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MODELING OF RADIATION PROCESSES OF DEFECT FORMATION IN MATERIALS IRRADIATED WITH IONS

Abstract

The consumption of materials is growing every day, which means that we will increasingly have to cope with the problems of natural resources and supply. Therefore, humanity is forced to expand its resource base finding ways to use existing raw materials more efficiently, turn previously unusable substances into useful materials and also produce completely new materials from substances that are available in abundance. One of the ways to create new materials is to irradiate a substance with charged ions. The article discusses this technique based on the cascade-probabilistic method, the purpose of which is to obtain as well as the next ensuing use of cascade-probabilistic functions (CPF) considering energy losses for ions. The CPF computations were executed depending on the number of collisions and the depth of surveillance for various incident ions and samples. When computing cascade-probabilistic functions and spatial distributions of vacancy clusters patterns of conduct and finding the real resulting region in gold and silver alloys were obtained. Selection of step and boundaries for calculation were automated. Results of the calculations performed are illustrated in the form of graphs and tables.

Key words: modeling, regularity, cascade-probabilistic function, concentration, ion irradiation.

Introduction

When materials are irradiated with various particles, corresponding defects are formed. To date, ion beams are mainly used to produce heavy-duty parts and materials in the case of ion radiation exposure defects in the form of cascade regions are formed [1–3]. The presence of defects in materials significantly accelerates or slows down various processes. As a result, this affects the formation of compounds and structures, the physicochemical properties of irradiated materials change. Simultaneously, it is needful take into consideration the full “physical” picture of the interaction process considering the types of falling particles (light or heavy) [4, 5]. When computing probabilistic characteristics difficulties arise in the case of ion irradiation, problems associated with the complexity of the mathematical description of these processes which served to create mathematical models describing the phenomena of the formation of vacancy clusters in dynamics [6–10].

For computations of cascade-probabilistic functions, spectra of primary knock-on atoms, concentrations of radiation defects (CRD) in gold and silver irradiated with various incident ions, an approximation expression for the interaction cross section was selected and the conforming approximation parameters were found.

Gold is a metal and a chemical element, the atomic number of which is according to the periodic table. Gold is a financial unit in the global economy and in the field of investment as well as a jewel that is used in the jewelry industry. Silver is a metal and a chemical element whose atomic number is according to the periodic table. Silver is not only a popular metal for investment in bullion, but also one of the most useful metals in the history of mankind and in the modern world. As the best conductor of heat and electricity of all metals, silver is used in a huge number of industrial, technological, and medical/hygienic products. Silver and gold are among the most common metals used in industry; therefore, alloys based on them will be considered in this paper.

Materials and methods

The interaction cross section for ions is computated according to the Rutherford formula [11]. The approximation cross section is computated using the following formula [1]:

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

where σ_0, a, k, E_0 – approximation parameters.

With ion irradiation, the mathematical model for calculating CPF, considering energy losses, is calculated by the formula [1]:

$$\psi_n(h', h, E_0) = \frac{1}{n!\,\lambda_0^n} \left(\frac{E_0 - kh'}{E_0 - kh}\right)^{-l} \exp\left(\frac{h - h'}{\lambda_0}\right) \left[\frac{\ln\left(\frac{E_0 - kh'}{E_0 - kh}\right)}{ak} - (\mathrm{h} - \mathrm{h}')\right]^n. \quad (2)$$

To calculate $\psi_n(h', h, E_0)$ a formula convenient for computations was used [1]:

$$\psi_n(h', h, E_0) = \exp\left[\begin{matrix} -\ln(n!) - n\ln(\lambda_0) - \frac{1}{\lambda_0\, ak}\ln\left(\frac{E_0 - kh'}{E_0 - kh}\right) + \\ + \frac{h - h'}{\lambda_0} + n\ln\left(\frac{\ln\left(\frac{E_0 - kh'}{E_0 - kh}\right)}{ak} - (\mathrm{h} - \mathrm{h}')\right) \end{matrix}\right]. \quad (3)$$

For ion irradiation, the following ratio is used to calculate the CRD [1]:

$$C_k(E_0, h) = \int_{E_c}^{E_{2\max}} W(E_0, E_2, h)\, dE_2, \quad (4)$$

$$E_{2\max} = \frac{4E_1(m_1c^2 m_2c^2)}{(m_1c^2 + m_2c^2)^2}.$$

Using the Bethe-Bloch formula we find the corresponding surveillance depths, considering that $\Delta E(h) = E_0 - E_1(h)$.

