Simulation of Plasma Immersion Ion Implantation into Silicon

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***Abstract*—A numerically efficient model for the simulation of ion implantation doping profiles in silicon after pulsed plasma immersion ion implantation is suggested. The model is based on an analytical formula for the energy distribution of the ions extracted from the plasma and on the application of this energy distribution in a Monte-Carlo simulator for conventional ion implantation. The model is verified using examples of BF_3 and AsH_3 plasmas for p-type and n-type doping in silicon, respectively.**

***Keywords*—plasma immersion ion implantation; BF_3 plasma; AsH_3 plasma; silicon**

I. INTRODUCTION

Plasma immersion ion implantation (PIII) has several advantageous features which make this method of semiconductor doping important for leading-edge semiconductor technology. An important advantage of PIII is its high productivity that reduces the implantation times from hours in conventional ion implantation setups to minutes or seconds in PIII. For a wide technological application of this doping method in semiconductor manufacturing reliable and numerically efficient simulation models of PIII are needed. The formulation of the universal models for PIII meets large challenges because of the diversity of the possible implementations of PIII tools and of plasma generation and extraction conditions. In this work, we show that the PIII model suggested in our previous work [1] is well applicable for the simulation of ion implantation profiles in silicon after PIII from different plasmas. BF_3 and AsH_3 plasmas are taken as examples to demonstrate the applicability of the same simulation model for both dopant types: BF_3 plasma for p-type and AsH_3 plasma for n-type silicon dopants.

II. EXPERIMENT

The experimental part of the work was performed using the PULSION® plasma doping tool developed by IBS [2] for PIII. In the PULSION® plasma implantation tool positively charged ions are extracted from the plasma by negative voltage pulses. In this work, we performed PIII into crystalline (100) silicon from BF_3 and from AsH_3 plasmas using different values of the extraction voltages in the range between 1 and 5 kV. The resulting doping profiles were characterized using high depth resolution SIMS (secondary ion mass spectrometry). The SIMS measurements were performed at Evans Analytical Group.

III. SIMULATION APPROACH

The energetic distribution of different molecular and atomic ions after extraction from the plasma is known to cover a range from a minimum energy E_{min} determined by the plasma potential and usually neglected as being below 100 eV to a maximum energy E_{max} which is equal to the product of ion charge times the maximum extraction voltage. The doping profiles in silicon after PIII from BF_3 and AsH_3 plasma were calculated in this work using the Monte-Carlo ion implantation module of the Sentaurus Process [3] simulator employing the plasma ion implantation model [1] and with the following formula for the energy distribution of the ions:

$$f(E) = \frac{5}{6(E_{\max}^{5/6} - E_{\min}^{5/6})} E^{-1/6}, E_{\min} < E < E_{\max} \qquad (1)$$

The energy distribution (1) follows from the theory of collisionless plasma [4], contains no fitting parameters, and is used as the initial energy distribution of the ions bombarding the target surface. Summarizing, the PIII model suggested consists of two components, the model for the energy distribution of the ions extracted from the plasma and comprised by (1) and the numerical simulation model that is responsible for the description of the doping profiles at each given ion energy. As the second component of the PIII model any numerical model that adequately describes the ion implantation profiles at any fixed ion energy is suitable. In this work, we used the Monte-Carlo ion implantation module of the Sentaurus Process simulator for the purpose of simulation of ion penetration for a given ion energy. There is a special user interface in this Monte-Carlo simulator to specify the user defined energy and angular distributions.

The trajectories of the ions inside the silicon target were simulated accounting for the channeling effect in crystalline silicon. Although all ions have the same universal energy distributions in the model suggested, each kind of ion hitting the target surface has a different velocity because of different ion masses. For example, the atomic masses of the ions BF_3^+, BF_2^+, BF^+, and B+ in the BF_3 plasma differ significantly and the resulting projected ranges of these ions in silicon differ as well. Fig. 1 illustrates this situation. Doping profiles for different ions resulted from the same energy distribution (1) for ions of different masses extracted from a BF_3 plasma are visualized here.

