

F.F. Komarov¹, T.A. Shmygaleva^{2*},
A.A. Kuatbayeva³, A.A. Srazhdinova²

¹Belarusian State University, Minsk, Belarus

²al-Farabi KazNU, Kazakhstan, Almaty

³IITU, Kazakhstan, Almaty

*e-mail: shmyg1953@mail.ru

COMPUTER SIMULATION OF VACANCY CLUSTERS CONCENTRATION IN TITANIUM IRRADIATED WITH IONS

Abstract. The process of irradiation of metals with ions is an effective method for changing various properties of materials, in particular titanium, as well as obtaining new materials. This work is devoted to modeling radiation processes in titanium irradiated with ions. Algorithms of cascade-probabilistic functions (CPF) computation depending on the number of interactions and the particle penetration deep number for various incident particles of the Mendeleev's periodic table in titanium are presented. Approximate value expressions for cross-sections are chosen, patterns of cooperation cross-sections demeanor, CP-functions depending on observation profound, number of interactions, target atomic number, primary particle initial energy are noted. Algorithms for calculating the radiation imperfections concentration in ion radiation have been developed and computations in titanium in ion radiation have been carried out. With the calculating CPF and the depth distribution of vacancy clusters, it is necessary to find the region of the result in which these characteristics of the process of formation of radiation defects in solids are exists. Regularities obtained when finding this area are formulated. The calculation results in the form of graphs and tables are presented.

Keywords: Modeling, algorithm, computation, ion, regularities, approximate value, CPF, cooperation cross-section, concentration, vacancy accumulations.

Introduction

For metals, ion irradiation is an effective method to alter properties such as metal durability, staining sustainability, weariness, deterioration, etc. At present, radiation physics makes a considerable investment to the development of nanophysics and its related application field - nanoelectronics.

In contradistinction to protons, α -particles, and electrons, (with energy > 1 MeV), Ion particles are able to form cascading regions (vacancy accumulations and accumulations of inter-node atoms). In contradistinction to protons, electrons, and α -particles process of interplay of ions with substance and their passing through substance is heavier task as during creature of physical and mathematical models [1-3]. This can be explained by the specific behavior of ions, for which the calculation of CPF, PVA spectra, the concentration of vacancy clusters, and the selection of approximations produce many

features that are eliminated in some way. Furthermore, with the aid of a definite diversity of flyable particles in a particular material it is possible to constitute a predefined structure and chemical compounds enough stable in a wide temperature range [4]. Then the physical and chemical properties of these materials will change. Therefore, when studying the process of ion irradiation of materials, it is necessary to consider and solve a block of physical and mathematical problems. Many papers have been devoted to the study of the interaction of particles with matter and the formation of vacancy clusters under ion irradiation [5]. The primary part of working in this directing is executed within the cascade probability way framework [6].

Main results

The probability of transition in n steps for ions is written as follows [1]:

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

where n – number of cooperation, h', h – Ion generation and registration deep, σ_0, a, E_0, k – approximate value factors related to cooperation mileage and specific energy loss factor, $\lambda_0 = l/\sigma_0$.

Cooperation of cross-sections was calculated according to the Reserford formula [1], deep of observations were based on spreadsheets of parameters of spatial allocation of ion-implanted admixture [7]. For ions forming primary- embossed atoms, the dependency of the approximate value

function on energy, which in turn depends on the profound of penetration, is represented as follows [1]:

$$\sigma(h) = \sigma_0 \left(\frac{1}{a(E_0 - kh)} - 1 \right), \tag{2}$$

Approximating curve dependencies of σ on h are given in figure 1 and in table 1. Agreement of approximate value and reference curves is very good.

