THREE-DIMENSIONAL MONTE-CARLO ION IMPLANTATION SIMULATION FOR MOLECULAR IONS

A. Hössinger[a], S. Selberherr[a], M. Kimura[b], I. Nomachi[c] and S. Kusanagi[c]

[a]Institute for Microelectronics, TU Vienna
Gusshausstrasse 27–29, A-1040 Vienna, Austria
[b]Advanced Devices Dept., ULSI R&D Laboratories
Semiconductor Company, Sony Corporation
4-14-1, Asahi-cho, Atsugi-shi, Kanagawa-ken, 243, Japan
[c]Center for Materials Analysis, Research Center, Sony Corporation
134 Godo-cho, Hodogaya-ku, Yokohama-shi
Kanagawa-ken, 240-0005 Japan

In modern semiconductor process technology Boron introduced by ion implantation is widely used to create p-type doped regions. BF_2 ions are preferred to Boron ions for the formation of shallow doping profiles because of their improved channeling behavior. We present a Monte-Carlo method that allows a rigorous simulation of the implantation of BF_2 ions into three-dimensional device structures. This molecular method calculates not only the distribution of the Boron atoms but also the distribution of the Fluorine atoms. Besides it can not only be applied to BF_2 ions but to arbitrary ionized molecules or atom clusters as long as their binding energy is significantly lower than the ion energy. The accuracy of the simulation results is evaluated by comparing the simulated Boron and Fluorine doping profiles with SIMS measurements. Finally the simulation results of a threshold voltage adjust implantation with BF_2 ions into a three dimensional MOS-transistor structure are shown.

INTRODUCTION

One of the key processes in the production of semiconductor devices is the formation of doped regions within the silicon substrate. Thereby ion implantation is commonly used to introduce doping atoms into the device structure because of its high controllability. Subsequent high temperature process steps often only repair the induced crystal defects while they barely redistribute the doping atoms. The distribution of the doping atoms in the final device is therefore mainly determined by the ion implantation step, and effects like channeling, which are caused by the anisotropy of the crystalline substrate, or effects resulting from non planar surfaces, can significantly influence the device behavior. Due to this reason analytical methods

which are often used to simulate an ion implantation process do not suffice to make a predictive process simulation. The alternative are Monte-Carlo methods which are able to overcome the problem of describing anisotropy and non planarity effects with the drawback of an increased computation time, which is especially a problem for three-dimensional simulations. The small device dimensions that are used in modern semiconductor technology require the application of three-dimensional process simulation, because severals effects have been brought to light that can not be reproduced by one-dimensional or two-dimensional simulations.

The most frequently used atoms for doping semi-conducting materials are Boron, Phosphorus and Arsenic. The implantation of these ion species has to be handled by an ion implantation simulator, but not single atomic ions only are used to introduce the dopants. For instance, BF_2 ions are often preferred to Boron ions to create shallow p-type doped areas. The doping profiles generated by BF_2 implantation are much shallower for comparable implantation energies, due to the higher mass of the BF_2 molecule. Thereby a reduction of the implantation time and of the production time is achieved. The disadvantage of using BF_2 ions is that not only Boron but also Fluorine atoms are brought into the device. These Fluorine atoms may influence the diffusion behavior of the dopants and the resulting electrical characteristics of the device.

Normally Monte-Carlo ion implantation simulators just consider the Boron ions when simulating the implantation of BF_2 ions. The molecule is treated in a way that the energy of the Boron ions is rescaled according to the mass ratio of the Boron atom and the BF_2 molecule.

We have introduced a new molecular method to our Monte-Carlo Ion Implantation simulator MCIMPL to rigorously simulate the implantation of arbitrary ionized molecules or atom clusters. The distributions of all species in the molecule are calculated as it will be demonstrated in the case of BF_2 ions.

THE SIMULATOR

The Monte-Carlo ion implantation simulator MCIMPL is a multi-dimensional simulator that is based on a binary collision algorithm (1),(2). This means that the interaction of an implanted particle with atoms and electrons of the target is continuously calculated when it moves through material, until it comes to rest. The simulator can handle arbitrary one-dimensional, two-dimensional and three-dimensional device structures consisting of several amorphous materials and amorphous/crystalline silicon.

