Accurate Three-Dimensional Simulation of Damage Caused by Ion Implantation

A. Hössinger and S. Selberherr

Institute for Microelectronics, TU Vienna
Gusshausstrasse 27–29, A-1040 Vienna, Austria, hoessinger@iue.tuwien.ac.at

ABSTRACT

We present a Monte-Carlo ion implantation simulation method that allows a very accurate prediction of implantation induced point defects, generation of amorphous areas, and impurity distributions. The implanted impurity profiles can be calculated as well as the distributions of impurities that are moved from one material to another during the implantation process. The simulation method can be applied to three dimensional device structures consisting of various materials. The accuracy of the simulated profiles is evaluated by comparing impurity profiles with SIMS measurements and point defect profiles with RBS spectra. Finally the simulation results of a source/drain ion implantation into a three-dimensional MOS-transistor structure are shown.

Keywords: ion implantation, damage, Monte-Carlo simulation

INTRODUCTION

In modern MOSFET process technologies the exact knowledge about silicon interstitials and vacancies caused by ion implantation, and the predictability of implantation induced amorphization and pollution of active areas is very important.

Rapid thermal annealing (RTA) processes and thereby the doping profiles are strongly influenced by point defects, because of pairing effects the diffusivity of doped atoms can be increased in the vicinity of point defects. During the first period of an RTA process, vacancy and interstitial recombination is in competition with these pairing effects. The dynamic of this process is very sensitive to the absolute values of the concentration of interstitials and vacancies and to their local ratio. Semi-analytical models which are normally used by Monte-Carlo ion implantation simulators to describe the damage generation behavior are not sufficient to study the whole complexity of this process. Especially the fact that the distribution of the vacancies and the interstitials have a different shape, can hardly be described by the analytical models with the required accuracy. Additionally it is interesting to know if amorphous areas are created by the implantation, because the recrystallization process during the annealing step can be enhanced along amorphous/crystalline interfaces.

Undesirable impurities which are pushed from overlaying materials to the active area by the implanted ions can degrade the device performance. Because of this knock on effect, atoms from isolating or masking materials are brought into the active area. Therefore measures have to be taken to avoid that these pollutions influence the device. These measures can be optimized if process simulation gives a deeper insight into the pollution process.

The small dimensions of modern semiconductor devices require not only accurate one-dimensional and two-dimensional process simulation, but also a detailed three-dimensional description of the devices, because many effects have been brought to light that can only be described by a full three-dimensional process simulation.

We have implemented a follow-each-recoil method to the Monte-Carlo ion implantation simulator MCIMPL [1],[2] which is capable of describing the doping profiles, the point defect profiles, the generation of amorphous areas, and the pollution effect with the required accuracy. Since MCIMPL simulator is a multi-dimensional simulator this follow-each-recoil method can also be applied to three-dimensional structures as will be demonstrated. Additionally we will evaluate the accuracy of the simulator by comparing SIMS measurements and RBS measurements to simulated doping and point defect profiles.

METHOD

The Monte-Carlo ion implantation simulator is based on a binary collision algorithm [1],[2]. The trajectory of each implanted ion is calculated until it comes to rest due to interactions with the atoms and the electrons of the target material. Since the simulator can be applied to devices consisting of several amorphous and crystalline materials, we often have to distinguish an amorphous case and a crystalline case as outlined in the following.

The electronic stopping power is described by a semi-empirical model based on the stopping of charged particles moving through a plasma of electrons [3]. For crystalline materials this model is modified by empirical expressions that take into consideration, that the

density of the electrons varies within a solid, mainly depending on the distance from lattice atoms [4], [5].

The interaction of an ion with a target atom is described by an elastic collision, which uses the Universal Screening Potential [6] to calculate the energy transfer and the scattering angle. To save computation time, the scattering process is not calculated rigorously for each collision but the scattering angle is interpolated from a table which contains the results of the scattering process for several energies and impact parameters [1]. Two methods are used to determine the position of the collision partner. If the ion moves trough an amorphous material the collision partner is randomly positioned, considering the density of the material and the direction of motion of the ion. If the target material has crystalline structure the collision partner is placed at the nearest crystal lattice position, in the direction of motion, offset by a random vector that describes the lattice vibration. The length of this vector follows a Gaussian probability distribution, whose standard deviation is derived from the wafer temperature by the Debye-model [7]. The type of the collision partner is determined randomly, depending on the composition of the target material. If the transfered energy exceeds the effective displacement energy a recoil is generated.