The spectrum of primary knock-on atoms (SPKA) is calculated by the formula [1]:

$$W(E_0, E_2, h) = \sum_{n=n_0}^{n_1} \int_{h-k\lambda_2}^{h} \psi_n(h') \exp\left(-\frac{(h - h')}{\lambda_2}\right) \frac{w(E_1, E_2, h')\, dh'}{\lambda_1(h')\, \lambda_2}. \quad (5)$$

In the range of acceptable values $\psi_n(h', h, E_0)$ n_0, n_1 are the minimum and maximum values of the number of collisions.

Computations of SPKA in the elementary act are executed according to the formula [1]:

$$\omega(E_1, E_2) = \frac{d\sigma(E_1, E_2)}{dE_2} \cdot \frac{1}{\sigma(E_1)}. \quad (6)$$

Main provisions

The aim of the study is to optimize the algorithms for calculating the probabilistic characteristics of the processes of radiation defect formation under ion irradiation. The object of research is metals, namely gold and silver. The subject of the study is cascade-probabilistic functions depending on the number of interactions and the depth of penetration of particles. The obtained mathematical models can be used in the future for numerical calculations of the spectra of primary knock-on atoms and the concentration of radiation defects in other metals and semiconductors, as well as in the study of similar phenomena. The obtained physical models and calculation results allow a deeper understanding of the processes of radiation defect formation in condensed media and can be used in their work by experimenters.

Literature review

It should be noted that many works have been devoted to the problems of radiation defect formation during the interaction of ions with matter, for example [2–10]. Energy losses due to ionization and excitation of the electron shells of the atoms of the medium were not considered, so the simplest CPF was used. When charged particles interact with matter, continuous energy losses occur along the path of their movement. These losses lead to a strong dependence of both the energy spectra of the incoming particles themselves and the primary knocked-out atoms (PKA) on the penetration depth. The range of interaction for the formation of PKA significantly depends on energy, and therefore it became necessary to obtain physical and mathematical models that consider the real dependences of various parameters of the elementary act on energy, depth. Previously, in most cases, the simplest cascade probability function (CPF) was mainly used for specific calculations, this is not always justified, since the interaction path depends on the energy [11]. It is necessary to investigate the behavior of the obtained CPF considering the energy losses for ions, to prove the properties that they should possess both from a physical and mathematical point of view, to develop calculation algorithms and perform calculations of CPF depending on the number of interactions and the depth of penetration of particles, and the concentration of radiation defects.

Results and discussions

To calculate $\psi_n(h', h, E_0)$ it is needful to calculate the interaction cross-section according to the Rutherford formula [11], find the surveillance depths from the tables of parameters of the spatial distribution of ion-implanted impurities [12] and determine the approximate parameters calculated by the formula (1), which are also included in the expressions for the PKA spectra, concentrations of radiation defects. The results of the selection of approximations are shown in figure 1. The approximation parameters and the correlation index for indium in gold at various values of E_0 are shown in table 1 (p. 58).