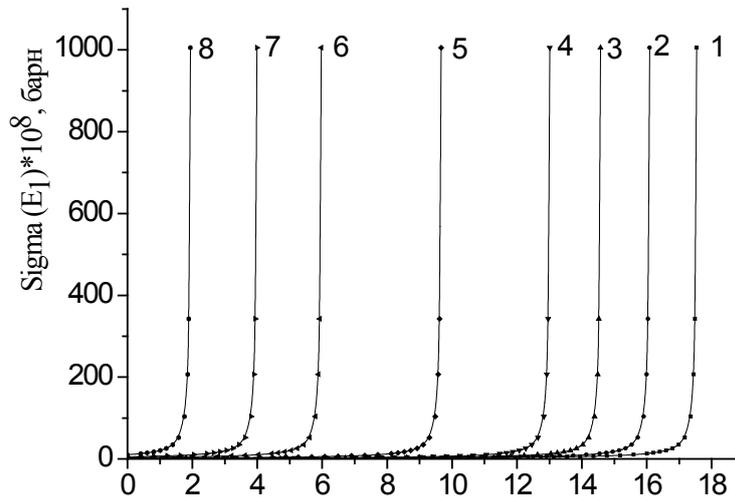


Figure 1 – Approximate value of modified section of CPF for aluminium in titanium $E_0 = 1000$ (1), 900 (2), 800 (3), 700 (4), 500 (5), 300 (6), 200 (7), and 100 (8) keV.
Points - Design Section Deep Dependency Data,
Solid Line – Approximate value

Analysis of the computations shows that the approximate value curves of the modified cooperation cross-sections are well described by formula (2), which makes it possible to calculate the CP-functions for aluminum in titanium with high precision. The theoretical correlation ratio ranges from 0, 99 to 0.999.

CPF computations were performed according to formula (1). All computations were made with double accuracy throughout the observation profound interval. The outcomes of the computations show that CPF, depending on h and on n , have the

following demeanor: increase, reach the maximum, then decrease. The figures show the relationship of the aluminum CPF in titanium to the number of cooperation (Figures 2, 3) and penetration profound. (Figures 4.5).

At CPF computation on computer depending on interplays number the following regularities arise:

1. Withal increase in atomic heft of the flyable particle the outcome finding area is displaced to the area of small deeps concerning h/λ and narrowed.
2. Withal a huge atomic heft of the flyable particle the CP-function maximum value is showed

to the square of small depths concerning h/λ already with little depths, and with huge profounds the outcome is in particularistic area (less than 1%, silver, gold). The narrowest region of the outcome is

acquired with a big atomic heft of the flyable particle and a tiny target at the end of the run and achieves hundreds of percent [8, 9]. The computation outcomes are given in Table 2.

Table 1 – Approximate value parameters for aluminum in titanium

E_0	$\sigma_0 \cdot 10^8$	a	E_0	k	η
1000	0.26338	0.2825	0.67741	385.67808	0.99932
900	0.29435	0.22033	0.6491	402.34914	0.98702
800	0.43114	0.18618	919318,00	987.37947	0.99942
700	0.40218	0.19447	0.67386	512.83839	0.99391
500	0.43023	0.19061	0.65982	677.91892	0.98702
300	0.66686	0.2023	0.83022	1384.2892	0.99944
200	0.56167	0.15111	0.62701	1562.21507	0.9994
100	0.81173	0.10855	0.61751	3138.50145	0.99937

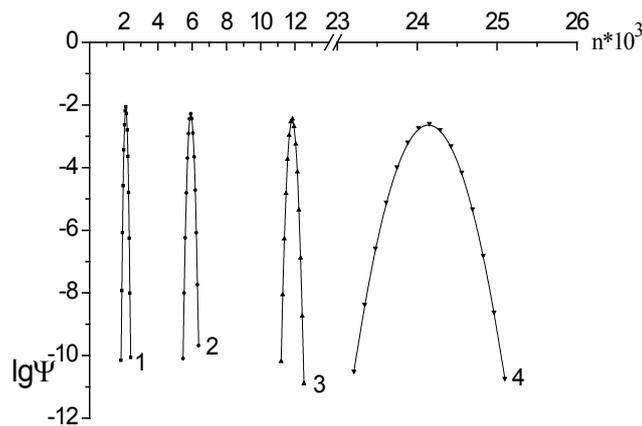


Figure 2 – CPF 's dependency on the interplays number for aluminum in titanium at $h = 1,5,9,13,17 (* 10^{-4})$ cm; $E_0 = 1000$ keV (1-4)