THE MOLECULAR METHOD

The molecular method assumes that a molecular ion dissipates when it enters the

substrate. This is true if the ion energy is significantly higher than the dissociation energy of the molecule which is of the order of 10 eV/atom. For ion energies in the keV-range this prerequisite is certainly met, with the exception of very large atom clusters, where additional surface effects would have to be considered. Once dissipated at the entrance into the target, all atoms of the molecule can be treated separately, while they interact with each other only by the damage which is produced when the ions move through the target.

The collisions of implanted particles with the atoms of the target are described by an elastic collision model. Since the target may consist of various materials, two methods are used for selecting collision partners. Within amorphous materials the type and the position of the collision partner are determined randomly, considering the density and the composition of the material. Within crystalline materials the collision partner is placed at the closest crystal lattice position in the direction of motion of the implanted particle, offset by a random vector that represents the lattice vibration. Crystalline defects are considered by randomly inserting and removing atoms. The probability for such a replacement is proportional to the quotient of the concentration of interstitials plus the concentration of vacancies, and the density of the material. During the simulation the point defects are generated when the elastic energy transfer to a target atom is larger than the displacement energy. The number of generated point defects caused by one collision is described by an empirical damage model (3). The vacancies are considered as being generated around the position of the elastic collision whereas the interstitials are offset by a distance that is proportional to the transfered energy.

The energy loss of an implanted particle to the electrons of the target material is also modeled empirically (4). For amorphous materials one parameter is necessary to quantitatively describe the electronic stopping behavior whereas four parameters are necessary for crystalline materials, because the crystalline model also describes anisotropic effects.

Each implanted particle has its own set of electronic stopping and damage parameters, but these parameters do not depend on whether the particle was implanted as a single atomic ion or was just a part of a molecule. Therefore measurements resulting from implantations with single atomic ions as well as molecular ions can be used for the calibration of the empirical parameters.

If the implanted molecule contains more than one atom of the same species, these atoms behave statistically identical. Thereby only one trajectory for each atom species has to be calculated. All other atoms of the same species are taken into consideration by multiplying the number of vacancies and interstitials, generated by a collision of one atom of this species, with the number of atoms of this species per molecule. The resulting distribution of the dopant is also weighted correspondingly. For BF_2 molecules two trajectories have to be calculated, one for the Boron atom and one for the Fluorine atoms.

Model Calibration for BF_2 Ions

In order to be able to apply the molecular method to the simulation of the implantation of BF_2 ions a set of the empirical parameters for the Boron and for the Fluorine atoms is necessary. We have calibrated the empirical parameters for Boron with SIMS measurements resulting from implantations with Boron ions and the parameters for Fluorine with SIMS measurements resulting from implantations with BF_2 ions.

Evaluation

We have evaluated the molecular method by comparing simulation results with SIMS measurements of Boron and Fluorine doping profiles resulting from implantations with BF_2 ions into a bare silicon wafer. SIMS profiles were measured for three ion energies 20 keV, 50 keV, 100 keV and two doses $5{\cdot}10^{13}$ cm^{-2}, $4{\cdot}10^{15}$ cm^{-2}. The comparisons are presented in Fig. 1, Fig. 2 and Fig. 3.