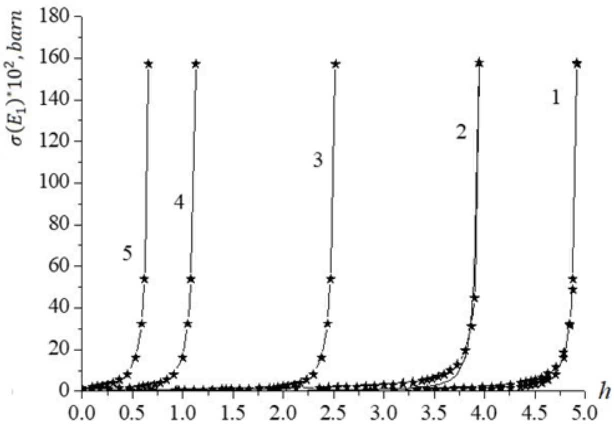

Figure 1 – Approximation of the modified $\psi(h', h, E_n)$ cross section for indium in gold: $E_0 = 1000$ (1), 800 (2), 500 (3), 200 (4), 100 (5) keV. Curves – approximation lines, asterisks – calculated data of the section dependence on h

Table 1 – Approximation coefficients for indium in gold

E_0	$\sigma_0 * 10^9$	α	E_0'	k	η	chi^2
1000	53.53353	0.23606	0.00599	8.57545	0.99667	33292.43045
800	102.8195	0.95274	0.00698	0.5697	0.99126	94088.98762
500	128.15188	0.52176	0.0222	143.41385	0.99095	109625.1123
200	163.07921	0.1802	0.05376	2524.30618	0.99641	66123.10731
100	129.54471	0.04733	0.12437	12034.90155	0.99925	20334.99881

Next, computations were executed $\psi(h', h, E_0)$, the areas of finding the result were revealed, the patterns that emerged when determining this region were set. Figure 2 and table 2 illustrate the results of the calculations.

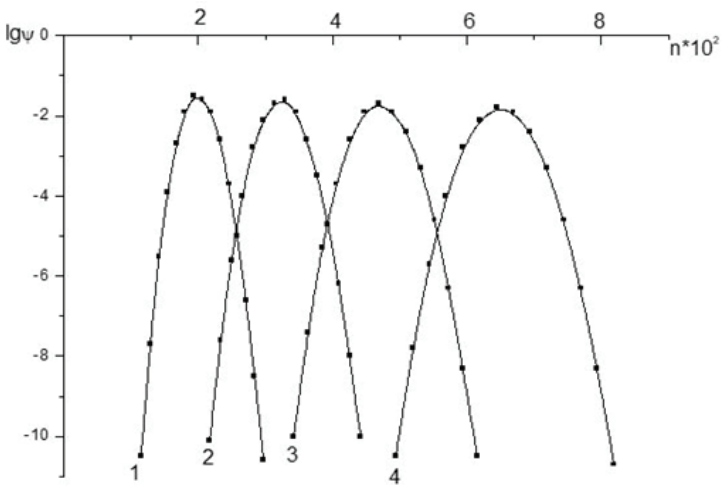

Figure 2 – Addiction of $E_0 = 100\ keV$ on for nitrogen in gold at $h = 0,5 \cdot 10^{-2};\ 0,9 \cdot 10^{-2};\ 0,13 \cdot 10^{-1};\ 0,17 \cdot 10^{-1}\ cm$ and $E_0 = 100\ keV$

Table 2 – Addiction of the percentage of displacement of the left and right boundaries of the resulting region on the surveillance depth for silver in gold at $E_0 = 1000\ keV$

$h * 10^6, cm$	$\frac{h}{\lambda}$, cm	$C_3, \%$	$C_3, \%$	N_h	$C_3, \%$
10	8682	-7,79	21	100	13,2
15	15483	-15,89	25	150	9,1
20	25015	-22,579	29	225	6,42
25	38912	-27,67	32	325	4,33
30	60433	-30,38	32,8	600	2,42
35	97168	-29,37	30,5	1300	1,13
40	171765	-22,835	23,1	5500	0,265
45	396151	-11,26007	11,2627	500000	0,00263

The results of computations of the concentration of radiation defects are illustrated in table 3 (p. 59).