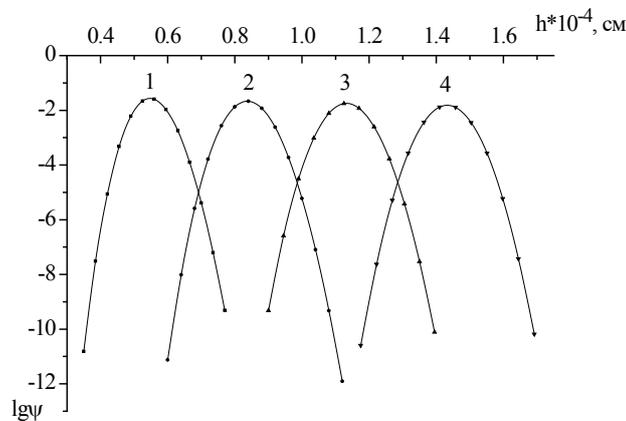


Figure 3 – Ratio of CPF for titanium carbon at deep at $E_0 = 300$ keV, $n = 215; 347; 498; 673$ (1-4)

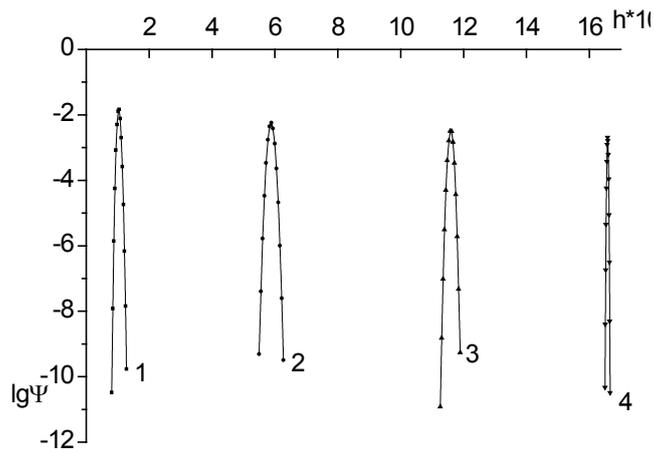


Figure 4 – Dependency $\psi_n(h', h, 0)E$ from deep for aluminum in titanium at $E_0 = 1000$ keV for $n = 677; 4704; 13054; 37124$ (1-4)

Table 2 – Left and Right Region Offset Percent Dependency. Outcome from the number of interplays for aluminum in titanium at $E_0 = 1000$ keV

$h * 10^4, \text{ cm}$	$B_1, \%$	$B_2, \%$	N_n	$B_3, \%$
1	26,23	24	23	50,23
3	22,4	2	40	24,4
5	26,2	-8,7	55	17,5
7	32	-20	65	12
9	39	-30,5	78	8,5
11	47,5	-41,2	95	6,3
13	57,6	-53,2	110	4,4
15	70,3	-67,8	135	2,5
17	89,58	-88,96	165	0,62

Similar patterns were revealed in CPF computations depending on penetration deep with the difference that the area of finding the outcome

is shifted to the area of greater deeps [9]. The outcomes of the computations are shown in Table 3.

Table 3 – The percent movement of the left, right edges of the outcome area depends on the penetration deep for titanium aluminum at $E_0 = 1000$ keV

$h*10^4, \text{ cm}$	$h/\lambda, \text{ cm}$	$C_1, \%$	$C_2, \%$	N_h	$C_3, \%$
1	677	19	31	24	50
3	2373	1	25	60	26
5	4704	-10	26	100	16
7	8031	-18,2	29,8	150	11,6
9	13054	-25,1	32,2	250	7,1
11	21325	-28,9	33	470	4,1
13	37124	-26,9	28,25	470	1,35

Computation of radiation imperfection concentration in case of ion radiation is performed by formula [10]:

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

E_2 – energy of the primary beaten-out atom, E_{2max} – Maximum kinetic energy the atom will receive, E_c – threshold energy, $W(E_0, E_2, h)$ – spectrum of primary - embossed atoms.