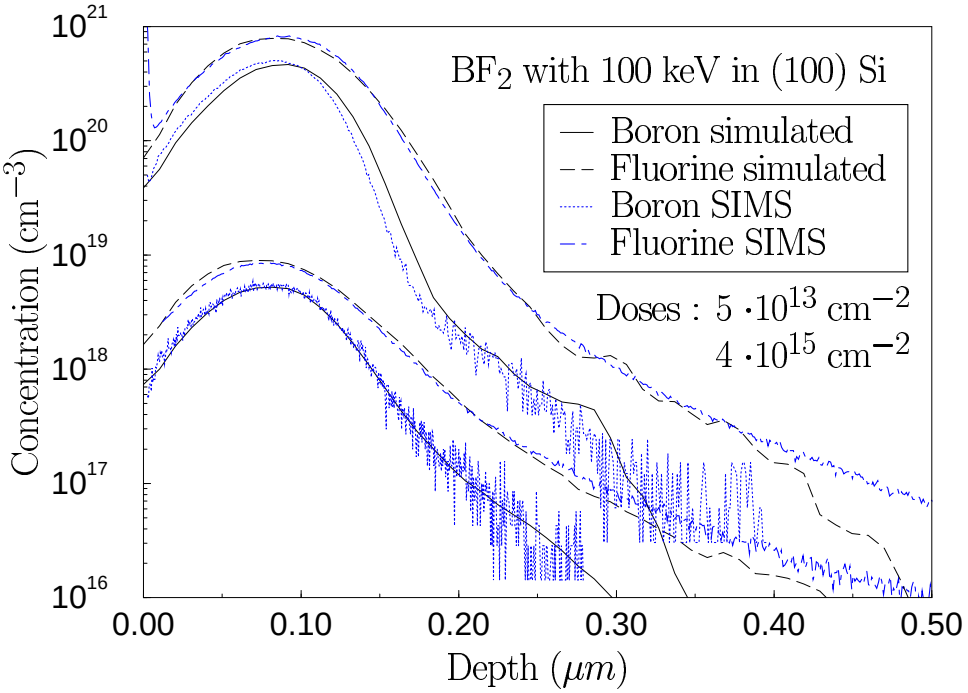

Fig. 1: Simulated Boron and Fluorine profiles compared to SIMS measurements for BF_2 implantations with energies of 100 keV. The ion beam was twisted by 22° for the implantations with a dose of $5{\cdot}10^{13}$ cm^{-2} whereas it was not twisted for the implantations with a dose of $4{\cdot}10^{15}$ cm^{-2}. In both cases the ion beam was tilted by 7°.

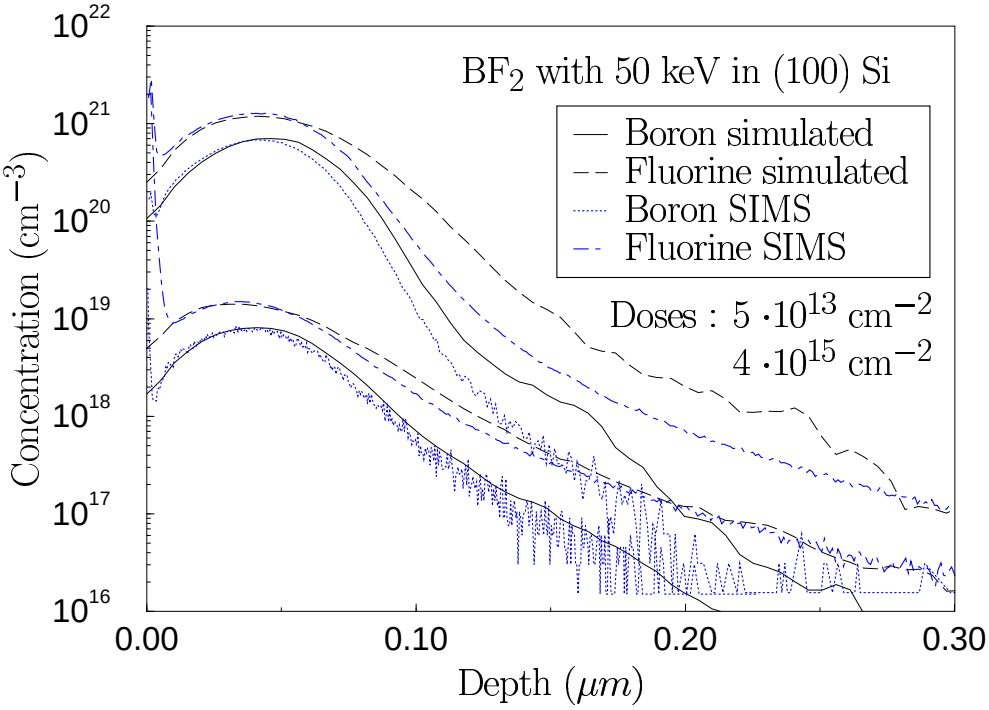

Fig. 2: Simulated Boron and Fluorine profiles compared to SIMS measurements for BF_2 implantations with energies of 100 keV and 50 keV. The ion beam was twisted by 22° for the implantations with a dose of $5{\cdot}10^{13}$ cm^{-2} whereas it was not twisted for the implantations with a dose of $4{\cdot}10^{15}$ cm^{-2}. In both cases the ion beam was tilted by 7°.

