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Computer modeling of radiation processes in solids is under ion irradiation

Abstract: The paper deals with the process of ion interaction with matter and the formation of radiation defects. The process of producing the cascade-probability functions (CPF) used further in the calculation of the spectra of primary sputtered atoms (PSA) and the concentration of radiation-induced defects. Presented CPF calculation algorithm is based on the number of interactions and the depth of particle penetration. The models calculate the spectra of primary sputtered atoms and the concentration of radiation defects in materials irradiated by different ions. This takes into account the atomic weight of the incident particle and the target, all options are: atomic weight of the incoming particle is less than the atomic number of the target, the atomic weight of the incoming particle is commensurate with target atomic number, atomic weight of the incoming particle larger atomic number of the target. The regularities of the behavior concentration of radiation defects.
Key words: Radiation defect formation, cascade and probabilistic function, primary beaten-out atom, an ion, the flying particle, a target.

Introduction

The process of ion interaction with matter and their passage through matter is a challenge to create the physical and mathematical models [1]. First of all, this is due to a catastrophic increase in the interaction cross sections of electrons and atoms of the medium. At the same depth of penetration of the ions in the material with increasing mass of the incoming particles decreases dramatically. In calculating the cascade-probability functions in this case it is necessary to use special methods and techniques. Set type of incident particles and the target is a huge amount of items. It is possible to consider various situations when the mass number of incoming ions A^1 smaller mass number of the target A^2, ie, $A_1 < A_2$, a case where A_1 becomes comparable with A_2, and finally completely unique processes, when $A_1 > A_2$. As shown by preliminary analysis, all of these cases be taken into account - in each of them manifest their laws.

In addition, by using a certain kind of projectile particles in concrete material can be formed preassigned structure and chemical compounds is quite stable over a wide temperature range. Naturally, in this and physicochemical properties of these compounds are different from the original. Work in this direction is carried out in the framework of cascade-probability method.

In [1] cascade-probability functions, taking into account the energy loss of electrons, protons and α--particles, performed their mathematical analysis, obtained by the mathematical model for calculating the spectrum of the primary-sputtered atoms (PSA) and the concentration of radiation defects and made their calculations were derived PC. For ions mathematical models of CPF get much more complicated. This is due to the fact that the cross section of interaction calculated by the formula Rutherford large ranges approximately from $n*10^7$ to $n*10^{12}$ (barns), where n - an integer, and running penetration is very small and is approximately $10^{-6} – 10^{-3}$ cm. Fluctuations due to the fact that with increasing atomic number of the element of interaction cross section increases and penetration mileage decreases.

The main results

For ions in contrast to the electrons, protons and α-particle approximation the dependence of the cross section of the energy factor is represented as follows [2]:

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

where σ_0, a, E_0, k - approximation coefficients.

Cascade-probability functions with regard to the ion energy loss can be obtained from the following recurrence relation [2]:

$$\psi_n(h', h, E_0) = \int_{h'}^{h} \psi_{n-1}(h', h'', E_0)\psi_0(h'', h, E_0)\frac{1}{\lambda_0}\left(\frac{1}{a(E_0 - kh'')} - 1\right)dh'' \quad (2)$$

In view of the above obtained recorded mathematical model CP - function energy taking into account the loss of ions in the form [2]

$$\psi_n(h', h, E_0) = \frac{1}{\lambda_0{}^n}\left(\frac{E_0 - kh'}{E_0 - kh}\right)^{-l} \exp\left(\frac{h - h'}{\lambda_0}\right) * \sum_{i=0}^{n} \frac{(-1)^i \ln^{n-i}\left(\frac{E_0 - kh'}{E_0 - kh}\right)(h - h')^i}{i!(n-i)!a^{n-i}k^{n-i}}. \quad (3)$$

Transforming the expression (3), we have

$$\psi_n(h', h, E_0) = \frac{1}{n!\lambda_0{}^n}\left(\frac{E_0 - kh'}{E_0 - kh}\right)^{-l} \exp\left(\frac{h - h'}{\lambda_0}\right) * \left[\frac{\ln\left(\frac{E_0 - kh'}{E_0 - kh}\right)}{ak} - (h - h')\right]^n. \quad (4)$$

Conditional probabilities ψ_0, ψ_1, ψ_2, ... ψ_n are transition probabilities for the Markov chain. When $k \to 0$, or $\alpha \to \infty$, CPF considering the energy loss becomes simple, and, consequently, in the Poisson distribution.

Calculation of cascade-probability functions, taking into account the energy loss of ions, represented by the expression (4), is particularly difficult for large values of the n (which is what we have in fact in most cases).

