2-блм **Раздел 2** **Section 2**

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MATHEMATICAL MODELING OF RADIATION DEFECT FORMATION PROCESSES ON LIGHT TARGETS

The article analyzes the problem of studying the mechanisms of radiation defect generation in materials under ion irradiation. During the research, algorithms were developed to calculate the cascade-probability function (CPF) and the concentration of cascade regions as a function of the depth of the irradiated material, which allowed for an increase in the accuracy of modeling defect formation processes. The calculations of the CPF and the concentration of cascade regions revealed patterns in the behavior of radiation defects depending on the physical parameters of irradiation. The comparison of the obtained calculated data with experimental results confirmed the validity of the developed algorithms and models. A distinctive feature of the proposed method is the application of an analytical cascade-probability approach, which allows tracking the dynamics of defect formation at any depth of the target, unlike traditional numerical methods that require significant computational resources.

These results can be explained by the fact that the process of particle interaction with matter and the formation of radiation defects is probabilistic, allowing for the determination of the probabilities of ion interactions with materials (CPF) at any depth of the irradiated material, which enables more accurate modeling of defect formation processes and their dependence on physical parameters such as energy and depth. The developed models and algorithms can be applied in materials science, micro- and nanoelectronics, and in predicting the radiation resistance of structural materials.

Key words: ion, algorithm, ion implantation, cascade-probabilistic function, concentration of radiation defects.

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Математическое моделирование процессов радиационного дефектообразования на легких мишенях

В данной статье анализируется проблема изучения механизмов генерирования радиационных дефектов в материалах при ионном облучении. В процессе исследования были созданы алгоритмы для расчета каскадно-вероятностной функции (КВФ) и концентрации каскадных областей в зависимости от глубины облучаемого материала, что дало возможность повысить точность моделирования процессов дефектообразования. Выполненные расчеты КВФ и концентрации каскадных областей позволили выявить закономерности поведения радиационных дефектов в зависимости от физических параметров облучения. Сопоставление полученных расчетных данных с экспериментальными результатами подтвердило достоверность разработанных алгоритмов и моделей. Отличительной чертой предложенного метода является применение аналитического каскадно-вероятностного подхода, который позволяет отслеживать динамику дефектообразования на любой глубине мишени, в отличие от традиционных численных методов, требующих значительных вычислительных ресурсов.

Эти результаты объясняются тем, что процесс взаимодействия частиц с веществом и образования радиационных дефектов является вероятностным и позволяет получить вероятности взаимодействия ионов с материалами (КВФ), на любой глубине облучаемого материала, что позволяет более точно моделировать процессы дефектообразования и их зависимость от физических параметров, таких как энергия, глубина. Разработанные модели и алгоритмы могут быть применены в материаловедении, микро- и наноэлектронике, при прогнозировании радиационной стойкости конструкционных материалов.
Ключевые слова: ион, алгоритм, ионная имплантация, каскадно-вероятностная функция, концентрация радиационных дефектов.

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Жеңіл нысталарда радиациялық дектіктердің қалыптасу процестерін математикалық модельдеу

Мақала ион сәулеленуі кезінде материалдардағы радиациялық ақауларды генерациялау механизмдерін зерттеу мәселесін талдайды. Зерттеу барысында сәулеленген материалдың тереңдігіне байланысты каскадты ықтималдық функциясын (КЫФ) және каскадтық аймақтардың концентрациясын есептеу үшін алгоритмдер әзірленді, бұл ақау түзілу процестерін модельдеудің дәлдігін арттыруға мүмкіндік берді. КЫФ және каскадтық аймақтардың концентрациясы бойынша жүргізілген есептеулер радиациялық ақаулардың физикалық сәулелену параметрлеріне байланысты мінез-құлқын анықтауға мүмкіндік берді. Алынған есептік деректерді эксперименттік нәтижелермен салыстыру әзірленген алгоритмдер мен модельдердің дұрыстығын растады. Ұсынылған әдістің ерекшелігі - ақау түзілу динамикасын мақсаттың кез келген тереңдігінде бақылауға мүмкіндік беретін аналитикалық каскадты ықтималдық тәсілін қолдану, дәстүрлі сандық әдістердің едәуір есептеу ресурстарын талап ететіндігімен салыстырғанда.
Бұл нәтижелер бөлшектердің затпен өзара әрекеттесу және радиациялық ақаулардың түзілу процесі ықтималдықты болып табылатындығымен түсіндіріледі, бұл иондардың материалдармен (КЫФ) өзара әрекеттесу ықтималдықтарын сәулеленген материалдың кез келген тереңдігінде анықтауға мүмкіндік береді, бұл ақау түзілу процестерін және олардың энергия, тереңдік сияқты физикалық параметрлерге тәуелділігін дәл модельдеуге мүмкіндік береді. Дамытылған модельдер мен алгоритмдер материалтану, микро- және наноэлектроникада, конструкциялық материалдардың радиациялық төзімділігін болжауда қолданылуы мүмкін.
Түйін сөздер: ион, алгоритм, иондық имплантация, каскадты-ықтималдық функция, радиациялық ақаулардың концентрациясы.