After the calculations $\psi(h', h, E_0)$ depending on the number of collisions and the depth of particles surveillance, the regularities of the behavior of the step and the resulting region for computation were identified.

Let 's pick out the patterns when choosing step:

1. For small values of the atomic mass A_r of the incident particle and small values of the depths, the step is significantly small (approximately in the range of 10–20) with an increase in the value of the surveillance depth, the step begins to increase.

2. Increasing the A_r value of the incident particle it also leads to an increase in the step.
3. If the A_r value of the incident particle is large and the sample is small, then the step begins to increase significantly.

Table 3 – Boundaries of the CRD determination area for titanium in silver at $E_c = 50\ keV, E_0 = 1000\ keV$

$h * 10^5$, cm	C_k, cm	E_1, keV	n_0	n_1	t
0,1	31762,9	1000	6	142	7''
3	34925,6	900	1559	2331	32''
6,1	39102,9	800	3617	4748	72''
9,1	44196,7	700	5930	7354	2'
12,2	51079,3	600	8731	10442	3'
15,3	60469,0	500	12092	14092	5'
18,4	74001,0	400	16272	18584	7'
19,9	82838,5	350	18722	21199	9'
21,5	95016,9	300	21778	24446	11'
22,1	100401,3	280	23076	25822	12'
22,7	106368,0	260	24477	27304	13'
23,3	112991,09	240	25996	28912	15'
23,9	120342,19	220	27661	30667	16'
24,4	126202,89	200	29176	32263	17'
25,0	134643,69	180	31183	34375	19'
25,6	143506,49	160	33445	36753	22'
26,2	152073,69	140	36036	39471	24'
26,7	153675,79	120	38525	42078	26'
27,3	151251,19	100	42057	45774	29'
27,9	124648,19	80	46458	50371	32'
28,1	83424,29	70	48202	52190	34'
28,4	13628,49	60	51186	55300	38'
28,7	0	50	54763	59027	43'

When calculating $\psi(h', h, E_0)$ depending on h, the regularities of the step behavior are revealed:
1. With a small value of A_r of the incident particle the step is significantly small, an increase in the value of the surveillance depth leads to a growth in the step at the end of the mileage it is significantly strong.
2. Reducing the particle E_0 will lead to a growth in the step, provided that the value of the surveillance depths does not change.
3. As the A_r value of the incident particle increases, the step begins to grow gradually and then very sharply, provided that the value of the surveillance depths does not change.
4. The dependence of the step on A_r can be represented as an increasing curve.

Patterns of conduct of the resulting domain for $\psi(h', h, E_0)$ calculated depending on *n*:

1. The maximum value of $\psi(h', h, E_0)$ is shifted to the region of shallow depths concerning to $\frac{h}{\lambda}$ when the value of A_r of the incident particle is large and at large depths the result is in a narrow region.
2. The most limited resulting region is turned out with a large value of A_r of the incident particle and a small value of the sample at the end of the mileage.
3. As the value A_r of the incident particle increases, the resulting finding area narrows and moves to the region of shallow depths concerning to $\frac{h}{\lambda}$.

Finding the resulting CRD region under ion irradiation revealed the following patterns:
1. The values of the CRD at the same depth of surveillance are significantly reduced.

2. Depending on h, the values of the CRD increase.
3. If the E_0 of the primary particle increases at the same value of threshold energy E_c and h then the values of the CRD begin to decrease.
4. Depending on E_c the boundaries of the resulting region remain constant provided that E and h remain unchanged.
5. The boundaries of the resulting CRD region, depending on h, increase and move to the region of great depths and the interval of boundary changes in the interval ranges from 0 to 5000.
6. The counting time t increases significantly for heavy incident particles and light samples.

