Iron ions distribution profile obtained by irradiating the silicon single crystal

A A Shemukhin¹, A V Kozhemiako², Y V Balakshin¹, V S Chernysh²

¹Skobeltsyn Institute of Nuclear Physics, 119991, Moscow, Russia.
²Lomonosov Moscow State University, Department of Physics, 119991, Moscow, Russia.

Abstract. Iron ions with energies of 90 and 250 keV and the irradiation dose of $10^{16}$ ions/cm² and xenon ions with energies of 100 keV and dose $7.7 \times 10^{14}$ cm⁻², 200 keV and dose $2.6 \times 10^{14}$ cm⁻² were implanted in the single crystal of silicon (110). The distribution profiles of implanted impurity, as well as the distribution profiles of the radiation defects in the crystal lattice, were studied by the Rutherford backscattering method in combination with channeling. The experimental results were compared with the results of simulations of binary collisions of the Monte Carlo method in the TRIM program. It is shown that the difference between the experimental data and the calculation program TRIM is more than 35% in all cases.

1. Introduction

Today, tens of nanometers semiconductor structures are the electronic components’ foundation. In such structures, the active element is realized in several and even single atom. Prototypes of monoatomic single-electron devices were demonstrated: a quantum bit [1-3], a quantum logic gate [4], devices for quantum metrology [5, 6], ultrasensitive charge sensors for biological applications [7]. The accuracy of simulation implemented impurities in depth largely determines the performance of the microcircuits elements. Implantation energies in the range of tens to hundreds keV are used to produce such structures.

There is a well-developed theory of interaction for accelerated charged particles with a solid body and there is an extensive experimental database for higher energies. Despite this, the programs that simulate penetration of impurities in the target, often exhibit the result characterized by tens of percent of that observed in the experiment [8-10].

The effect of irradiation on the target structure, especially in the case of single crystals, is an extremely important factor in the application of semiconductors. Creation of thin films of high crystallinity level is required for high-frequency semiconductor technology with a high degree of integration. In some cases, the creation of thin-film structures requires the removal of crystal lattice defects obtained during the growth of layers of one material on a crystalline substrate of another material. The ion implantation method in combination with high-temperature recrystallization makes it possible to obtain multilayer structures of a high crystallinity level when the parameters of the film and substrate lattices vary within 10%. In particular, the works [11-13] shows the effect of defect formation under the effect of irradiation on the quality of the recrystallized silicon film. The defects formation in the crystal structure of silicon at different irradiation parameters is considered in work [14]. According to the results of works, the direction of recrystallization and the quality of the resulting film depend of destruction level of the defective layer, as well as the location and thickness...
of the undamaged layer serving as a seed for recrystallization. Since the defect formation process under ion irradiation has not been sufficiently studied. It is necessary to select ion irradiation parameters for obtaining films of the best quality, which is a resource-consuming task.

This paper present the experimental results on the study defect distribution profiles formed after the implantation of iron ions with energies of 90 and 250 keV into a silicon single crystal. The experimental data were compared with calculations obtained with the TRIM program. The choice of iron ions for modifying the silicon conditioned by that this material has a promising magnetic and optical properties [11,15,16]. Iron can form silicides. It is necessary to determine the impact of this effect on the defect distribution profile. For this, implantation of xenon ions with energies of 100 and 200 keV was carried out.

2. Experimental technique
Implantation was performed based on HVEE-500 heavy ion accelerator complex [17]. Experiments of implantation iron ions Fe⁺ with the ion beam energies of 90 and 250 keV and xenon ions with energies of 100 and 200 keV in silicon Si(110) were carried out. The implantation energy is chosen to explore the expected difference between the experimental distribution profiles implanted particles with theoretical calculations at an energy in the range from 1 to 4 keV/nucleon. To minimize the effect of ordering the target structure on the dopant distribution profile, the dose of 10¹⁶ ions/cm² was selected. At xenon implantation, the doses were 7.7×10¹⁴ cm⁻² at 100 keV and 2.6×10¹⁵ cm⁻² at 200 keV.

Upon irradiation, the sample was scanned by a beam in two mutually perpendicular directions to achieve uniformity of the lateral distribution of the impurity. The samples were studied using the Rutherford backscattering method by 1800 keV He⁺ ions with a backscattering angle 165° [18].

The calculation of the implemented particles distribution profiles was performed using the TRIM program [19,20]. Program is based on the Monte Carlo method with the following assumptions: collisions are considered paired, target material - completely amorphous, not taken into account the recombination of interstitial atoms with vacancies, changes in the structure and composition of the target at the time of implantation are absent, that is the ions are always implanted into the net and a static target.