1 Introduction

Research in the field of ion implantation and radiation-induced defect formation has been conducted and continues to be an important topic for the scientific community to this day.

This area is particularly relevant for the advancement of science in Kazakhstan, as many organizations are engaged in experimental studies on the effects of various types of radiation, including electron (1–10 MeV), proton and alpha (1–50 MeV), and ion (100–1000 keV) irradiation. There is a need for further explanation and analysis of experiments related to ion irradiation.

The relevance of the topic is confirmed by a number of factors. First, with the increasing consumption of materials and the growing demands for their properties, it is essential to

develop new methods for their production and processing. It is expected that in the coming years, the demand for structural materials will significantly increase, highlighting the need to optimize ion irradiation processes to enhance radiation resistance and other key properties of materials. Second, the results of research in this area can have a substantial impact on their practical applications. The development of algorithms for calculating defect distribution will allow for more accurate predictions of material behavior under various operating conditions. This, in turn, could lead to the creation of more efficient and reliable structural materials, contributing to the advancement of technologies and increasing their competitiveness in the market. For example, the Institute of Nuclear Physics in Almaty has a proton accelerator and an alpha-particle accelerator (light ions), a cyclotron, and a nuclear reactor. The Eurasian University in Astana has an ion accelerator, and work is being conducted at the National Nuclear Center in the city of Kurchatov. Similar research is being carried out in countries near and far abroad.

Previously, mathematical models were developed to describe the processes of radiation defect formation within the framework of an analytical CP-method using the simple CPF (probability of transition in n steps) that did not account for energy losses due to ionization and excitation. Mathematical models have been developed taking into account energy losses for alpha particles, protons, electrons and ions. Unlike electrons, protons, and alpha particles, for ions it is necessary to find the actual result area for calculating transition probabilities and the concentration of cascade regions.

The object of the study is a solid body. The subject of the research is the CPFs depending on the number of interactions and the depth of particle penetration, the concentration of cascade regions during ion irradiation. The aim of the research is to mathematically model the processes of radiation defect formation in materials irradiated with ions, taking into account energy losses. Accordingly, the following tasks have been formulated:

- to develop algorithms for calculating the CPFs and the concentration of cascade regions as a function of the depth of the material irradiated with ions, and to create a software package (SP) for performing the calculations of these characteristics;
- to carry out calculations of the CPFs and the concentration of cascade regions;
- to verify the developed algorithm through a comparison of the simulation results with experimental data..

2 Literature review and problem statement

The paper [1] presents the results of research aimed at assessing the suitability of glassy carbon as a material for packaging nuclear waste. It is shown, that ion bombardment with xenon leads to the amorphization of the glassy carbon structure, which is confirmed by Raman spectroscopy analysis. However, unresolved questions remain regarding the influence of defects and radiation damage on the microstructure and surface of glassy carbon. This may be due to objective difficulties related to the lack of data on the behavior of glassy carbon under radiation exposure. A way to overcome these difficulties could be the use of computer modeling methods to predict material behavior. This approach was used in article [2], but the results indicated that a broader range of factors affecting the microstructure needs to be considered. All of this suggests that it is advisable to conduct research for a deeper understanding of the impact of radiation defect formation.