The following convenient upgraded formula for calculating used for calculating CPF:

$$\psi_n(h', h, E_0) = \exp\left[-\ln(n!) - n * \ln(\lambda_0) - \frac{1}{\lambda_0 ak}\ln\left(\frac{E_0 - kh'}{E_0 - kh}\right) + \frac{h - h'}{\lambda_0} + n * \ln\left(\frac{\ln\left(\frac{E_0 - kh'}{E_0 - kh}\right)}{ak} - (h - h')\right)\right], \quad (5)$$

where n - the number of interactions, h',h - the depth of ion generation and detection, λ_0, a, E_0, k - the parameters of the approximation.

The calculation of the concentration radiation defects under ion irradiation is performed by the formula [3]:

$$C_k(E_0, h) = \int_{E_c}^{E_{2\max}} W(E_0, E_2, h)dE_2, \quad (6)$$

$$E_{2\max} = \frac{4m_1c^2 m_2c^2}{(m_1c^2 + m_2c^2)^2}E_1, \quad (7)$$

m_1c^2 – the rest energy of the ion.

The spectrum of primary sputtered atoms is determined by the following equation [3]:

$$W(E_0, E_2, h) = \sum_{n=n_0}^{n_1} \int_{h-k\lambda_2}^{h} \psi_n(h')\exp\left(-\frac{h - h'}{\lambda_2}\right)\frac{w(E_1, E_2, h')dh'}{\lambda_1(h')\lambda_2}, \quad (8)$$

where n_0, n_1 - initial and final value of the number of interactions in the domain of cascade-probability functions.

Cascade-probability functions $\psi_n(h')$ in expression (8) is as follows

$$\psi_n(h') = \frac{1}{n!\lambda_0^n}\left(\frac{E_0}{E_0 - kh'}\right)^{\frac{1}{\lambda_0 ak}} \exp\left(\frac{h'}{\lambda_0}\right)\left(\frac{\ln\left(\frac{E_0}{E_0 - kh'}\right)}{ak} - h'\right)^n, \quad (9)$$

$$\text{where } \lambda_1(h') = \frac{1}{\sigma_0 n_0\left(\frac{1}{a(E_0 - kh')} - 1\right)} * 10^{24} \text{ (cm)}, \qquad \lambda_2 = \frac{1}{\sigma_2 n_0} * 10^{24} \text{ (cm)}. \quad (10)$$

Cross section σ_2 is calculated by the formula of Rutherford. The spectrum of PSA in the elementary act is calculated by the following formula [3]:

$$\varpi(E_1, E_2) = \frac{d\sigma(E_1, E_2) \Big/ dE_2}{\sigma(E_1)}, \quad (11)$$

$$\frac{d\sigma(E_1, E_2, h)}{dE_2} = 4\pi a_0^2 E_r^2 z_1^2 z_2^2 \frac{1}{E_1 E_2^2} 10^{24} \quad (12)$$

Substituting the expression for $w\left(E_1, E_2, h'\right)$ in the formula (6), (8) we obtain:

$$C_k\left(E_0, h\right) = \frac{E_d E_{2\max}}{E_{2\max} - E_d} \int_{E_c}^{E_{2\max}} \frac{dE_2}{E_2^2} \sum_{n=n_0}^{n_1} \int_{h-k\lambda_2}^{h} \psi_n(h') \exp\left(-\frac{h-h'}{\lambda_2}\right) \frac{dh'}{\lambda_1(h')\lambda_2}. \quad (13)$$

Doing transformation, we arrive at the following expression:

$$C_k\left(E_0, h\right) = \frac{E_d}{E_c} \frac{E_{2\max} - E_c}{E_{2\max} - E_d} \sum_{n=n_0}^{n_1} \int_{h-k\lambda_2}^{h} \psi_n(h') \exp\left(-\frac{h-h'}{\lambda_2}\right) \frac{dh'}{\lambda_1(h')\lambda_2}. \quad (14)$$

Calculate the concentration of radiation defects by the formula (14), if we substitute $\psi_n(h')$ its expression in the form (9), it is impossible, as every member of CPF overflow occurs. The expression for $\psi_n(h')$ use in the form (5).

For light incident particles and light curves of targets increases, reaching a maximum and then decreases to zero. With the increase of the initial energy of the particle curves are shifted to the right. With the increase in the concentration of E_c values threshold energy decreases, and the curves are much lower, the transition through a maximum is carried out smoothly. At energies E_0 =100 keV curve decreases. With the increase in atomic weight of the incident particles function value at the maximum point is increased and thus pass above the curves, while the depth value decreases. With increasing atomic number of the target for the same value of a function of the incident particle at the maximum point slightly increased depth value decreases.

The calculation results are shown in Figures and Tables 1.2 to 1.2.

