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Three-Dimensional Monte Carlo Simulation of Boron Implantation into <100>Single-Crystal Silicon Considering Mask Structure

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Abstract

A new and computationally efficient three-dimensional Monte Carlo ion implantation simulator, TRICSI, has been developed to investigate three-dimensional mask effects for low-energy boron implantation into <100>single-crystal silicon. The simulator accurately and efficiently simulates three-dimensional implanted doping profiles under the mask structure and window. All of the typical implant parameters such as dose, tilt angle, rotation angle, in addition to energy are considered. The orientation of silicon substrate, ion beam divergence, presence of native oxide layer, wafer temperature, orientation of masking edge, masking layer thickness, and structure and size of window are also taken into account.

1. Introduction

In the crystalline silicon, one-dimensional(1D) or two-dimensional(2D) Monte Carlo(MC) ion implantation simulations have been made by many authors [1], [2], [3]. However, three-dimensional(3D) MC simulations of ion implantation in the crystalline silicon have been rarely reported and have yet to predict 3D effects depending on the mask structure and the size of the open window for ion implantation. The 3D MC simulation of ion implantation in the crystalline silicon is strongly needed to understand the 3D behaviors of implanted impurity and to compactly control the depth and lateral doping profiles of implanted impurity under smaller implant area at ever lower energy. In addition, the 3D implantation simulation based on the physical approach becomes more important under the circumstances that the 3D experiments of the implanted doping profiles are not available for the present. In this paper, we have investigated and predicted 3D mask effects by using our simulator, TRICSI (TRansport Ions into Crystal SIlicon) which is coded based on TRIM [4] and MARLOWE models [5]. A newly developed searching algorithm for a collision atom in <100>single-crystal silicon and an effective cumulative damage model for boron implantation are implemented in the simulator. In the following section, we describe the details of models employed in TRICSI.

2. Model Details

Recently, UT-MARLOWE code [1] has been developed for 1D boron implantation simulation in the crystalline silicon, and the results show a good agreement with the SIMS

experiments, but it is reported that the simulation time is increased by 50% compared with that of MARLOWE because it has considered and calculated that the variation of electronic density through which the moving ion has got along its trajectory. In this paper, in order to efficiently simulate the whole volume for 3D simulation, we have newly defined and modified the value of the average electronic density for the use of ABS electronic stopping model [6] which the implanted ion has experienced along its trajectory. The value of the average electronic density used for the good agreement with the SIMS experiments [1], [7] was found 0.735 electrons/$Å^3$ over the range of the simulated energies, from 5 to 80 keV. A *priori* damage function (1) is also introduced into the cumulative damage model for boron implantation by manipulation of the maximum impact parameter P_{max} which is the same as the TRIM calculation [4]. The P_{max} is determined by the function of the ion energy, the ratio of moving ion mass to stationary silicon atom mass, and the minimum transferred energy, which is set initially to 1.5 eV for zero tilt angle and 5 eV for any tilt in our simulation. For all of collisions, the new impact parameter P'_{max} as a function of the cumulative damage probability $f(X)$ [8] is calculated by the following function, where the value of $f(X)$ is predetermined not to exceed 1 initially in the simulation.