In article [3], the problem of understanding how the energy transferred to electronic and atomic subsystems can affect defect dynamics in materials is addressed. The interaction of displacement and ionization cascades induced by irradiation in silicon carbide (SiC) is investigated. It is shown that under ion irradiation, a delay in damage accumulation is observed, which linearly depends on both the increase in ionization and the energy transferred to the material. However, unresolved questions remain regarding the evolution of defects and their influence on material properties. This may be due to the limitations of existing models, making the investigation of this issue relevant. A way to overcome these difficulties could be the use of more complex models, such as Monte Carlo methods, which are classified as statistical trial methods and are numerical approaches to solving mathematical problems by predicting random variables. This method began to be widely applied in the 1970s for statistical modeling of particle trajectories and calculating the energy distribution transferred from ions to the atoms of the material. This approach was used in article [4], allowing for the calculation of particle penetration depth and the determination of radiation defect concentrations, such as vacancy clusters and interstitial atoms, which became the basis for quantitative analysis of radiation damage to materials. However, the results indicated that the dynamics of defect interactions need to be considered, as the algorithm only allows for the calculation of the distribution and concentration of primary defects, without accounting for their subsequent evolution.

In article [5], the method of pulsed ion bombardment was used to investigate the interaction of noble gas ions with potassium tantalate (KTaO3) and its influence on damage formation and amorphization. It was shown that the mechanism of amorphization is primarily due to defects caused by ion irradiation. However, the results indicated that additional factors influencing defect dynamics need to be considered.

Article [6] presents the results of a study dedicated to the formation of nanostructured TiAlN coatings on AISI 304 stainless steel substrates using reactive magnetron sputtering. It is shown that irradiation of the coatings with argon ions at an energy of 200 keV leads to changes in their mechanical properties, including hardness and Young's modulus. However, the calculations only considered the distribution of implanted ions, not the defects generated by them.

Article [7] employs a more detailed analytical method, such as scanning electron microscopy. However, the results indicated that the influence of various irradiation conditions on mechanical properties needs to be taken into account.

Thus, existing research highlights the need for further investigation into the effects of ion implantation and irradiation on material properties, opening new horizons for scientific research.

One of the key issues of ion implantation is the formation of radiation defects. First and foremost, it is essential to know the distributions of defects generated in atomic collision cascades. Despite the well-known numerical methods and models, analytical methods have undeniable advantages over them, even if they can only approximate certain phenomena. In this regard, a cascade-probabilistic method has been developed using a CPF, which allows for the creation of mathematical models in analytical form and, consequently, provides the opportunity to track the entire defect formation process at any depth of the irradiated material dynamically.

Previously, a simple CPF was used [8], which did not account for the actual changes in

the range and angle of ejection of particles after each collision. This is not always justified, especially if the interaction range depends on energy. Such an approach can at best be used only for estimating results. Therefore, work has been conducted in this direction, resulting in mathematical models of the CPF that consider energy losses, the dependence of range and cross-section on energy for electrons, protons, alpha particles, and ions [9, 10].

This research aims to address the specified problems, which will allow for the management of defect generation and evolution, ultimately leading to the production of materials with desired properties.

3 Materials and methods

The interaction cross-section for ions is calculated using the Rutherford formula [11]. The observation depths are based on data from tables [12]. The obtained interaction cross-section values are approximated by the following expression:

$$\sigma(h) = \frac{1}{\lambda_0}\left(\frac{1}{a(E_0 - kh)} - 1\right), \tag{1}$$

where λ_0, a, k, E_0 – approximation parameters.

It is not possible to use the provided formula (1) from [13] for the calculations of the CPF, as it leads to overflow issues when λ_0 is small or when n takes on large values (which can reach several million). By modifying this formula, we obtain:

$$\psi_n(h', h, E_0) = exp\left(-\left(\frac{h - h'}{\lambda_0}\right) + \frac{1}{\lambda_0 ak} ln\left(\frac{E_0 - kh'}{E_0 - kh}\right)\right) * \prod_{i=1}^{n}\left(\frac{h - h' - \frac{ln\frac{(E_0 - kh')}{(E_0 - kh)}}{ak}}{\lambda_0 i}\right), \tag{2}$$

where n – number of interactions; h', h – depths of ion generation and registration, $l = \frac{1}{\lambda_0 ak}$

In order to optimize the algorithms for calculating the CPF as a function of n and h, as well as the concentration of cascade regions, Stirling's formulas (5) and (6) from [14] are applied. To automate the determination of the CPF result area based on n, h, and the concentration of cascade regions, Binary [15] and Ternary [16] search algorithms are used. When ions interact with matter, defects are formed in the form of cascade regions, which consist of vacancy clusters and interstitial atom aggregates.