This recoil is treated as a new particle inside the simulation domain. Starting from the position of its generation the trajectory of the recoil is calculated in the same way as the trajectory of an implanted ion. Therefore a recoil itself can also generate recoils. The starting conditions of recoiled particles are stored on a stack until the calculation of the trajectory of the ion which has generated the recoil is finished. The first particle which has been stored on the stack is the first one that is calculated when the stack is processed. The stopping position of all particles are stored during the simulation and are used to calculate the concentrations for each particle species.

The effective displacement energy is a modification of the physical displacement energy. It is the energy, which is required to remove an atom irreversibly from its current position in the solid, modified by a factor that represents a spontaneous recombination process initiated by locally removing an atom. In MCIMPL this factor is a parameter that can be calibrated depending on the wafer temperature during the implantation process.

Not only the stopping position of a particle is stored, but also the position of the recoil generation, because the remaining material defect can influence the trajectories of succeeding particles. In amorphous materials the density (ρ_M) is modified according to the concentration of removed (ρ_V) or added (ρ_I) atoms. There is one ρ_V and one ρ_I for each atom species the target material consists of. In consequence the average free flight-path of a particle between two nuclear collisions, which is derived from the density, is locally changed.

$$\rho_{M(mod)} = \rho_M + \sum_{atomspecies} (\rho_I - \rho_V) \tag{1}$$

In crystalline silicon two types of recoils are distinguished. First a silicon atom can be removed from a crystal lattice position. Thereby a vacancy/interstitial pair is generated. The vacancy stays at the position where the recoil was generated, whereas the interstitial penetrates deeper into the target. Second an interstitial silicon atom can be recoiled, with the consequence that no vacancy is generated, but the interstitial silicon atom is moved to another position. We do not consider the recoiling of doping atoms, because the probability for such a process is at least one order lower. The interstitials and vacancies affect the trajectories of a particle when the collision partner for a nuclear collision process is selected. Instead of placing the collision partner at a crystal lattice position it is sometimes placed randomly, as is the case in amorphous materials. The probability (P_α) for random positioning is proportional to the sum of the concentration of interstitials (ρ_I) and vacancies (ρ_V) as long as it is lower than the amorphization concentration (ρ_α). ρ_M is the particle density of the material.

$$\begin{aligned} P_\alpha &= \tfrac{\rho_I+\rho_V}{\rho_M}, \quad & \rho_I + \rho_V < \rho_\alpha \\ P_\alpha &= 1.0, & \rho_I + \rho_V > \rho_\alpha \end{aligned} \tag{2}$$

When a silicon recoil has reached its final energy which is of the order of the lattice vibration energy, a recombination model [8] is used to decide whether an interstitial is generated, or whether the silicon atom recombines with a vacancy in its near surrounding. The probability for a recombination is proportional to the concentration of the vacancies.

$$P_{rec} = r_{rec} \cdot \frac{\rho_V}{\rho_M} \tag{3}$$

r_{rec} can be interpreted as recombination radius of a vacancy which is moving through the target by thermal processes. This recombination radius can be calibrated as the effective displacement energy according to the wafer temperature.

Since computation time is a very critical aspect, we make use of two statistical methods which allow a reduction of the number of calculated trajectories without increasing the statistical noise.

