Calculation of the spatial distribution of defects and cascade-probability functions in the materials

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Abstract. In this article we carried out the calculations of the depth distribution of implanted ions of arsenic and indium, loss of energy and cascade-probability functions in silicon. Comparison of the calculations with the experimental data is in the satisfactory agreement. The computer simulation and analysis of the characteristics of ions depending on the depth of penetration and the number of interactions were carried out.

1. Introduction
It is known that the high-energy particles produce in solids, as well as in semiconductor materials, a number of consecutive interactions with electrons and atoms condensed matter. As a result the energy of the primary and secondary radiation is transferred to this substance that causes the radiation-chemical transformations in the material by the ionization and excitation of atoms and molecules. In addition we observe the cascade of secondary particles (primary sputtered atoms) having a sufficiently high kinetic energy to generate secondary sputtered atoms and molecules. It should be noted that the charged particles (electrons, ions, etc.) produce in condensed media direct ionization of atoms and molecules, and the photon and neutron radiations produce indirect ionization due to the interaction of this radiation with the medium, whereby the charged particles are formed.

Further, electrons and atoms of a material, absorbing the energy of the primary interactions become ancestors of a large number of further consecutive interconnected events at the atomic and molecular level, which ultimately leads to a change in the structure and various properties of the irradiated material. Consequently, after irradiation we can observe the irreversible changes in the structure and properties of materials accompanied by a set of effects that are characterized by dose or integral effects, since the degree of their activity depends primarily on the energy and intensity of the radiation and absorbed dose. As a rule, radiation effects occur at the atomic and molecular level in the form of various radiation-induced defects.

The most typical type of radiation defects in the structure of solids are Frenkel pairs in the form of interstitial atoms and vacancies in the crystal lattice. In this case, the colliding neutral or charged particles interact elastically with the nucleus (the target) and shift their its field of the nodes of crystal lattice [1-4]. At the elastic interaction the total kinetic energy of the displaced atom and the primary particle remains unchanged. The primary knock-on atom with kinetic energy sufficient for subsequent interactions with the atoms of the crystal lattice, may cause further displacement.
regularities of formation of the secondary displaced atoms are considered in various models and theories of cascades. Moreover, different types of ionizing radiation have different ability of formation of secondary etc. displacements [1-3].

Despite the large amount of works in this field, there are little calculations and analysis of the characteristics of interactions and the depth of observation. In this paper, we carried out the calculations of the spatial distributions of defects, loss of energy, concentration of knocked-on atoms and cascade-probability functions in silicon irradiated by ions of arsenic and indium.

2. Calculation procedure
The computer simulation of the spatial distributions of implanted ions was carried out using the standard program Srim.

The calculations of cascade-probability functions (CPF) were made by the formula (2):

$$\psi_n(h, E_0) = \frac{1}{n! \sigma_0^n} \left( \frac{E_0}{E_0 - kh} \right)^{-l} \exp \left( \frac{h}{\frac{E_0}{E_0 - kh}} \right)^* \left[ \ln \left( \frac{E_0}{E_0 - kh} \right) \frac{ak}{1} - h \right]^n,$$

where $h$ is the depth of the particle detection, $n$ is a number of interactions, $E_0$ is the energy, $K$ is the specific particle energy loss factor, $\sigma_0, a, l$ are the approximation coefficients.

The CPF has the following physical meaning: it is the probability that the primary particle with energy $E$ reaches a depth $h$ after $n$ interactions.

For ions unlike electrons, protons and $\alpha$-particles dependence of the approximation coefficient of cross section on energy is represented as:

$$\sigma(h) = \sigma_0 \left( \frac{1}{a(E_0 - kh)} - 1 \right).$$

In finding the approximation parameters of (1) and (2) we used the following (Table 1):

1. The cross section of atom-atom interactions were calculated by the Rutherford formula.
2. The observation depths and other parameters were found out using tables of parameters of the spatial distribution of ion-implanted impurities [3].

2. Results and discussion
As an example, Figures 1 - 4 show the distribution of implanted ions of arsenic and indium and energy loss in depth in irradiated silicon as a function of depth for different energies of the incident ions: 1 – 245; 2 – 350; 3 – 500 keV.

The distribution curves of implanted ions for different energies as for arsenic and indium have distinct maxima, and their concentration is irregularly distributed across the depth of silicon.

As calculations show the distribution of energy losses for the ionization and excitation in the depth of the material represents quite sharply decreasing functions. The distributions of knocked-on atoms in depth at a certain extent repeat the distribution of the implanted impurity. Comparing the calculations of the distributions of implanted particles for arsenic (245 keV) and indium (350 keV) in silicon, we can observe a good agreement between them. The small difference of calculations and experimental data [5] for arsenic is connected with the incomplete survey on the temperature environment effect.
The calculations of cascade-probability functions were performed in double precision over the entire interval of observation depths. The correlation coefficient (Table 1) between $\sigma$ calculated by the formula (2) and using the Rutherford formula is more than 0.99, that testifies about a good approximation (2). The calculation results show that the CPF depending on $h$ and $n$ have the following behavior: they increase, reaching a maximum and then they decrease. The ratio dependence of the displacement of left and right boundaries of the domain results CPF on the penetration depth for arsenic (245 keV) and indium (350 keV) in silicon are shown in Tables 2 and 3. It follows from them that the real region of existence of the CPF on various parameters displacement of boundaries (C1, C2, C3) may differ from $h/\lambda$ to 30%. Although all the curves at first glance have the same behavior, the areas of result findings are different. All the CPF dependencies are located in a very narrow range of depths and number of interactions. Depending on $n$ the CPF with increasing the depth of observation is displaced to the right, the function value at the maximum point is decreased, the distance between two adjacent curves increases. With the increase of atomic weight of the incident particle and the target the CPF behavior is similar. Depending on $h$ the CPF with increasing number of interactions is also shifted to the right, the values of functions at the maximum point decrease, with increasing atomic number of the incident particle and the target the distance between two adjacent curves, the real area a results finding and the values of the maxima are significantly decreased (Figures 5 and 6). The obtained results can significantly improve understanding of radiative processes in materials and simplify the calculations of other parameters and characteristics of the particles and defects.