To calculate the concentration of cascade regions, the following formula from [9] is used:

$$C_k(E_0, h) = \int_{E_c}^{E_{2max}} W(E_0, E_2, h)\, dE_2, \tag{3}$$

$$E_{2max} = \frac{4(m_1 c^2 m_2 c^2)}{(m_1 c^2 + m_2 c^2)^2} E_1,$$

E_1 – the energy of the particle after energy losses at h, E_0 – the initial energy of the ion, $C_k(E_0, h)$ is defined considering that the energy of the particle at depth h is $E_1(h)$, E_{2max} –

the maximum possible energy gained by an atom, E_c – the threshold energy, E_2 – the energy of the primary knocked-out atom, m_1c_2 – the rest energy of the ion, m_2c_2 – the rest energy of the atom.

The spectrum of primary knocked-out atoms (PKA) is calculated using the (4.26) from [9]. Modifying equation (3) , we obtain:

$$C_k(E_0,h) = \frac{E_d}{\lambda_2 E_c}\frac{(E_{2max}-E_c)}{(E_{2max}-E_d)}\sum_{n=n_0}^{n_1}\int_{h-k\lambda_2}^{h} exp\left(-\frac{h-h'}{\lambda_2}\right)\psi_n(h')\frac{dh'}{\lambda_1(h')}, \tag{4}$$

where $\psi_n(h')$ is used as (2), E_d – the average displacement energy, n_0, n_1 –the initial and final values of the number of collisions from the area of the CPF, k – is an integer greater than one.

$$\lambda_1(h') = \frac{1}{\sigma_0 n_0(\frac{1}{a(E_0-kh')}-1)} * 10^{24}\ (cm),$$

$$\lambda_2 = \frac{1}{\sigma_2 n_0} * 10^{24}\ (cm).$$

The cross-section σ_2 is calculated using the Rutherford formula; λ_1, λ_2 – are the mean free paths for ion-atomic and atomic-atomic collisions, respectively, $\sigma_0 = 1/\lambda_0$.

4 Results and discussions

When approximating curves, difficulties arise in specifying the initial data λ_0, a, E_0, and k in the approximation formula. The approximation expression best describes the cross-section values, as the theoretical correlation coefficient is sufficiently close to 1. The approximating curves of the dependence of σ on h are shown in Fig. 4.1. Table 1 presents the approximation parameters and the theoretical correlation coefficients for boron in silicon at various initial energy values. The targets are metal - aluminum and semiconductor - silicon.

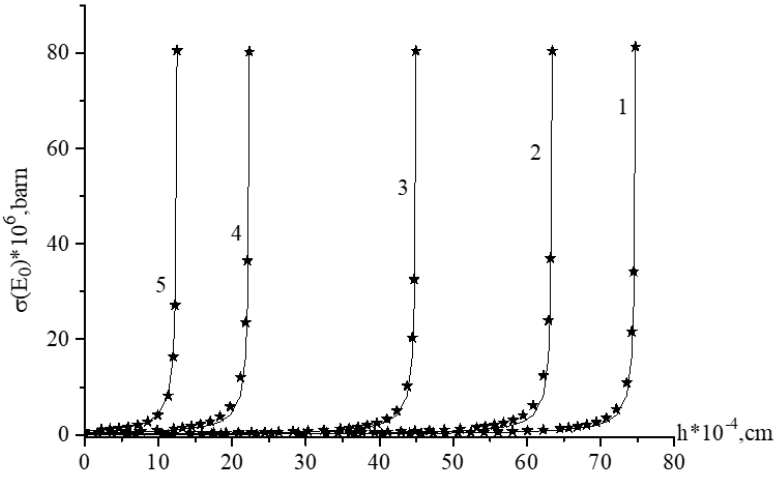

Figure 4.1: Approximation of the modified cross-section of the CPF for boron in silicon: $E_0 =$ 1000, 800, 500, 200, 100 (1-5) keV. Solid lines – approximation values, stars – calculated data for the dependence of the cross-section on h

Table 1: Approximation parameters for boron in silicon

E_0	$\sigma_0 * 10^6$	a	k	E_0'	η
1000	1,96808	0,2161	584,57	4,3801	0,9961
800	1,96898	1,199	91,07	0,57988	0,9954
500	1,61508	2,01	55,807	0,2519	0,9887
200	4,16808	0,254	921,908	2,0801	0,978
100	3101242	0,32	2342,4	3,041	0,9811

The CPF represents the probability that a particle generated at a certain depth h' will reach a specific depth h(registration depth) after n collisions.