Conclusion

In this paper, the expressions of the CPF are obtained, considering the energy losses for ions in an analytical form. The approximation expression is selected, and the approximation parameters are chosen so that the correlation index is close to one. Computation algorithms have been developed and computation of cascade probabilistic functions has been optimized, considering energy losses depending on the number of interactions and the depth of surveillance particles, the concentration of vacancy clusters under ion irradiation. Computations were executed and patterns of conduct of the resulting region of the CPF and the step for computation were found depending on the number of collisions and the depth of surveillance particles. It is shown that the resulting region is significantly affected by the initial energy of the primary particle, the surveillance depth, the atomic number of the incident particle and the sample. Comparisons of the computation results by time before and after optimization are performed. The computations were executed using a software package developed in Microsoft Visual Studio 2017 and the database was created in MS SQL Server 2019.

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ИОНДАРМЕН СӘУЛЕЛЕНГЕН МАТЕРИАЛДАРДАҒЫ АҚАУДЫҢ ПАЙДА БОЛУЫНЫҢ РАДИАЦИЯЛЫҚ ПРОЦЕСТЕРІН МОДЕЛЬДЕУ

Аңдатпа

Материалдарды тұтыну күн сайын артып келеді, бұл өз кезегінде табиғи ресурстар және жабдықтау мәселелерімен жиі күресудің пайда болуын білдіреді. Сондықтан адамзат қолданыстағы шикізатты тиімді пайдалану, бұрын жарамсыз болған заттарды пайдалы материалдарға айналдыру мен қолданылған заттардан мүлдем жаңа материалдар шығару жолдарын табу арқылы өзінің ресурстық базасын кеңейтуге мәжбүр. Жаңа материалдарды жасау тәсілдерінің бірі – затты зарядталған иондармен сәулелендіру. Мақалада иондар үшін энергия шығынын ескере отырып, каскадты ықтималдық функцияларын (КЫФ) алу және пайдалану мақсатындағы каскадты ықтималдық әдісіне негізделген тәсіл қарастырылады. КЫФ есептеулері соқтығыстардың санына және әртүрлі құлаған иондар мен үлгілердің бақылау тереңдігіне байланысты жүргізілді. Каскадты ықтималдық функцияларын және бос кластерлердің кеңістіктікте таралуын есептеу кезінде алтын мен күміс қорытпаларындағы нақты нәтиже аймағын табу мен метал қасиеттерінің заңдылықтары алынды. Есептеу үшін қадамдар мен шекараларды таңдау автоматтандырылған. Орындалған есептеулердің нәтижелері графиктер мен кестелер түрінде ұсынылған.

Тірек сөздер: модельдеу, заңдылық, каскадты ықтималдық функциясы, концентрация, иондық сәулелену.

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МОДЕЛИРОВАНИЕ РАДИАЦИОННЫХ ПРОЦЕССОВ ДЕФЕКТООБРАЗОВАНИЯ В МАТЕРИАЛАХ, ОБЛУЧЕННЫХ ИОНАМИ

Аннотация

Потребление материалов растет с каждым днем, а это значит, что нам все чаще придется справляться с проблемами природных ресурсов и снабжения. Поэтому человечество вынуждено расширять свою ресурсную базу, находя способы более эффективно использовать существующее сырье, превращать ранее непригодные вещества в полезные материалы, а также производить совершенно новые материалы из веществ, которые доступны в изобилии. Одним из способов создания новых материалов является облучение вещества заряженными ионами. В статье рассматривается данный способ, основанный на каскадно-вероятностном методе, цель которого состоит в получении, а также последующем использовании каскадно-вероятностных функций (КВФ) с учетом потерь энергии для ионов. Проведены расчеты КВФ в зависимости от количества соударений и глубины наблюдения для различных падающих ионов и образцов. При расчете каскадно-вероятностных функций и пространственных распределений вакансионных кластеров получены закономерности поведения и нахождения реальной результирующей области в сплавах из золота и серебра. Автоматизирован подбор шага и границ для расчета. Результаты выполненных вычислений проиллюстрированы в виде графиков и таблиц.

Ключевые слова: моделирование, закономерность, каскадно-вероятностная функция, концентрация, ионное облучение.

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