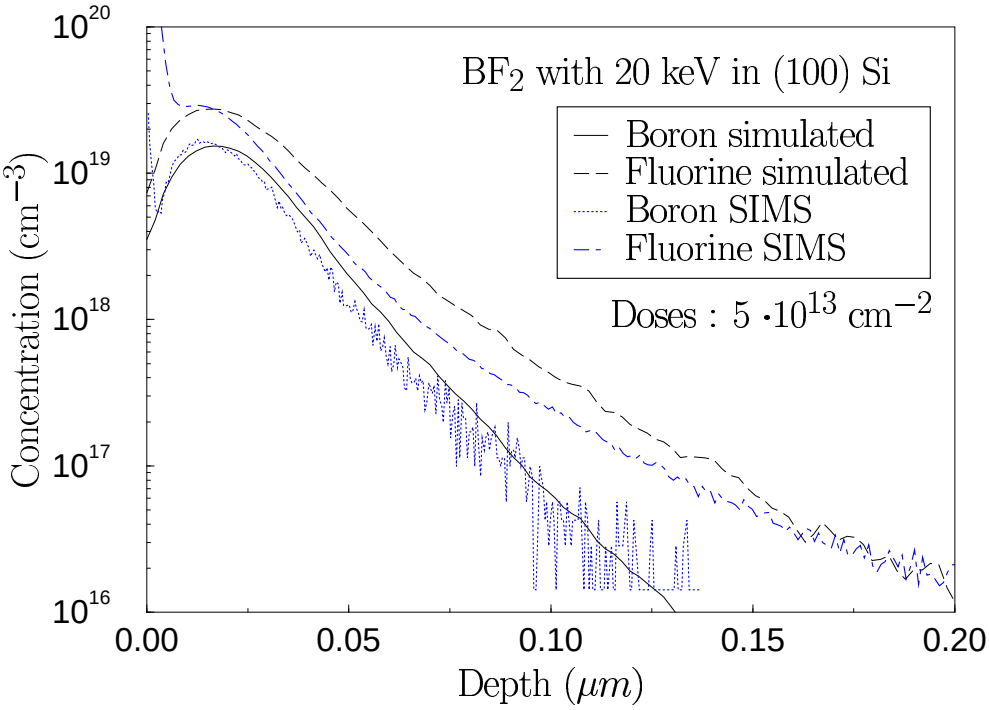

Fig. 3: Simulated Boron and Fluorine profiles compared to SIMS measurements for a BF_2 implantation with an energy of 20 keV and a dose of $5{\cdot}10^{13}$ cm^{-2}. The ion-beam was twisted by 22° and tilted by 7°.

There is quite a good agreement between simulation results and measurements especially for low implantation doses. Worth mentioning is that for low energies the measured profile is slightly shallower than the simulated profile. The lower the energy of an ion the more the nuclear stopping dominates the behavior of the ion. In this case an inaccuracy in the inter-atomic potential, which is an average for a wide range of ion target combinations, can have a significant influence on the simulation results. At very high doses, the simulated profile is also slightly deeper than the measured profile, because the analytical damage model dose not properly consider the amorphization of the silicon.

Three-dimensional simulation

To make the molecular method applicable also for three-dimensional simulations we are using statistical methods to reduce the noise of the simulation results. Thereby the quality of one-dimensional simulation results can be reached without a tremendous increase in the number of simulated ion trajectories. Within amorphous materials we make use of a trajectory-reuse method. The surface of the simulation domain is split into several areas. In one of those areas an ion trajectory is calculated for each material the ion moves through. These trajectories are reused in all other areas. They are just translated and rotated according to the new entrance vector.

This method cannot be applied within crystalline materials since they are not isotropic. Alternatively we are using a trajectory-split method (5). When an ion moves to a region of low concentration it is split into virtual particles that behave physically like a real ion, but the number of interstitials and vacancies that are generated by a virtual ion are weighted by the number of virtual particles originating from the same ion. The effect of the trajectory-split method is that statistical errors are reduced by just slightly increasing the CPU-time requirement.