Let's conduct a study of the CPF and examine its main properties:

1. Domain of the function: $E_0/ak(k-1) < h < E_0/k$.
2. $lim_{h\to h'}\psi_n(h', h, E_0) = 0$, $lim_{h\to h'}\psi_0(h', h, E_0) = 1$.
3. $lim_{k\to 0}\psi_n(h', h, E_0) = \frac{1}{n!}(\frac{h-h'}{\lambda})^n exp(-\frac{h-h'}{\lambda})$, that is the probability of transitioning over n steps, taking energy losses into account, reduces to the simplest CP-function without considering energy losses.
4. The sum of the CPF over all interactions is equal to 1, i.e., $K_\infty = \sum_{n=0}^{\infty}\psi_n(h', h, E_0) = 1$.
5. $lim_{n\to 0}\psi_n(h', h, E_0) = (\frac{E_0-kh'}{E_0-kh})^{-l} exp(\frac{h-h'}{\lambda_0}) = \psi_0(h', h, E_0)$
6. $lim_{n\to\infty}\psi_n(h', h, E_0) = 0$, that is the probability of a particle experiencing an infinite number of collisions while traversing a depth from h' to h is undoubtedly equal to zero.
7. $\int_{h'}^{h}\frac{\psi_n(h',h,E_0)dh}{\lambda(h)} = 1$, where $\lambda(h) = 1/(\sigma(h)n_0)$.

The results of the CPF as a function of n are presented in Figs. 4.2 and 4.3.

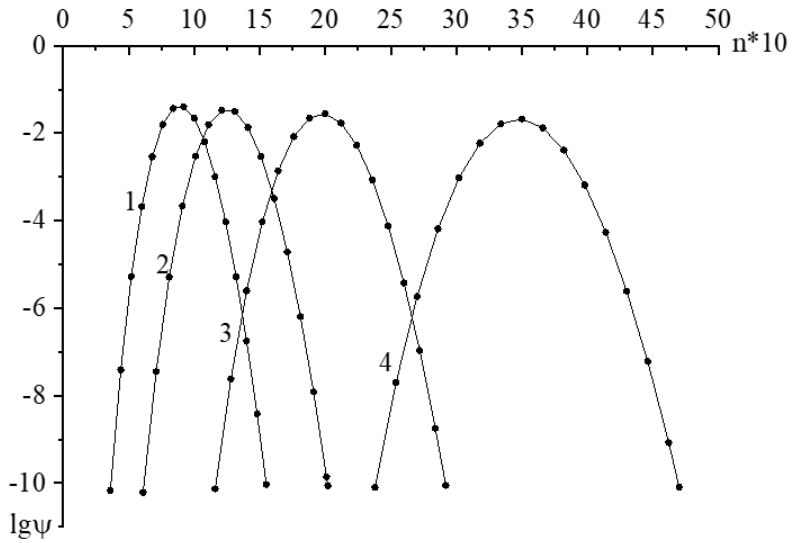

Figure 4.2: Dependence CPF on n for boron in silicon at $E_0 = 800\ keV$; $h = 5,0\times10^{-3}; 5,5\times 10^{-3}; 6,0\times10^{-3}; 6,3\times10^{-3}$ (cm.) (1–4)

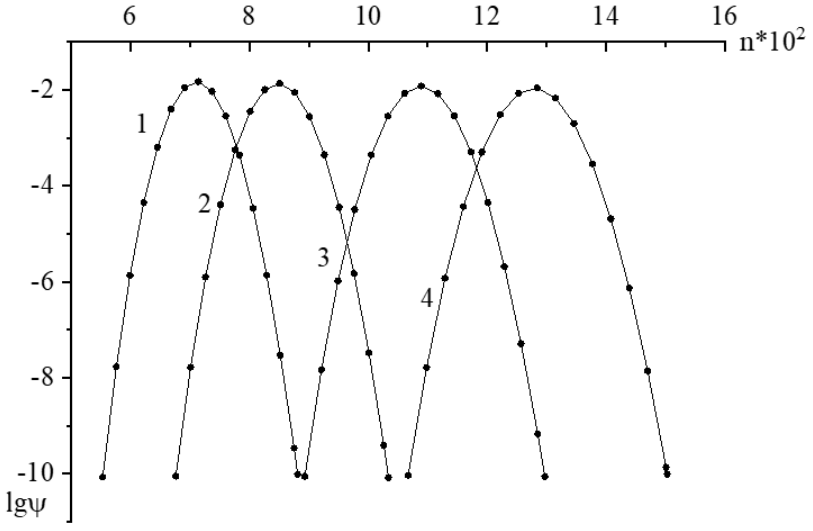

Figure 4.3: Dependence CPF on n for selenium in aluminum at $E_0 = 200\ keV$; $h = 1,5\times 10^{-4}; 1,7\times10^{-4}; 2,0\times10^{-4}; 2,2\times10^{-4}$ (cm.) (1–4)

The results of the CPF as a function of h are presented in Figs. 4.4 and 4.5.