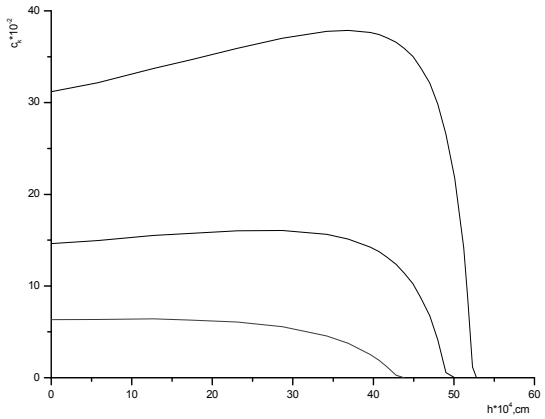

Figure 1 – The dependence of the concentration of radiation defects on the depth under ion irradiation for silver in titanium at E_0= 1000, E_c= 50 (1), 100 (2), 200 (3) keV

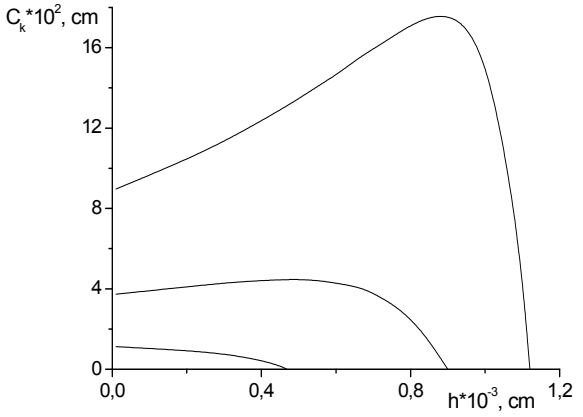

Figure 2 – Dependency of concentration radiation defects of depth by irradiating nitrogen ions, titanium for E_0 = 500 keV, 50 keV E_c = (1), 100 keV (2), 200 keV (3)

Table 1 – The boundaries of the area of determining the concentration of radiation defects in the aluminum titanium at E_c = 50 keV and E_0 = 1000 keV

h*10⁴, cm	**$C_к$, cm**	**E_0, keV**	**n_0**	**n_1**
0,1	3286,5	1000	7	139
1,4	3560,9	900	645	1155
3	3964,6	800	1645	2410
4,5	4419,5	700	2735	3698
6,2	5068	600	4172	5344
7,9	5908,4	500	5882	7260
9,7	7124,1	400	8100	9707
10,6	7910,7	350	9427	11156
11,5	8858,2	300	10951	12811
11,9	9358	280	11707	13628
12,3	9907,8	260	12521	14507
12,7	10513,5	240	13404	15457
13,1	11178,9	220	14365	16490
13,5	11906,1	200	15421	17621
13,9	12689,6	180	16589	18871
14,3	13508,5	160	17898	20268
14,7	14298,7	140	19383	21850
15,2	15536,3	120	21570	24174
15,6	15644,2	100	23691	26421
16	13843,2	80	26303	29183
16,2	11101,2	70	27876	30843
16,4	5544,9	60	29700	32765
16,6	-5926,2	50	31870	35049

Table 2 – The boundaries of the area of determining the concentration of radiation defects in titanium silver for the E_U = 50 keV, E_0 = 800 keV

h*10 ^{4}, cm	$C_к$, cm	E_0, keV	n_0	n_1
0,01	3050,95	800	0	22
0,57	3149,61	700	192	441
1,14	3247,18	600	476	830
1,70	3330,05	500	786	1229
2,25	3379,15	400	1114	1623
2,52	3378,35	350	1284	1835
2,79	3348,35	300	1459	2048
2,90	3324,76	280	1532	2132
3,0	3288,37	260	1599	2213
3,11	3242,87	240	1673	2297
3,21	317,84	220	1742	2367
3,32	3096,25	200	1819	2459
3,42	2983,01	180	1889	2545
3,53	2833,87	160	1967	2626
3,63	2625,95	140	2040	2713
3,73	2323,90	120	2113	2806
3,87	1914,65	100	2216	2922
3,95	1244,71	80	2276	2981
4,0	758,55	70	2314	3055
4,06	102,06	60	2360	3080
4,14	0	50	2421	3156

Conclusion

In work ions interaction process with substance and radiation defects formations is considered. Process receiving the cascade and probabilistic functions (CPF) used further at calculation ranges the primary beaten-out atoms (PBOA) and concentration on radiation defects is described. The calculation algorithm on CPF depending on interactions number and depth on particles penetration is presented. Calculation models on primary beaten-out atoms ranges and radiation concentration defects in the materials irradiated with various ions are developed. Thus the nuclear weight on the flying particle and target is considered, all options are considered: the nuclear weight the flying particle is less than atomic number on a target, the nuclear weight on the flying particle is commensurable with a target atomic number, the nuclear weight on the flying particle is more than a target atomic number. Regularities on concentration behavior on radiation defects are revealed.

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