$$P'_{max} = P_{max} \times (1 + f(X)^3) \quad (1)$$

As a result of the new P'_{max}, the collisions of the implanted ions are increased, and the otherwise channeled ions are dechanneled. The increased rate of their random smatterings decreases the depth channeling tail. The relatively simple damage model has well simulated the low-dose profiles below 1E15 ions/cm^2. To consider the lattice vibration effect, Debye model [9] has been implemented and the average displacement X_{rms} from the lattice site of the silicon is calculated by using the Debye temperature of 543K [9] for the crystalline silicon. It is assumed that the displacement due to the lattice vibration is randomly determined in 3D coordinates. We can directly calculate the impact parameter in a collision by considering the random displacement from the 3D original site of the silicon lattice atom as X_{rms} multiplied by the random number between 0 and 1. The 10Å native oxide layer is considered as an amorphous layer on the silicon substrate and the 0.5° beam divergence is also included assuming that the incoming ion beam spreads isotropically within a cone defined by the divergence angle. Also, using the vector analysis for the direction vector of the moving ion after a collision, we can calculate two direction angles defined as azimuthal angle and the scattering angle in 3D coordinates. The nearest collisional row is first searched according to the azimuthal angle from Z axis defined in Fig. 1. Each silicon atom which is spacing by the silicon lattice constant of 5.43095Å from the initial reference atom in the detected collisional row is examined one by one by using the scattering angle from X axis parallel to <100> direction. If a collision fails to be found in the first nearest row, the search is continued until the collision is found in the next sequential detected row or the ion energy is exhausted by the electronic collisions. Consequently, after searching for a collision in the single-crystal silicon, we can directly and accurately calculate the impact parameter and the flight-path length between collisions in 3D coordinates without the random selection of the impact parameter in the simulation of the amorphous silicon target.

3. Simulation Results

In Fig. 1, 1D simulation results obtained by using the 3D simulator have been compared with the SIMS experiments in order to demonstrate its capability and reliability. The definitions of tilt angle, rotation angle, and 3D coordinates for the simulation structure are also shown. The simulator accurately and efficiently calculates the 1D depth profiles under the area of implant window in the mask. The calculated 3D locations of implanted ions

have been projected onto the desired 3D plane, so that the resulting doping profile is presented as a 2D doping profile on each projected plane. In order to investigate 3D effects due to the mask structure and the size of implant window, boron pseudoparticles were uniformly and randomly implanted into the entire area of implant window. The masking layer was assumed to be impenetrable and have the window for the implanted region with vertical edges. Fig. 2 shows the corner rounding effect that the lateral concentration profiles in the regions near the masking corners are decreased compared with those in the regions near the masking edges. The dilutes of ion concentrations around corners are due to the decrease of scattered ions into the regions near those corners, while the lateral concentration profile in the region near one specific masking corner in the structure of the window of 2500×2500×3/4 is enhanced because of superposed increase of ions scattered into that region from two adjacent masking edges. In addition, in Fig. 3, the narrow window effect on the change of the lateral doping profile in a reduction of the window size has been presented: the lateral doping profile becomes circular as the size of the perfect-square window is reduced from 500×500 nm^2 to 20×20 nm^2. The tilt and the rotation angle in the simulation shown in Fig. 2, 3 are all zero. In Fig. 4, two different profiles on each projected plane in cases of 15° tilt and 0° tilt without rotation are presented to show the difference of the profiles of two different tilt cases. For the 15° tilt angle profiles, the asymmetric profile on the x-y plane is due to the 15° tilt angle, the symmetric profile on the x-z plane is due to the zero rotation angle, and the iso-concentration contours on the y-z plane are slightly shifted downwards and shrunk in the shadowed region due to the shadow effect of the masking thickness compared with 0° tilt angle profiles on the same planes.

4. Conclusions

3D low-energy boron implantation into <100>single-crystal silicon has been modeled and simulated by using the physical approach, MC method. The newly constructed MC approach assures the accuracy of the simulation as shown in the comparison of the 1D data with the SIMS experiments. The simulation results also clearly show 3D mask effects such as the corner rounding effect and the narrow window effect. The doping profile near the mask corner is enhanced or diluted due to the mask structure. In the narrow window, the impurity dilute phenomena is well presented and it finally gives circular contours of two-lateral doping profile on the <100>silicon surface. This effect arises from the fact that the lateral scattering of implanted ions is more concentrated or more diverse in the mask corner than in the mask edge. In addition, not only the planar channeling in the two-lateral doping profile, but also the axial channeling in the depth and lateral doping profile has been presented for the case of very low energy of 5 keV. It shows that the planar and axial channeling effect occurs strongly in the small implant window due to the increased critical angles for the planar and the axial channeling.