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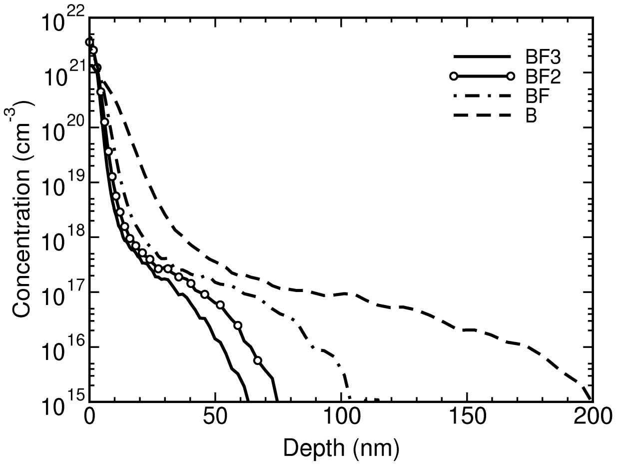

Fig. 1. Boron implantation profiles from single ionized ions of BF_3^+, BF_2^+, BF^+, and B^+ for extraction voltage of 2 keV.

The boron ion B^+ exhibits the largest penetration range because of its lowest mass. Further, the heavier the ion is, the shorter is its penetration into the silicon crystal. If there is a mix of different ions in the plasma, ions of different mass contribute to different depths in the resulting doping profile. The deeper part of the doping profile is only reached by the boron ions B^+. The fact that different ions contribute to different depths allows us to reproduce the experimentally observed doping profiles by a proper choice of the plasma composition in the model.

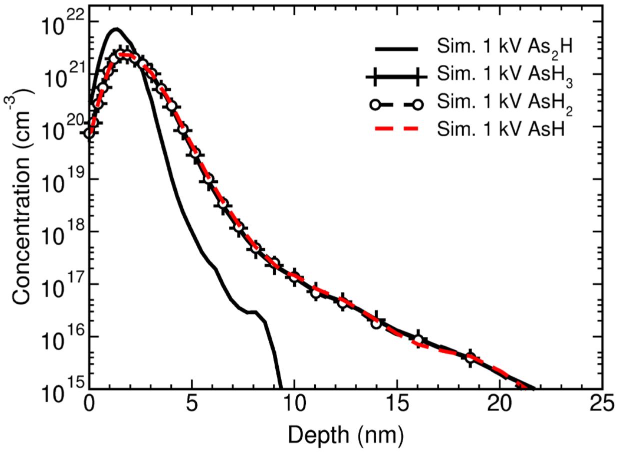

Fig. 2. Arsenic implantation profiles from single ionized ions of AsH_x^+ and $As_2H_x^+$ for extraction voltage of 1 keV.

In the case of a AsH_3 plasma, less ion types have to be considered. This is illustrated in Fig 2. Because of the small mass of the H atom in comparison to As in an AsH_3 plasma the ions containing one As atom, As+, AsH^+, AsH_2^+ and AsH_3^+, all have very similar projected ranges after ion implantation at the same energy. Therefore we have to distinguish only two ion fractions, first of type AsH_x^+ and second of type $As_2H_x^+$, the latter one having a significantly smaller mean penetration depth into silicon when implanted with the same energy.

Although the energy distribution of the ions extracted from the plasma has a universal character, the relative abundance of different ion fractions is a property that depends on the conditions of plasma excitation and ion extraction. Since different fractions of the ions that show up in the model contribute to the implantation profiles of dopants at significantly different depths, the results of the extraction of the relative abundance of separate ion fractions by the variation of the abundance and minimization of the deviation between the measurement of the doping profiles and the simulation is well reproducible.

Moreover, after considering doping profiles obtained for different extraction voltages we found that the abundance of the ions extracted from BF_3 and AsH_3 plasma remained about constant for the investigated range of extraction voltages. Therefore, we optimized the relative abundances of the ions used in the simulation model for the PULSION® plasma implantation tool so as to obtain best reproduction of the doping profiles without changing the ion abundance with the extraction voltage. The results of such optimization of the model parameters are presented in Tables I and II below.