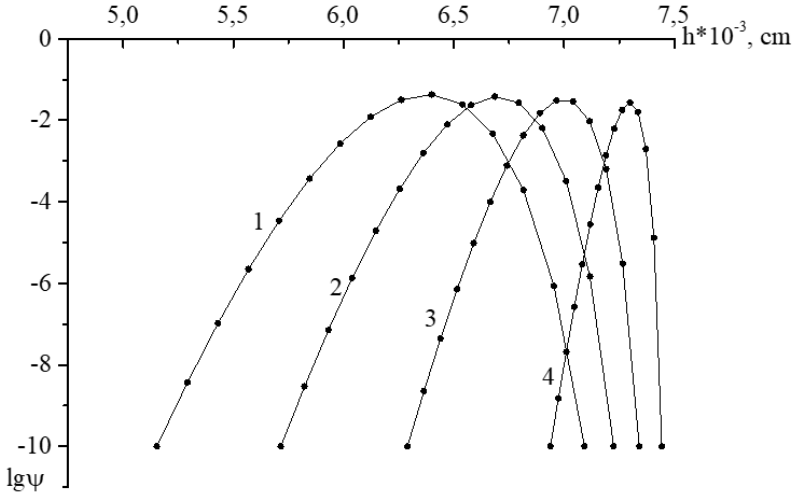

Figure 4.4: Dependence CPF on h for boron in silicon at $E_0 = 1000\ keV$; $n = 116611; 306622; 651245; 1421513$ (cm.) (1–4)

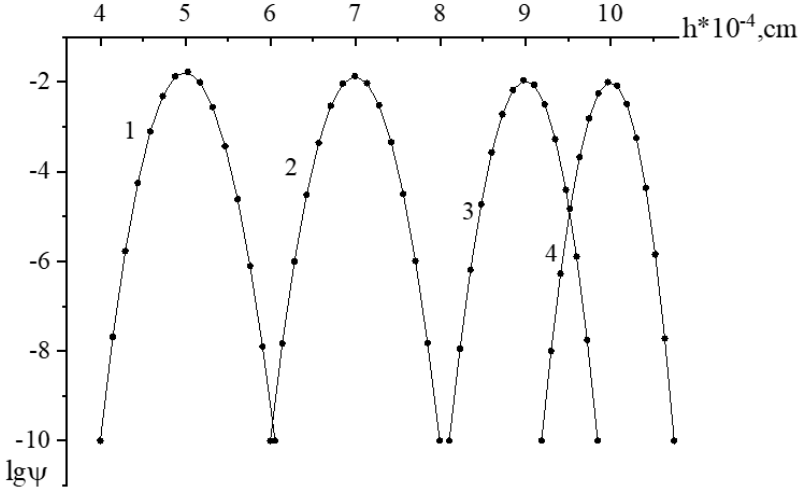

Figure 4.5: Dependence CPF on h for selenium in aluminum at $E_0 = 800\ keV$; $n = 549; 866; 1288; 1564$ (1–4)

The results of the calculations of the concentration of cascade regions for boron in silicon are presented in Fig. 4.6 and Table 2 and for selenium in aluminum in Fig. 4.7 and Table 3.