- Trajectory reuse method
- Trajectory spilt method

In amorphous materials a trajectory reuse method is applied. The surface of the simulation domain is divided into several subareas. A trajectory for one ion in one sub-area is calculated. This trajectory is split

into sub-trajectories which are completely in one material. The information about the physical behavior for all sub-trajectories that belong to amorphous materials are stored for later reuse. The trajectories for the recoils originating from the ion are also calculated and subdivided in the same way, as long as there is one recoil that belongs to an atom species with an already calculated trajectory. If a sub-trajectory exists for the material, the recoil currently moves trough, and if the recoil energy is within the initial-energy and the final-energy of the sub-trajectory, the sub-trajectory is transformed to the position and the momentum of the recoil. Doing so, the subsequent behavior of the recoil can be derived from the sub-trajectory as long as the end of the sub-trajectory is reached or the recoil changes into another material. The same procedure is used for all other recoils and for all particles in the other subareas of the simulation domain. If there is no suitable sub-trajectory for a certain particle the trajectory is calculated and added to the list of sub-trajectories.

The trajectory reuse method can not be applied to crystalline materials, because it requires isotropy of the materials but a trajectory split method is used instead [9]. When an ion moves to a region of low concentration it is split into virtual particles which behave physically identical to a real ion, but their contribution to the doping distribution is weighted according to the number of virtual particles originating from the same ion. The contribution of the recoils generated by a virtual particle, to the overall particle distribution is also weighted correspondingly. The gain of the trajectory split method is that the effective number of trajectories which contribute to the doping distribution in regions of low concentration is increased, without an increase of the total number of trajectories that have to be calculated. The trajectory split method is not applied to recoiled particles, because the number of recoil trajectories is much higher than the number of ion trajectories. Nevertheless, it has to be mentioned that the follow-each-recoil method requires more computational resources than an analytical damage model, because the number of trajectories to be calculated is significantly higher.

SIMULATION

We have evaluated the follow-each-recoil method by comparing simulated doping profiles to SIMS measurements resulting from implantations with phosphorus and arsenic ions [10] (Figure 1) and we have compared the simulated damage profiles of these implantation to RBS spectra. Since the RBS measurements do not directly yield a point-defect concentration but the amorphization percentage, we have summed up the concentration of interstitials and vacancies and divided this value by the amorphization level. Figure 2 shows the resulting profile in comparison to the RBS spectra.

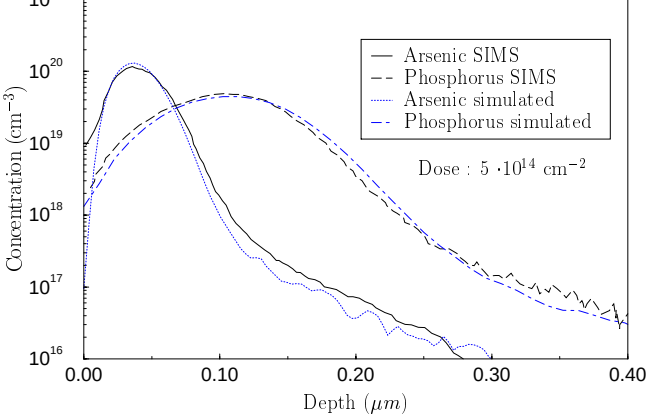

Figure 1: Simulated phosphorus and arsenic profile compared to SIMS measurements. The phosphorus ions were implanted with an energy of 80 keV whereas the arsenic implantation was done with an energy of 50 keV. A dose of $5 \cdot 10^{14}$ cm^{-2} was used for both implantations.

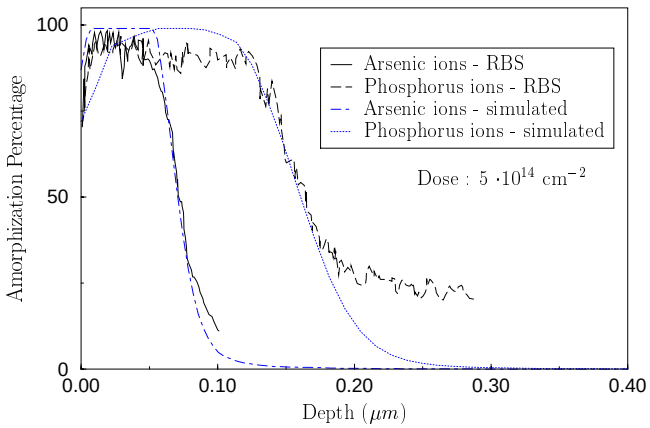

Figure 2: Simulated amorphization of crystalline silicon caused by implantations with arsenic ions and phosphorus ions compared to RBS measurements. The phosphorus ions were implanted with an energy of 80 keV whereas the arsenic implantation was done with an energy of 50 keV. A dose of $5 \cdot 10^{14}$ cm^{-2} was used for both implantations.

