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Two Dimensional Monte Carlo Simulation of Ion Implantation in Crystalline Silicon Considering Damage Formation

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Abstract

One- and two-dimensional concentration profiles of high-dose boron implants have been computed using our Monte Carlo simulator IMSIL. In the 1-D case they have been compared with experiments obtaining very good agreement. The lattice damage formation is taken into account according to the modified Kinchin-Pease model. A factor of 1/8 was found to properly describe the self-annealing process reducing the amount of lattice defects. In the 2-D case it is observed that the channeling in directions leading below the mask edge is not suppressed in contrast to vertical channeling.

1. Introduction

In recent years considerable research activities on modeling 1-D implantation profiles in crystalline silicon have been carried out. 2-D simulations of ion implantation in crystalline silicon have been rare and have neglected damage formation [1], [2]. Souce/drain profiles of MOSFET's, however, require high implantation doses, and therefore considering damage formation and its influence on the channeling and dechanneling of ions is mandatory. Furthermore, the knowledge of the damage profile resulting from the implantation process is useful in modeling diffusion phenomena.

In this paper we have extended our Monte Carlo simulator [2] in order to calculate 2-D dopant profiles considering damage formation. We have called the program IMSIL (IMplantation in SILicon). In the following section we describe the physical models implemented in IMSIL. Afterwards we present the results of our simulations and finally we discuss them.

2. Models Implemented in the Monte-Carlo Simulator

In our studies we use an extended version of the Monte Carlo simulator described in [2]. The version includes an improved model of the electronic stopping power [3], a modified Debye temperature of 490K [4] for the description of lattice vibrations, and the damage model to be discribed below. Furthermore, the present version is not restricted to point responses, but allows to perform the implantation in the whole simulation area.

This is important because the superposition of point responses cannot be used to get the dopant distribution at a mask edge, if implantation damage is taken into account. The increasing lattice damage during the implantation is dynamically recorded as a function of the space coordinates, so we have permanent knowledge of the actual defect distribution. The lattice damage encountered by an ion along its trajectory is considered by carrying out amorphous collisions with a probability proportional to the local number of displaced atoms. This presumes as a physical background the existence of quasi-amorphous zones embedded in the crystal lattice.

During every collision the ion transfers energy to the lattice atom. If this energy exceeds the displacement energy, the target atom leaves its lattice site and may produce further damage on its way through the crystal. Restricting ourselves to boron implantations, we may neglect the recoil range. The amount of damage is taken into account using the modified Kinchin-Pease model [5]. Although self-annealing is a complicated process, we found it sufficient for our purpose to use a factor to reduce the amount of created damage resulting from the modified Kinchin-Pease model [5]. Comparing many simulated implantation profiles with experimental results we found a value of 1/8 for this factor at a temperature of 300K.

3. Results and Discussions

In all simulations boron has been implanted into amorphous or (100) silicon with a 5A native oxide layer. Figure 1 shows the dose dependence of the 1-D concentration profile of a boron implantation at 35keV in random direction (7° tilt, 15° rotation from the [110]-direction). Comparing the profiles we see that, at a dose of 10^{16} cm^{-2} (curve 1), we obtain a shallower profile than in the simulation of the same implantation without taking damage formation into account (curve 3).

At a dose of 10^{14} cm^{-2} (curve 2), the implantation profiles with and without damage are almost the same, so lattice amorphization can be neglected. We remark the paralellism of the profile calculated for the dose of 10^{16} cm^{-2} without taking damage formation into account (curve 3) and the profile for the dose of 10^{14} cm^{-2} (curve 2). This is due to the fact, that in the absence of damage only lattice vibrations and the native oxide layer [6] influence the channeling and dechanneling of implanted ions regardless of the dose, while at a dose of 10^{16} cm^{-2} lattice amorphization becomes the major dechanneling mechanism. For both doses there is excellent agreement between simulation (curves 1,2), and experiment [7].

In Figures 2,3, and 4 we see the 2-D dopant profiles resulting from 5keV boron implantations near a mask edge in amorphous target, in crystalline target without damage consideration and in crystalline target with taking lattice amorphization into account, respectively. The simulations into crystalline silicon were performed with 7° tilt and 45° rotation from the [110]-direction.

At the low implantation energy used, channeled ions have a far larger range than non-channeled ions. Therefore, the profiles resulting from the implantation in the crystalline target are much deeper than in the amorphous case.