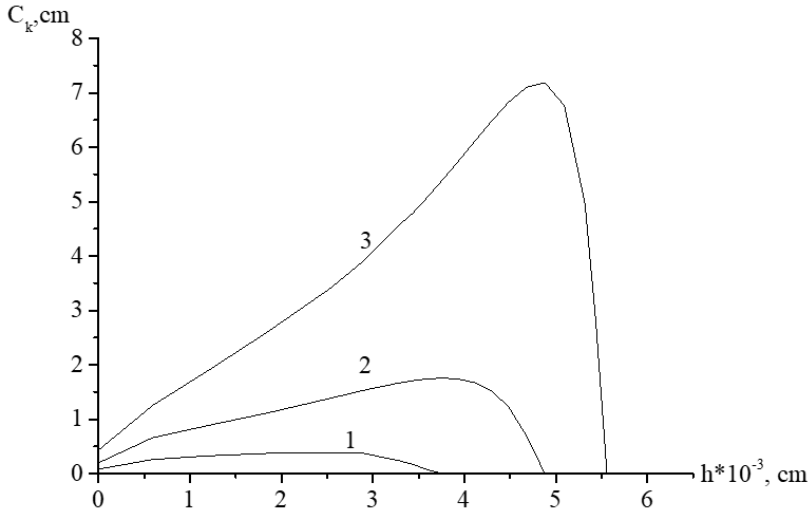

Figure 4.6: Dependence of concentration of cascade regions on h during the irradiation of silicon with boron ions for: $E_0 = 800\ keV$, $E_c = 200\ keV$ (1), 100 keV (2), 50 keV (3)

Table 2: The boundaries of the region for determining the concentration of cascade regions for boron in silicon at $E_c = 50\ keV$, $E_0 = 1000\ keV$

$h * 10^{-3}$, cm	C_k, cm	E_0, keV	n_0	n_1
0,1000	0,011332	1000	1	9
0,5000	0,1567	900	1	14
1,1286	0,52027	800	1	20
1,7200	0,946	700	1	27
2,3330	1,3808	600	1	34
2,9770	1,91	500	1	44
3,6600	2,61075	400	1	57
4,0270	3,0578	350	1	65
4,4070	3,5944	300	1	75
4,5860	3,6484	280	1	77
4,7270	4,1036	260	1	85
4,8930	4,3868	240	1	90
5,0640	4,536	220	1	96
5,2390	5,012	200	2	103
5,4204	5,3427	180	4	110
5,6080	5,63	160	6	119
5,8030	5,9128	140	9	129
6,0070	5,9962	120	13	141
6,2215	5,7033	100	18	156
6,4470	4,1819	80	25	175
6,5640	2,40099	70	30	187
6,6860	0	60	36	200

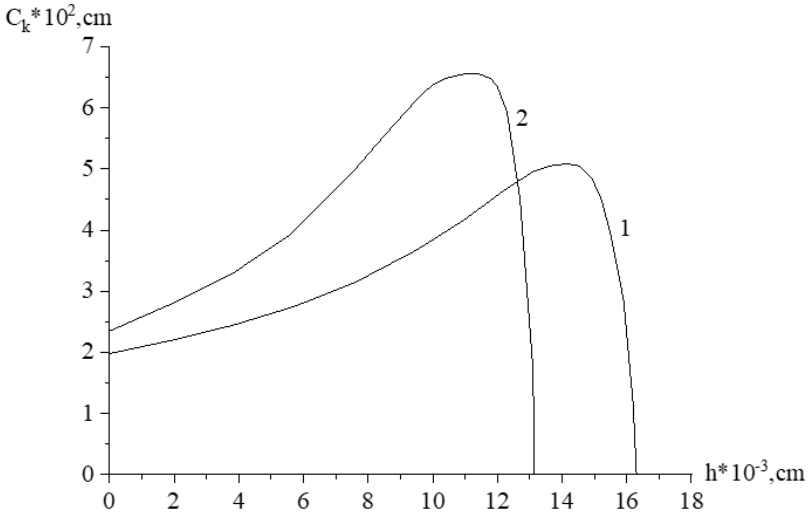

Figure 4.7: Dependence of concentration of cascade regions on h during the irradiation of aluminum with selenium ions for: $E_c = 100\ keV$, $E_0 = 1000\ keV$ (1), 800 keV (2)

Table 3: The boundaries of the region for determining the concentration of cascade regions for selenium in aluminum at $E_c = 50\ keV$ $E_0 = 1000\ keV$

$h * 10^{-4}$, cm	C_k, cm	E_0, keV	n_0	n_1
1,15	451,7	1000	21	173
2,21	477,7	900	74	288
4,33	544,8	800	214	521
6,71	417,84	700	320	678
8,49	412,58	600	429	831
10,23	406,59	500	671	1154
27,6	408,17	400	1713	2441
28,1	397,25	350	1749	2483
29,3	383,21	300	1835	2584
30,6	376,91	280	1925	2695
32,1	369,6	260	2036	2822
33,1	360,18	240	2109	2907
34,2	348,9	220	2189	3001
35,3	335,06	200	2270	3095
36,2	317,6	180	2336	3172
37,6	295,92	160	2440	3292
38,1	266,74	140	2477	3335
39,4	228,11	120	2573	3447
40,9	173,37	100	2686	3577
41,8	89,97	80	2754	3655
42,4	30,11	70	2799	3707

For comparison with experimental data, Fig. 8 shows the distributions of implanted boron

ions with depth in irradiated silicon as a function of depth at an energy of 50 keV.