Furthermore, we have performed a fully three-dimensional simulation of a source/drain implantation which is part of a 0.6 μm MOS-Transistor process. We have simulated an implantation with arsenic ions into the NMOS-Transistor. Figure 3 shows the input geometry that is used for the simulation: One have of the NMOS-Transistor, which is cut through the gate. The silicon substrate (grey) is covered by silicon dioxide (dark grey). The active area in the center of the simulation domain is surrounded by a LOCOS isolation. The gate area is made of polysilicon (light grey) and covered by silicon

dioxide. As a result of the simulation we show the amorphous area generated by the source/drain implantation. In order to give an impression of the three-dimensional result the amorphous area within three cuts through the source/drain region is presented in common with an outline of the transistor structure (Figure 4).

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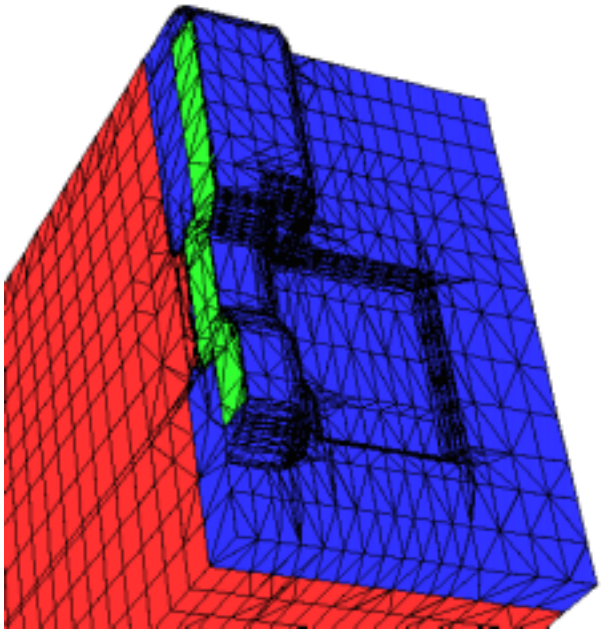

Figure 3: Structure of one half of the 0.6 μm NMOS-transistor which is used as input for a source/drain ion implantation simulation. Because of symmetry the transistor is cut through the gate region.

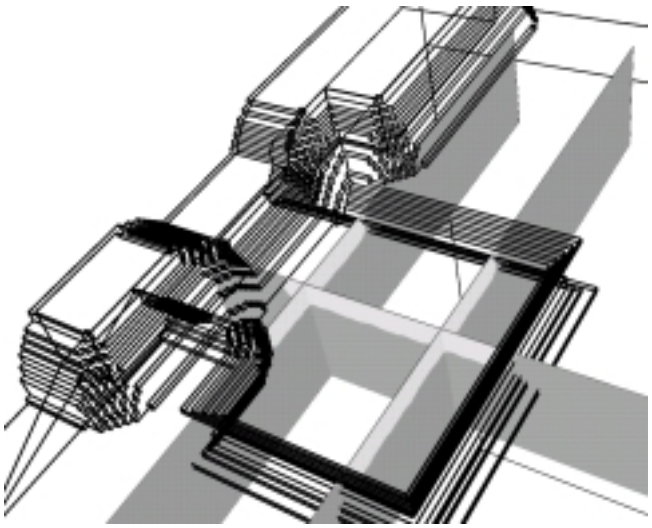

Figure 4: Simulated amorphization of the source/drain region of a 0.6 μm NMOS-transistor by a source/drain implantation with arsenic ions with an energy of 90 keV and a dose of $4{\cdot}10^{15}$ cm^{-2}. The figure shows three cuts through the source/drain region. The light gray area denotes the amorphous region.