Using these statistical methods it is possible to perform three-dimensional simulations within reasonable time. We have simulated a threshold voltage adjust implantation with BF_2 ions, which is a part of a 0.6 μm MOS-transistor process. The input to the simulation is shown in Fig. 4. It is one half of an NMOS-transistor, which is cut through the gate. The silicon substrate (light) is covered by silicon dioxide (dark). The active area in the center of the simulation domain is surrounded by a LOCOS-Isolation.

The simulation with the molecular method was performed with ~2.300.000 effective ions and took about 5 hours of CPU-time on a DEC-600 workstation. Fig. 5 and Fig. 6 show the simulated distribution of the Boron an of the Fluorine atoms. In order to visualize the three-dimensional result we are presenting an outline of the simulation domain in common with the doping profiles within three planes inside the device.

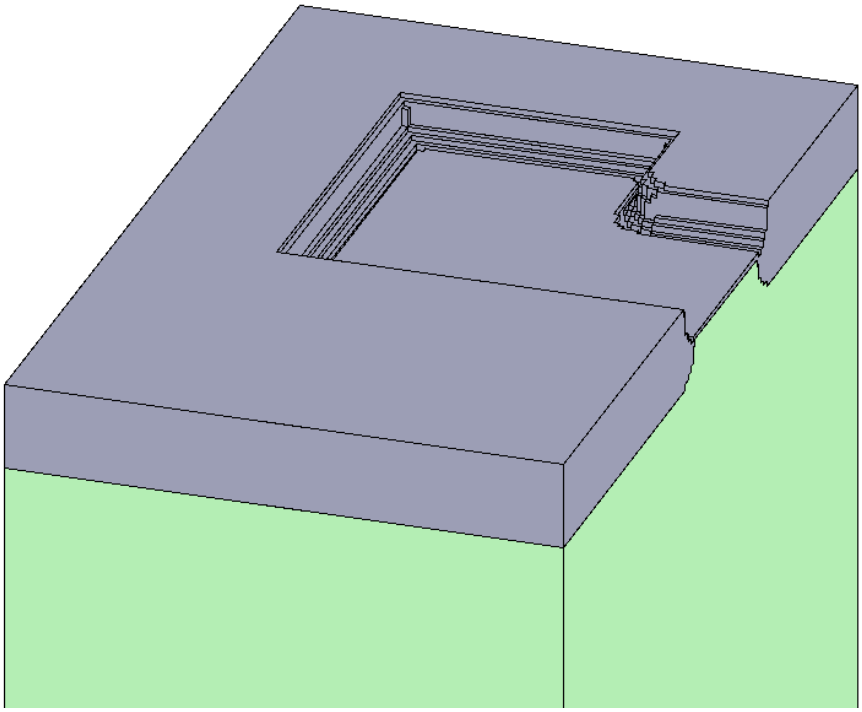

Fig. 4: Structure of one half of a 0.6 μm NMOS-Transistor before the threshold voltage adjust implantation.