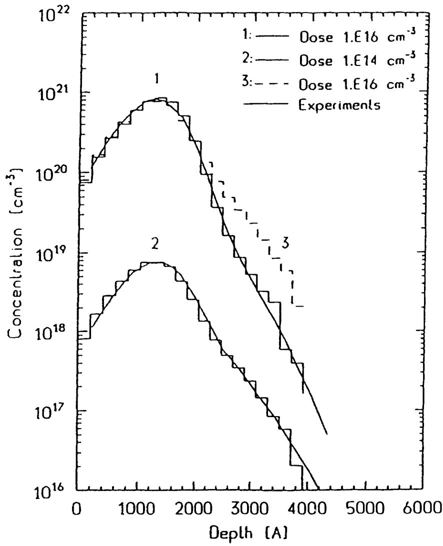

Figure 1: 35 keV boron implantation into (100)-silicon with 7° tilt and 30° rotation.

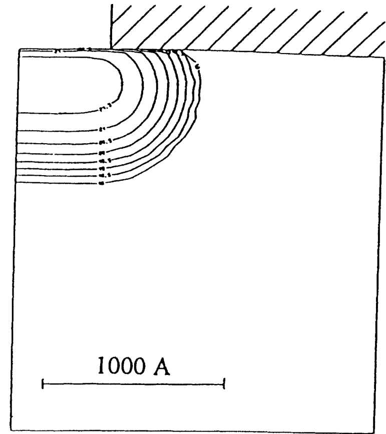

Figure 2: 5keV boron implantation into amorphous silicon near a mask edge.

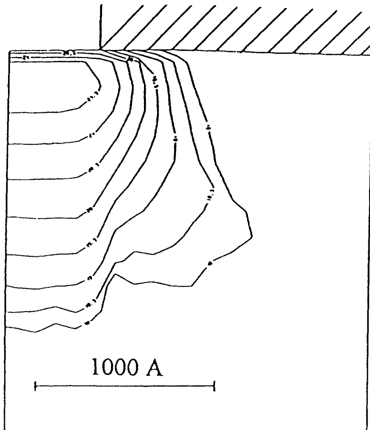

Figure 3: 5keV boron implantation into (100)-silicon near a mask edge without considering lattice amorphization.

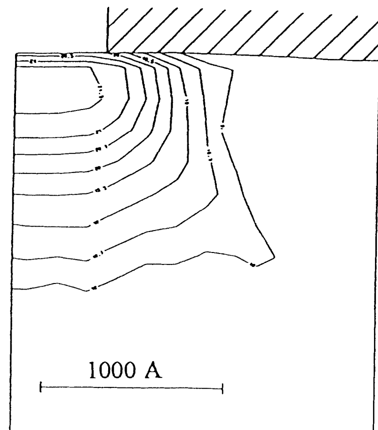

Figure 4: 5keV boron implantation into (100)-silicon near a mask edge considering lattice amorphization

The 2-D simulations were performed with 7° tilt and 0° rotation and an implantation dose of $2 \cdot 10^{16}$ cm^{-2}. There are two contour lines per decade of concentration.

Comparing Figure 2 on the one hand and Figures 3 and 4 on the other hand, we remark the major effect of channeling on the dopant profile in the crystalline case. At the considered high implantation dose ($2 \cdot 10^{16}$ cm^{-2}) damage formation becomes the dominant channeling and dechanneling mechanism, resulting in significant differences of the 2-D implantation profiles with and without taking lattice amorphization into account (Figures 3 and 4 respectively). When considering damage formation (Figure 4) we notice, analogous to the 1-D case, the considerable suppression of the channeling effect in vertical direction.

In directions leading below the mask edge the channeling tendency is favorized. In order to explain this behaviour, we first notice that the region below the mask contains less damage than the silicon region which is not covered by the mask. However, this is not true when comparing the region below the mask (where lateral channeling occurs) with the deeper part of the region not covered by the mask (where vertical channeling occurs). Therefore we need additional explanations.

The first reason of the observed behaviour is that ions which are scattered out of the vertical channel by lattice damage are available with some probability for the lateral channels, while the reverse process, i. e. the scattering out of a lateral channel into the vertical channel, is less likely due to the smaller number of ions channeled lateraly as compared to those channeled vertically. The second reason is that a displaced lattice atom is more effective in scattering the ion into a channel than a regular lattice atom. This effect is similar to the enhancement of the channeling probability by a screening oxide [6].

4. Conclusions

We have presented for the first time 2-D implantation profiles calculated by Monte-Carlo simulations taking into account damage formation. The results show that lateral channeling at a mask edge is not suppressed in contrast to vertical channeling. The validity of the results is confirmed by the good agreement with 1-D experimental profiles and by the physical approach using the Monte-Carlo method.

5. References

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