TABLE I. EXTRACTION PROBABILITIES OF DIFFERENT ION SPECIES FROM BF_3 PLASMA

Ion species	**B**	***BF***	***BF₂***	***BF₃***
Probability, %	5	15	80	0

The lightest ions of atomic boron, contributing more than other ions at larger depths, are present in a fraction of 5%. Since the experimental profiles in the tail part are more prone to statistical fluctuations, the accuracy of the extraction of this parameter may be influenced by these fluctuations. On the other hand side, also at smaller depths the shape of the doping profile for boron ions differs from the profiles typical for heavier ions containing both boron and fluorine atoms (Fig. 1). Specifically, the slopes of the doping profiles at depths between 10 and 50 nm is specific for each of the ion species, changing from shallow sharp falling profile for BF_3^+ to each time smoother profiles for BF_2^+, BF^+, and B^+. Therefore the final doping profile in the simulation of PIII at these depths becomes smoother if more light ions are present among the extracted species. The high contribution of BF_2^+ ions resulted from the shape of the experimentally measured profiles at small depths below 20 nm.

TABLE II. EXTRACTION PROBABILITIES OF DIFFERENT ION SPECIES FROM AsH_3 PLASMA

Ion species	***AsHₓ***	***As₂Hₓ***
Probability, %	10	90

Arsenic profiles from AsH_3 plasma could be reproduced well assuming constant extraction probabilities of 10% for ions with one arsenic atom and 90% for the ions with two arsenic atoms. Because the profiles for the ions that differ only in the number of hydrogen atoms are about identical (Fig. 2) we cannot identify the value of the index *x* in the ions of type AsH_x^+ and $As_2H_x^+$.

IV. Comparison of Simulations with Measurements

Figs. 3 and 4 demonstrate the ability of the universal simulation model to well reproduce the experimentally measured doping profiles for boron and arsenic ions for varying plasma extraction voltages. Fig. 3 shows the boron depth profiles in silicon after plasma immersion ion implantation into crystalline silicon.