Finding the region of the outcome of the concentration of vacancy accumulations in ion radiation revealed the following patterns:

1. As the atomic number of the flyable particle increases, the range of the outcome region is significantly shifted to the region of greater depths and magnifications, the concentration value at the maximum dot and the concentration values themselves are extremely enlarged.

2. With a huge atomic heft of the flyable particle, the counting time is greatly increased.

3. Depending on the deep of permeation, the elementary and final values of the number of cooperation is increasing, the interval of the outcome square (n_0 n_1) also increases and changes to the greater profound area.

The computations outcomes are given in Figures 6.7 and Table 4.

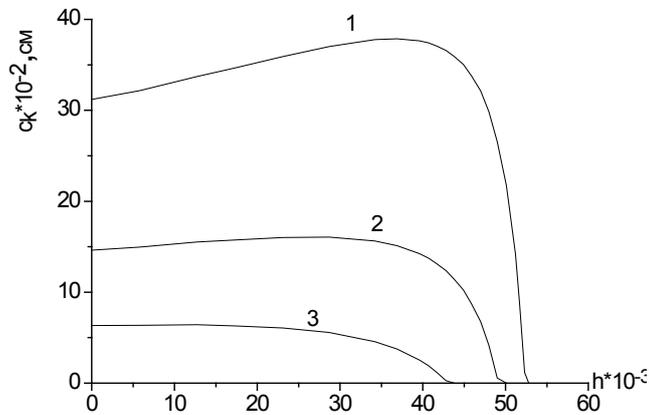


Figure 5 – Dependency of vacancy accumulations concentration on deep of titanium radiation with carbon ions at $E_0=800$ keV, $E_c=50$ keV (1), 100 keV (2), 200 keV (3)

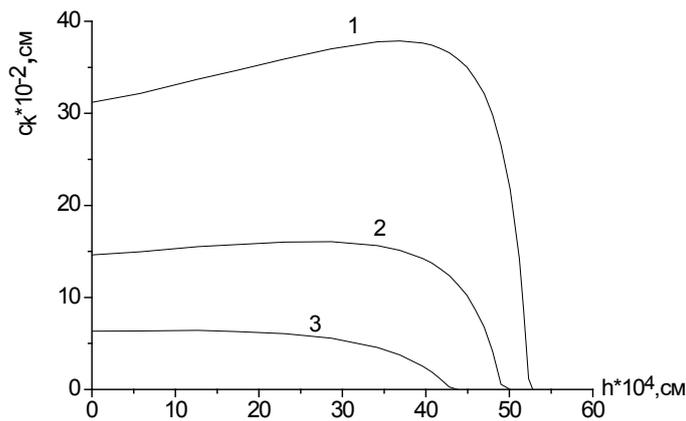


Figure 6 – Dependency of vacancy accumulation concentration on deep of ion radiation for silver in titanium at $E_0=1000$, $E_c=50$ (1), 100 (2), 200 (3) keV

Table 4 - Limits of the radiation imperfections concentration determination area for silver in titanium at $E_c=100$ keV, $E_0= 1000$ keV

$h \cdot 10^4$, cm	C_k , cm^{-1}	E_0 , keV	n_0	n_1	τ
0,01	1462,93	1000	0	25	2"
0,58	1495,87	900	196	444	3"
1,27	1552,12	800	546	925	4"
1,74	1575,49	700	809	1253	5"
2,31	1601,31	600	1152	1669	7"
2,87	1604,77	500	1512	2095	9"
3,42	1563,53	400	1900	2539	14"
3,69	1511,67	350	2083	2765	16"
3,96	1424,11	300	2284	2990	17"
4,07	1374,71	280	2367	3090	20"
4,17	1312,41	260	2444	3174	29"
4,28	1237,09	240	2530	3274	31"
4,38	1141,89	220	2609	3363	31"
4,49	1023,67	200	2697	3466	33"
4,59	871,74	180	2778	3563	23"
4,70	675,75	160	2868	3656	23"
4,80	414,37	140	2951	3747	24"
4,90	56,05	120	3035	3847	25"
5,01	0	100	3129	3948	26"

