implantation with similar conditions [3], we neglect the contribution from BF$_3^+$ ions.

The simulation of the final boron implantation profiles used a fixed relative abundance of BF$_3^+$, BF$_2^+$, BF$^+$, and B$^+$ as shown in Table 1. These are shown in Figures 2 and 3 alongside the experimental results with a boron implantation dose of 1×10$^{15}$ cm$^{-2}$ for comparison. Silicon amorphization was also accounted for. An amorphization is certainly expected during the
BF$_3$ plasma implantation because of the large atomic mass of the fluorine atoms present in positive ions containing both boron and fluorine.

A thicker amorphization layer in silicon is expected for higher extraction voltages. Amorphization depths of 3, 5, and 8 nm were assumed in the simulations for extraction voltages of 1, 2, and 4 keV, respectively. The thickness of the amorphous layer in the simulations corresponded to a depth at which the concentration of the implanted boron reaches a concentration of about $3 \times 10^{20}$ cm$^{-3}$. Accounting for amorphization leads to somewhat shallower profiles due to more ions scattering in this amorphous layer than would otherwise in crystalline silicon.

The good agreement of the simulation results with the measurements for all three values of the extraction voltage shown in Figure 2 supports both the physical assumptions of the simulation model about the independence of the ion species abundance on extraction energy and the necessity to account for an amorphous layer in silicon at boron implantation doses of $10^{15}$ cm$^{-2}$ and higher. The suggested model allows for the prediction of the implantation profiles after PIII doping for different extraction voltages.

2D AND 3D SIMULATION OF PLASMA IMMERSION ION IMPLANTATION

Although the physically based Monte-Carlo simulation model presented in the previous section is well suited to describe one-dimensional doping profiles after plasma immersion ion implantation, its application to more complicated non-planar device structures is not straightforward. There are two problems that have to be solved. The first problem is that only constant angular distributions of the ions can be defined in the input for Sentaurus Process; however, the direction of ion impact during plasma immersion implantation into non-planar structures is not constant but is dependent on the topography of the implanted surface. The second problem is that the simulation time of the Monte-Carlo method grows proportionally to the area of the simulated structure and the simulation time becomes prohibitive if real device structures have to be simulated. Therefore, analytical simulation methods, similar to those used for the simulation of conventional ion implantation, are attractive for practical applications.

For the analytical simulation of plasma implantation, we modified the IMP3D software module that was initially envisaged for the simulation of conventional ion implantation to account for peculiarities of plasma implanted doping distributions. The modifications of IMP3D for plasma immersion implantation included implementation of the following criteria: 1) the source of the ions to be implanted is uniformly distributed over the sample surface that is in contact to the plasma; 2) ions are implanted in direction of the local normal to the exposed sample surface; 3) at the corners, where the direction normal to the surface is not defined, the implantation direction is taken along the direction of the closest distance between the grid point in question and the exposed surface. The accurate implantation depth profile which is needed for the analytical modeling in IMP3D was

**FIGURE 2.** Boron implantation profile from BF$_3$ plasma immersion ion implantation for extraction voltage of 1 keV (a), 2 keV (b) and 4 keV (c)
first calculated in advance using the Monte-Carlo-based model and then approximated by a Pearson type distribution.

One of the attractive technological capabilities of the plasma immersion ion implantation is the possibility to perform a uniform near-surface doping of the fine-structured device features such as the fins of FinFET transistors. As recently shown experimentally [4], the method of PIII is able to uniformly dope near-surface layers of silicon also in strongly non-planar nano-structured samples.

**FIGURE 3.** Boron distribution simulated analytically for BF3 plasma immersion ion implantation into a non-planar structure for an extraction voltage of 1 keV and a dose of $1 \times 10^{15}$ cm$^{-2}$.

Figure 3 shows an example of the simulation of a boron doping distribution near the silicon surface after BF$_3$ plasma immersion ion implantation into a test structure that is similar to the one presented in Ref. 4. The lateral pitch size of this silicon structure is 127 nm, the height of the fin-like structures is 180 nm. The analytical simulation exhibits a uniform thickness of the boron-doped area which is independent of the surface orientation and of the shadowing. This simulation result is in a good qualitative agreement with the measurement results of Ref. 4.

After an analytical model for plasma implantation was implemented in IMP3D, implantation into any device structure can be efficiently simulated. Figure 4 presents an example of the analytical 3D simulation of the BF$_3$ plasma immersion source/drain implantation into a FinFET transistor with a gate length of 25 nm. The active area of this transistor in the shape of a silicon fin has a height of 25 nm and a width of 6.25 nm. The BF$_3$ implantation was performed at an extraction voltage of 1 keV and with a dose of $1 \times 10^{14}$ cm$^{-2}$. For the best visibility of the shallow doping distribution inside the active area, the transistor in the Figure 4 was cut by a vertical plane through the middle of the active area along source/drain direction and only a part of the FinFET transistor is visualized in Figure 4.

**FIGURE 4.** 3D boron distribution in a FinFET device structure after BF3 plasma immersion ion implantation

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**REFERENCES**