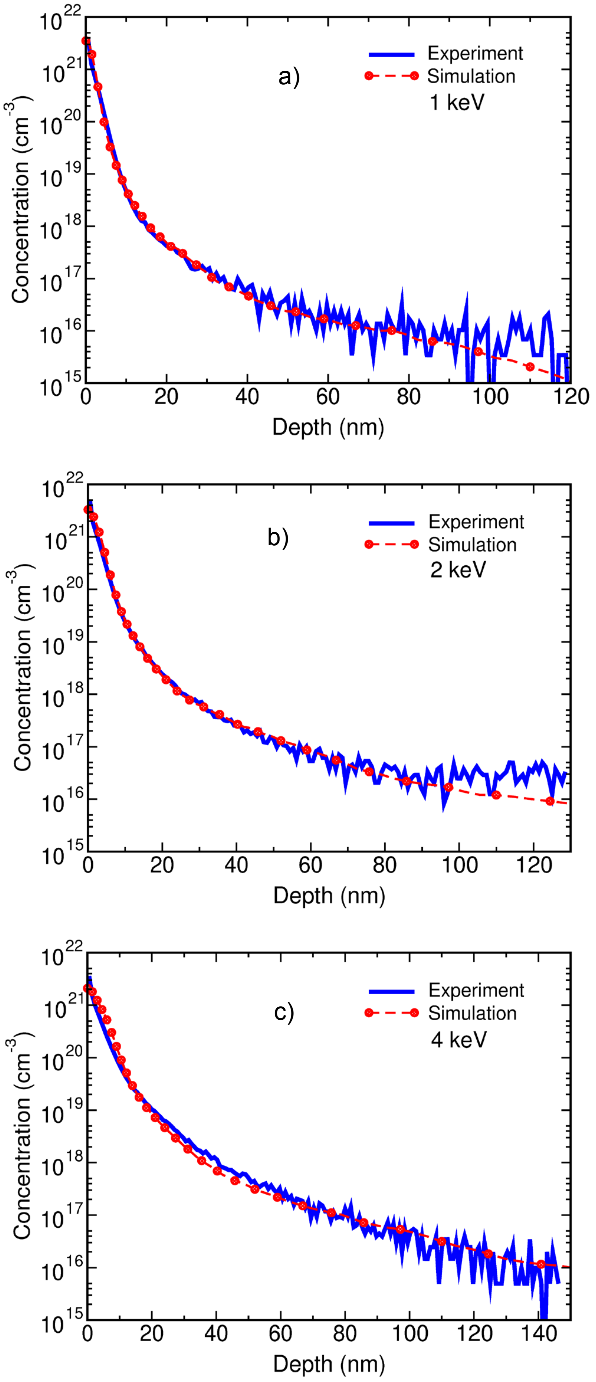

Fig. 3. Boron implantation profiles from BF_3 plasma immersion ion implantation into silicon for an implantation dose of 1×10^{15} cm^{-2} and a maximum extraction voltage of 1 keV (a), 2 keV (b) and 4 keV (c).

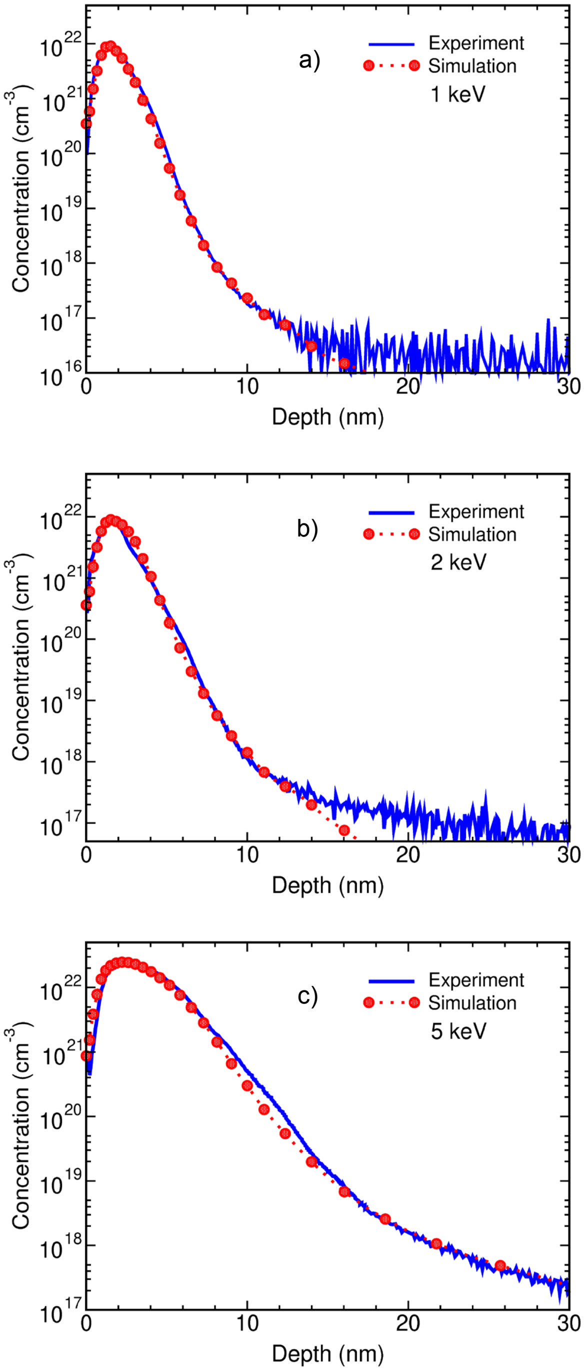

Fig. 4. Arsenic implantation profiles in silicon from AsH_3 plasma with a maximum extraction voltage of 1 kV (a) and 2 kV (b) for an implantation dose of 5×10^{14} cm^{-2}, and for 5 kV and an implantation dose of 5×10^{15} cm^{-2} (c).

The maximum concentration in the experimental boron doping profiles is at the surface. In the simulation, the maximum concentration is also at the surface, if the minimum energy of the ions extracted from plasma is assumed to be zero, E_{min}=0 in (1). A small difference in the shape of the doping profile in the first nanometers of depths can be explained due to the ion beam mixing effect during the SIMS analysis. The ion beam mixing leads to a surface peak of the boron signal in the SIMS profiles.