**Figure 1.** The distribution of the implanted As in depth of silicon at the irradiation by ion beams of different energies

1 – 245 keV; 2 – 350 keV; 3 – 500 keV; 4 – experiment (245 keV)
Figure 2. The distribution of the energy loss in depth when irradiated silicon by As ions of the different energies.

1 – 245 keV; 2 – 350 keV; 3 – 500 keV

Figure 3. The distribution of the implanted In in depth of silicon when bombarded by the streams of the particles of the different energies.

1 – 245 keV; 2 – 350 keV; 3 – 500 keV; 4 – 350 keV; experiment
1 – 245 keV; 2 – 350 keV; 3 – 500 keV

**Figure 4.** The distribution of the energy loss in depth when irradiated silicon by In ions of the different energies

**Table 1.** The approximate parameters for arsenic and indium in silicon

| $E_0$, keV | $\sigma_0 \times 10^4$ | $a$ | $E_0$ | $k$ | $\eta$ | $\chi^2$ |
|------------|-----------------|-----|-------|-----|-------|---------|
| 245 arsenic | 0.39188 | 0.23283 | 0.74915 | 1311.42461 | 0.99619 | 14.85065 |
| 350 indium  | 0.7804  | 0.15684 | 0.66457 | 1108.63961 | 0.99372 | 225.53162 |

**Table 2.** The ratio dependence of the displacement of left and right boundaries of the domain results CPF on the penetration depth for arsenic in silicon at $E_0 = 245$ keV

| $h \times 10^4$, cm | $h/\lambda$, cm | $C_1$, % | $C_2$, % | $N_h$ | $C_3$, % |
|---------------------|-----------------|---------|---------|-------|---------|
| 1                   | 116611          | -9.1    | 12.5    | 500   | 3.4     |
| 2                   | 306622          | -20.24  | 22.15   | 1000  | 1.91    |
| 3                   | 651245          | -28.625 | 29.58   | 2200  | 0.955   |
| 4                   | 1421513         | -29.36  | 29.65   | 6500  | 0.29    |

**Table 3.** The ratio dependence of the displacement of left and right boundaries of the domain results CPF on the penetration depth for indium in silicon at $E_0 = 350$ keV

| $h \times 10^4$, cm | $C_1$, % | $C_2$, % | $N_h$ | $C_3$, % | $h/\lambda$, cm |
|---------------------|---------|---------|-------|---------|-----------------|
| 1.5                 | -13.75  | 15.1    | 1300  | 1.35    | 689775          |
| 2                   | -18.68  | 19.7    | 1900  | 1.02    | 1044469         |
| 2.5                 | -23.25  | 24.05   | 2400  | 0.8     | 1506130         |
| 3                   | -27.12  | 27.685  | 3000  | 0.565   | 2128270         |
| 3.5                 | -29.65  | 30.035  | 4500  | 0.385   | 3007239         |
| 4                   | 29.925  | 30.14   | 8000  | 0.215   | 4335823         |
3. Conclusions

1. The computer simulation of the implanted arsenic and indium ions distributions in depth with energies $E = 245$, $350$ and $500$ keV, as well as energy loss in the silicon. It was found that the curves for different energies for arsenic and indium in silicon have distinct maxima, and their concentration is irregularly distributed in depth. With the energy increasing the curves are shifted to the right and the value of their maxima decreases. Comparison of the calculations for arsenic (245 keV) and indium (350 keV) gives a good agreement with experiment.
2. The calculations show that the distribution of energy losses for the ionization and excitation in the depth of the material (arsenic and indium in silicon) represents quite sharply decreasing functions for all the calculated energies (245, 350, 500 keV).

3. The computer modeling of cascade-probability functions depending on the depth of penetration of arsenic and indium in silicon was carried out. As it follows from the calculations, all CPF dependences are located in a very narrow range of depths and number of interactions. Depending on $n$ the CPF are shifted to the right relatively $h/\lambda$ with increasing the depth of observation, the value of the maximum point is decreased. With increasing atomic weight of the incident particle and the target the CPF behavior is similar. Depending on the depth the CPF (relative to $h/\lambda$) with increasing number of interactions is also shifted to the right, the values of functions at the maximum point and the real area of the result finding is significantly decreased.

4. The analysis of the characteristics of ion was executed depending on the depth of penetration and the number of interactions. It is found that the approximation coefficient of the cross section (Eq. 2) is quite good (with a correlation coefficient of more than 0.99) describes a similar value calculated using the Rutherford formula and energy losses listed in Tables Kumahova-Komarova. The percentage displacement of the left and right boundaries of the domain results of the CPF depending on the penetration depth for arsenic and indium ions in silicon (C1, C2, C3) may differ (relative $h/\lambda$) by 30%.

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