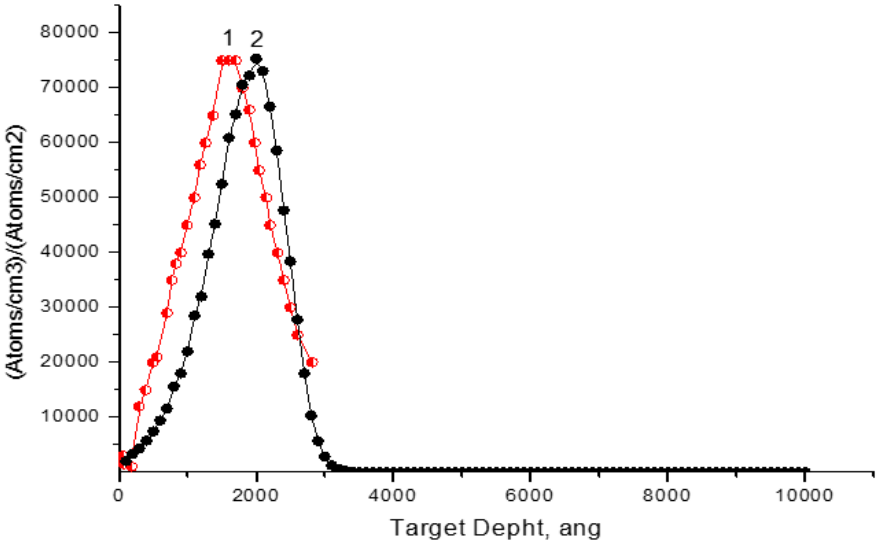

Figure 4.8: Distribution of implanted boron atoms with depth in Si: 1 – Experiment (50 keV); 2 – SRIM (50 keV)

The distribution of implanted boron atoms in Si exhibits clear maxima, and their concentration is unevenly distributed with depth. Comparing the calculated distributions of implanted boron ions (50 keV) in silicon with experimental data shows a good agreement. The slight discrepancies between the calculations and experimental data for boron are attributed to the incomplete consideration of the influence of the ambient temperature.

Unlike previously developed mathematical models of radiation defect formation that used simple CPF [8], this work proposes improved models that:

– take into account energy losses due to ionization and excitation of the medium's atoms, as well as the dependence of interaction range and cross-section on energy, achieving a closer agreement of the obtained results with physical experimental data (within 15%);

– they provide the ability to observe the entire process of ion interaction with the substance as a function of h.

Unlike electrons [17], protons [18], and alpha particles [19], modeling the interaction process of ions with matter is more complex [10], [13], [20–23]. In the proposed approach:

– it is possible to perform calculations for various incoming particles and targets from the periodic table;

– patterns of cascade regions distribution are identified based on threshold energy, penetration depth, and initial ion energy;

– the actual region of the result is found when calculating the transition probabilities and the concentration of cascade regions.

5 Conclusion

Algorithms and SP have been developed to calculate transition probabilities as a function of the number of collisions, the penetration depth of particles, and the concentration of cascade

regions for ions. This enables the identification of patterns in the behavior of radiation defects based on the physical parameters of irradiation. All CPF calculations were performed using (2) , and concentrations were calculated using (4) in C#, with MS SQL Server 2022 used as the database management system.

The developed SP enables the calculation of interaction cross-sections, ionization losses, observation depths, and the determination of approximation coefficients. The created algorithms have enabled the automation of the area of result finding and the identification of patterns in the behavior of this area.

An analysis of the CPF has been conducted, and the properties that these functions should possess have been outlined. A comparison of the calculation results of the distributions of implanted particles for boron (50 keV) in silicon has been made with experimental data.

The study of the distribution of implanted ions and energy losses is crucial for understanding the processes occurring during ion implantation. The application of the obtained results can significantly enhance the understanding of radiation processes related to defect formation in materials irradiated by charged particles.

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