Depth profiles of arsenic ions from AsH_3 plasma implantation (Fig. 4) differ from the boron profiles. The maximum of the profiles is not at the surface but at a depth of about 1.3 to 2 nm. In all measurement, a distinct depletion of arsenic concentration towards the surface is observed. This depletion amounts to about a factor of 1/50 from the maximum. To reproduce the effect of depletion towards the surface in the simulation, we introduced a minimum energy E_{min} in (1). The higher is E_{min}, the stronger is the surface depletion of arsenic. A value of 0.1 keV for E_{min} was sufficient to explain the surface depletion as observed in the measurements.

The accuracy of the simulated doping profiles depends on the accuracy of the basic algorithm of the Monte-Carlo simulation program. It should be noted that the accuracy of the basic Monte-Carlo algorithm for simulation of ion implantation in Sentaurus Process is confirmed by many years of its exploitation in industry and research. Also the channeling effect plays an important role in the formation of the shape of the doping profiles in crystalline silicon, therefore a good calibration of the Monte-Carlo code at low ion energies is a prerequisite for an adequate description of the plasma immersion ion implantation. In this work, we used the default stopping power models of [3] for arsenic atoms moving in silicon but we modified the stopping power model for boron ions.

For boron, the default model of electronic stopping contains two contributions, the local and the nonlocal contribution. The local stopping power [5] is due to a direct interaction of the moving ion with the non-uniformly distributed electrons in the channels of the silicon crystal. The non-local electronic stopping contribution is due to plasmonic excitations which are not localized and therefore this contribution does not depend on the position of the ion trajectory in the channel. Such kind of electronic excitations are only possible for swift ions and should be neglected for low energetic ions of boron as in the situation considered here. Therefore, we set the parameter *nloc.pre=0* for the electronic stopping power of boron. Such a choice of the stopping power parameters enlarges the maximum range of channeled boron ions and improves the agreement of the simulations with measurements of boron profiles.

The model of damage accumulation for BF_3 plasma implantation was also modified so as to reproduce the ion scattering effect on the amorphous layer which is built during the PIII from BF_3 plasma [6]. The following parameters responsible for damage accumulation were used for boron and fluorine: *amor.par=3.0, surv.rat=1.0.* The damage generation rate and damage accumulation in silicon irradiated by boron and fluourine ions is higher when using these parameters in comparison to the default damage accumulation model of Sentaurus Process. In the BF_3 plasma, most damage comes from fluorine ions which are heavier than boron ions and so contribute more to damage generation in silicon. In AsH_3 plasma, arsenic atoms, having a larger mass, create enough damage to produce an amorphous layer in crystalline silicon at doses of implantation considered. The default model of damage accumulation for arsenic ions was used in these simulations. The presence of an amorphous layer on the surface of crystalline silicon reduces the probability of channeling and leads to a relative reduction of the channeling tail part of the profiles.

V. CONCLUSION

A model for the simulation of plasma immersion ion implantation [1] was calibrated and evaluated in this work for two plasmas, BF_3 and AsH_3. The model is based on a universal energy distribution of the ions that follows from the general theory of the collisionless plasma. This universal energy distribution was introduced into the Monte-Carlo module for ion implantation of the commercially available Sentaurus Process simulator. The probabilities for ions of different mass to be extracted from the plasma are treated as free parameters in the model. These probabilities depend on the properties of the plasma setup, the manner of plasma excitation, plasma density, dimension of the plasma chamber etc. In this work, we determined the probabilities of ion extraction for the plasma immersion implantation tool PULSION® of the company IBS. The quantification of the ion extraction probabilities was performed by fitting these model parameters so as to reproduce the shape of experimentally measured doping profiles after plasma immersion ion implantation at different extraction voltages. An assumption of the extraction probability that is independent of extraction voltage is an acceptable approximation for the simulation model in the range of the extraction voltages between 1 and 5 keV. The model describes well the evolution of the doping profiles with varying extraction voltages even if a constant extraction probability for the ions for a certain plasma type is assumed in the model.

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