3. Results and discussion
Table 1 shows the parameters of the experiments and the corresponding value of average projected range. Doses are given in units of dpa - the number of displacements per atom. This method is universal. This makes it possible to compare the profiles of defects obtained by irradiation with different elements at different energies, doses [ion/cm²], and other parameters of irradiation. Dose recalculation from units [ion / cm²] to dpa units was carried out using TRIM.

| Ion type | Energy  | Dose   | Average projective range, nm | Straglling, nm |
|----------|---------|--------|-----------------------------|----------------|
|          | keV/    | keV    | DPA            | ion/cm² | 220 | 80 |
| Fe⁺      | 1,6     | 90     | 48.6           | 10¹⁶    | 50  | 80 |
|          | 4,6     | 250    | 41.2           | 10¹⁶    | 220 | 170|
| Xe⁺      | 0.8     | 100    | 6.0            | 7.7×10¹⁴ cm⁻² | 65  | 40 |
|          | 1.5     | 200    | 2.1            | 2.6×10¹⁴ cm⁻² | 120 | 50 |

A comparison of the defect profiles, determined experimentally, with the defect profiles calculated by the TRIM program was performed. The selected dose in dpa units for 90 keV energy was 48.6 dpa, and for energy 250 keV - 41.2 dpa. A comparison of the defect distribution determined experimentally (curve A) with a defect profile calculated by TRIM (curve B) for an beam energy of 90 keV is shown in Figure 1. The RBS amorphisation parameter shows the ratio of the signals to the spectra taken in the channeling direction and in the direction not containing the open channels. In comparison with the theoretical calculations, the authors considered the silicon single crystal to be completely disordered when the number of displacements is equal to the number of atoms in the layer. That is, the completely
disordered region on the experimental defect distribution corresponds to $4.9 \times 10^{22}$ vacancies/cm$^3$ on the graph of the theoretical distribution (shown by a solid red line). According to TRIM calculations, such a number of displacements is observed at a depth of 155 nm. However, according to experimental data, amorphization is observed only to 110 nm, which is 30% less than the theoretical value. Further, the disordering level falls to 35% at 180 nm from the surface. The absence of a fall in the yield of the backscattered particles to the level of the initial structure in the channeling regime is explained by the dechanneling of the helium ion beam as it passes deep into the crystal through the region destroyed by the ion irradiation.

Figure 2 compares the defect distribution profiles determined experimentally (curve A) with the defect profile calculated by TRIM (curve B) for the beam energy of implanted ions of 250 keV. According to the experimental curve, amorphization occurred only at 54 nm. And up to a depth of 360 nm, the average RBS disorder was 95%. According to calculations, amorphization occurs at a depth of up to 365 nm. In addition, for these experiment parameters, the formation of defects deeper than 450 nm does not occur. However, according to the experimental data at 450 nm, the RBS amorphisation parameter is 60%. In this case, in contrast to figure 1, there are more decanalized particles, since the ion irradiation modified layer is thicker.

A similar difference in the experimental data with the TRIM calculation is also observed in the analysis of the impurity distribution profiles [21].

The observed difference between the results can be caused by the fact that TRIM does not take into account the effect of the radiation dose on the character of defects accumulation. Therefore, smaller doses were chosen for the following experiments. That the peak from the impurity was as well visible on the RBS spectra, xenon was chosen as the impurity. It is an element with a larger atomic mass and, consequently, with a large scattering cross section. Similarly, since xenon is a noble gas, unlike iron, it does not form silicides, which could also affect the defect profile.

Consider the profile of the defects formed during the 200 keV xenon implantation of xenon (Figure 3). What is 1.5 keV/nucleon. This energy is close to the case of 90 keV (1.6 keV/nucleon) iron implantation. The dose was 2.1 dpa, which is an order of magnitude less than with the corresponding of iron implantation. The figure shows that according to TRIM, the number of displacements corresponding to complete amorphization is observed at a depth of 105 nm, and according to the experimental data – 65 nm. The discrepancy between the theoretical and experimental data was 38%. A similar discrepancy was observed in the 90 keV iron implantation.

Now consider the defects profile produced by implantation with a larger dose, but less energy: $7.7 \times 10^{14}$ cm$^{-2}$; 100 keV (0.8 keV/nucleon). The corresponding profile is shown in Figure 4. According to the experimental curve, amorphization occurred only to a depth of up to 35 nm. According to
calculations, amorphization occurs up to 77 nm. In this case, the discrepancy between the theoretical and calculated data is 55% and it is even greater than in the previous case.

Figure 3. Defects distribution profile formed after 200 keV Xe\textsuperscript{+} ions irradiation. A – experimental data; B – TRIM simulation.

Figure 4. Defects distribution profile formed after 200 keV Xe\textsuperscript{+} ions irradiation. A – experimental data; B – TRIM simulation.

4. Conclusion
An analysis of the defects formed at 1.6 keV/nucleon and a dose of 48.6 dpa shows that TRIM gives an overestimate of 30%. According to experimental data, with an energy increase to 4.6 keV/nucleon, there is no complete disordering of the crystal structure of silicon by the penetration depth of iron ions. However, the calculation for these implantation parameters in the TRIM program shows the formation of a significantly larger number of vacancies. The use of the dpa dimension in the study of defect formation is not clear and convenient.

In the study of defects formed after 1.5 keV/nucleon Xe\textsuperscript{+} implantation with dose of 2.1 dpa, also there is a significant discrepancy (38%) of the experimental data with the calculation results. With a further decrease in energy to 0.8 keV/nucleon, the divergence increases to 55%.

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