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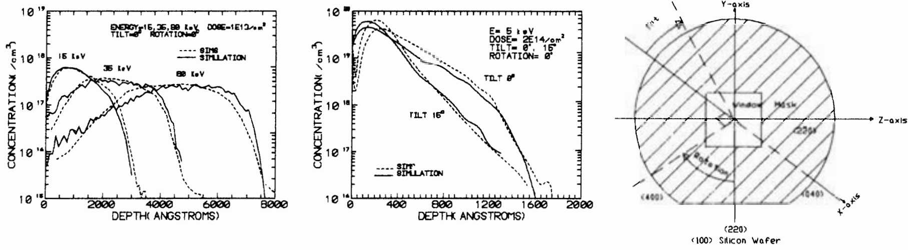

Figure 1: Comparison of 1D simulation results with the SIMS experiments [1], [7], and definitions of tilt angle, rotation angle, and 3D coordinates for the simulation structure.

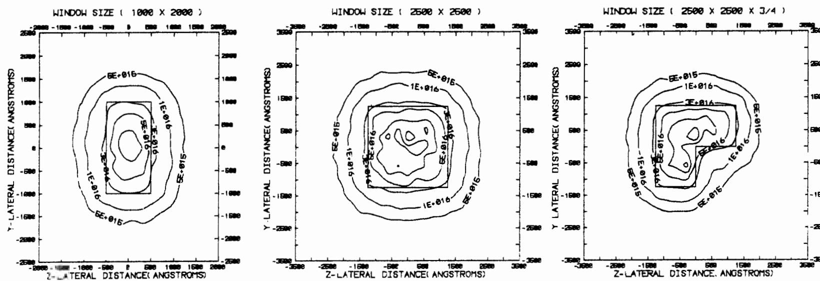

Figure 2: The corner effect of 3D ion implantation at Energy 15 keV, Dose 1E13 ions/cm^2.

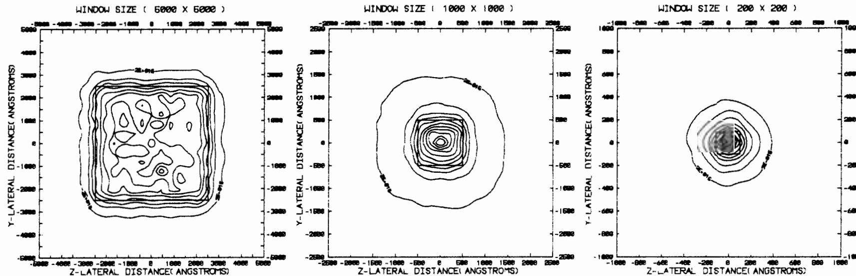

Figure 3: The narrow window effect of 3D ion implantation at Energy 15 keV, Dose 1E13 ions/cm^2.

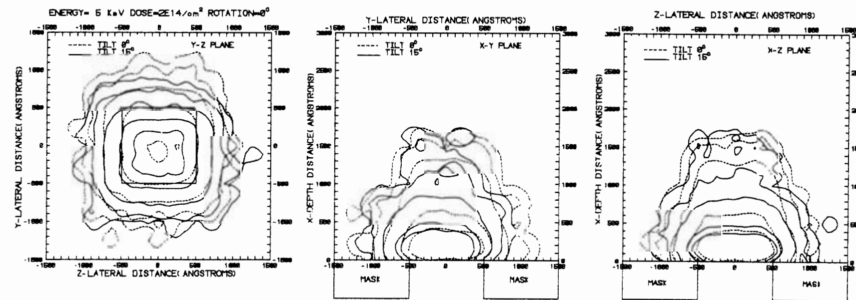

Figure 4: Comparison of the doping profiles between at 0° tilt and at 15° tilt without rotation, where the thickness of the masking layer is 500 Å; for the solid or dashed contour lines, the concentration of the outermost contour is 1E15/cm^3 and from the outermost one, the concentration is increasing by one order of magnitude. The maximum concentration presented is 2E18/cm^3.