Conclusion

Thus, the work represents mathematical models of cascade-probabilistic functions with considering energy losses for ions, an approximate value expression for the cooperation cross-sections calculated from the Reserford formula. Based on the models obtained, vacancy accumulation concentration models were obtained. Approximate value expression was chosen and approximate value coefficients were found for different flyable particles in titanium. Computations of CPF are performed depending on cooperation number and particle penetration depth for flyable ions in titanium. The demeanor patterns in the outcome area are shown. The vacancy accumulations concentration has been calculated. Patterns of finding the region at the vacancy accumulations concentration outcome for various flyable particles and target titanium have been revealed.

References

1. E.G. Boos, A.A. Kupchishin, A.I. Kupchishin, E.V. Shmygalev, T.A. Shmygaleva. *Cascade and probabilistic method, solution of radiation and physical tasks, Boltzmann's equations. Communication with Markov's chains.* - Monograph. Almaty: KazNPU after Abay, Scien.

Res. Inst. for New Chem. Techn. and Mat. under al-Farabi KazNU (2015).

2. Zinovieva A.F, Zinovyev, V.A., Nenashev, A. V., Zhivulko, V., Mudryi, A. "Photoluminescence of compact GtSi quantum dot groups with increased probability of finding and electron in Ge." *Scien. Rep.* 10 (2020).

3. Sahul, M., Smyrnova, K., Harsani M, Babincova, P., Vopat, T. "Effect of lanthanum addition on the struture evolution and mechanical properties of the nanocomposite Ti-Si-N coatings." *Mat. Let.* 276 (2020).

4. Kodanova, S.K., Issanova, M.K., Ramazanov T.S., Khikmetov, A.K., Maiorov, S.A. "Simulation of positronium plasma by the molecular dynamics method." *Contr. to Pl. Phys.* 59 (2019).

5. Kozhamkulov, B.A., Akitaj, E., Dzumadillaev, K.N., Primkulova, Z.E., Kyrykbaeva, A.A. "Destruction of Silicon – Organic Composites Irradiated by High-Energy Electrons." *Mech. of Comp. Mat.* 55 (2019): 637-642.

6. Pak, V.K., Ghyngazov, S.A., Miklin, M.B., Lysenko, E.N., Kupchishin A.I. "Hole localization in Thallium Nitrate (I)." *Rus. Phys. J.* 62 (2019): 756-762.

7. Voronova, N.A., Kupchishin A.I., Niyazov, M.N., Taipova, B.G., Abdukhairova, A.T. "Research of electron irradiation effects upon plexigals strain

during bending test.” *IOP Conf. S.: Mat. Scien. and Eng.* 289 (2018).

8. Kozhamkulov, B.A., Kupchishin A.I., Bitibaeva, Z. M., V.P. “Radiation-Induced Defect in Composite Materials and Their Destruction Under Electron Irradiation.” *Mech. of Comp. Mat.* 53 (2017): 59-64.

9. Voronova N.A., Kupchishin, A.I., Kupchishin, A.A., Kuvatbayeva A.A., Shmygaleva, T.A.

“Computer Modeling of Vacancy Nanoclusters Depth Distribution in Ion-Irradiated Materials.” *K. Engin. Mat.* 769 (2018): 358-363.

10. Anatoliy Kupchishin, Nataliya Voronova, Tatyana Shmygaleva, and Alexander Kupchishin. Computer Simulation of Vacancy Clusters Distribution by Depth in Molybdenum Irradiated by Alpha Particles. *K. Engin. Mat.* 781 (2018): 372.