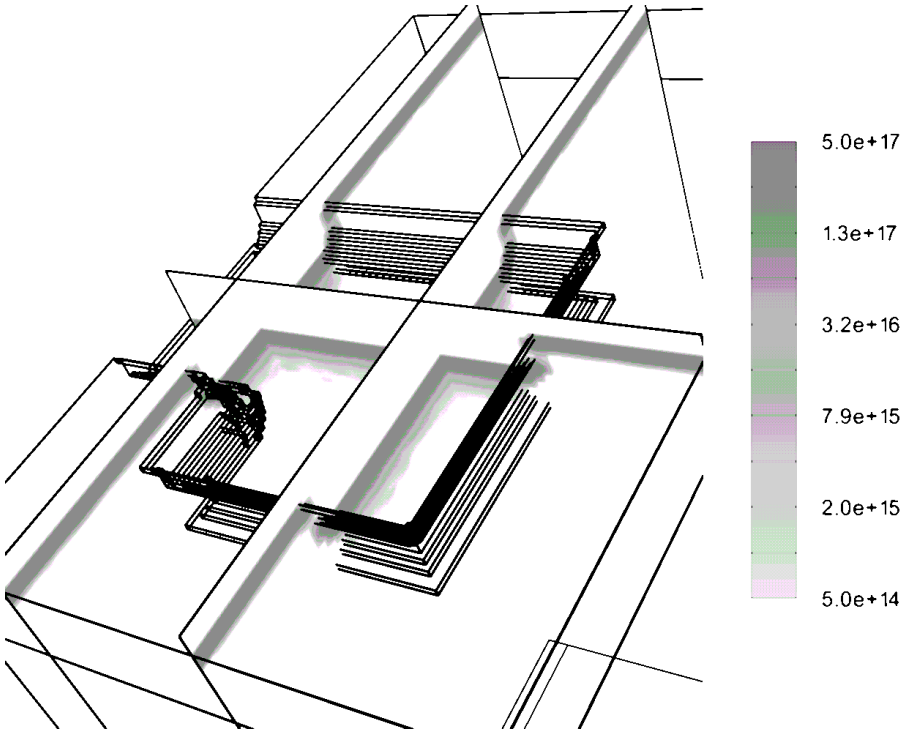

Fig. 5: Simulated Boron profile resulting from a threshold voltage adjust implantation into a 0.6 μm NMOS-transistor with BF_2 ions with an energy of 50 keV and a dose of $3{\cdot}10^{12}$ cm^{-2}. The figure shows an outline of the transistor structure and the doping profile within three cuts through the gate and source/drain region.

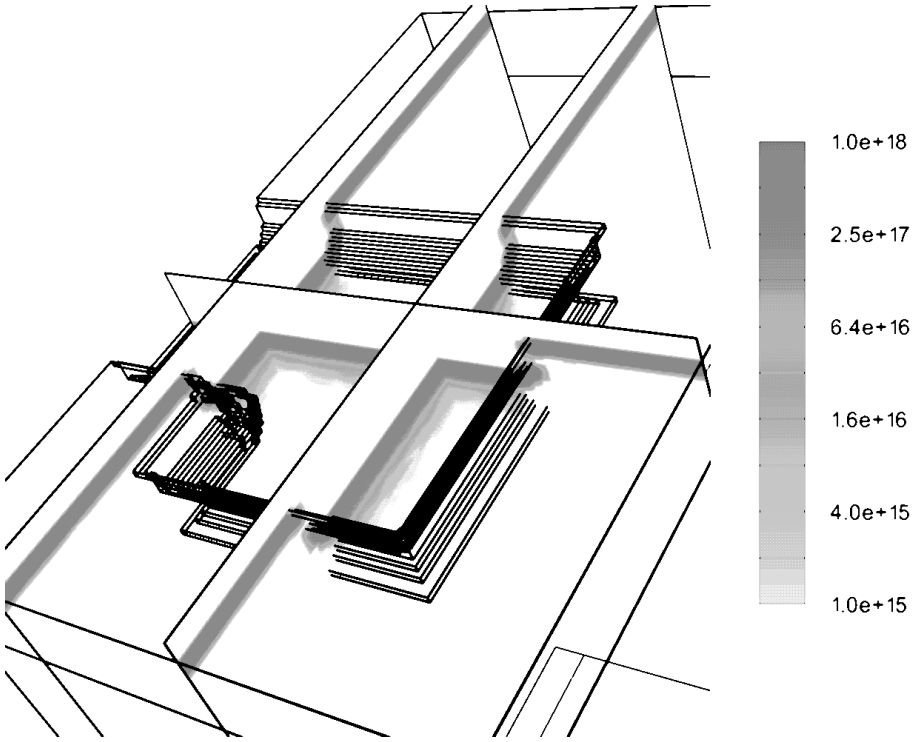

Fig. 6: Simulated Fluorine profile resulting from a threshold voltage adjust implantation into a 0.6 μm NMOS-transistor with BF_2 ions with an energy of 50 keV and a dose of $3{\cdot}10^{12}$ cm^{-2}. The figure shows an outline of the transistor structure and the doping profile within three cuts through the gate and source/drain region.

ACKNOWLEDGMENTS

This research project is supported by the European Community ESPRIT project 24038 PROMPT-II.

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