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Mathematical modelling of radiation defect formation processes in the materials irradiated with protons and alpha particles

Abstract. Metals and alloys still remain constructional, instrumental and other materials basis. An important factor in their properties formation are the crystalline grid nano-defects arising, in particular, in case of radiation. By the ionic bombing receiving high-quality, dense metal films and coverings on substrates could be realized. Such materials search and development rely on clear understanding nano-defects radiation creation mechanisms. In the work process of interaction protons and alpha particles with substance and radiation defects formations is considered. For calculation the cascade and probabilistic functions, the primary beaten-out atoms (PBOA) ranges, radiation defects concentration needs to execute approximating expression selection and to find approximation coefficients for interaction section. Interaction section for protons and alpha particles is calculated by Rutherford's formula. Analytical expression on cascade and probabilistic function taking into account energy losses for protons and alpha particles from recurrence relations for transition probabilities is received. The cascade and probabilistic function calculation algorithm, primary beaten-out atoms range, radiation defects concentration is given.
Key words: Proton, alpha particle; approximation, cascade and probabilistic function, interaction section, a range of primary beaten-out atoms, concentration; radiation defects.

Introduction

When passing particles through substance quite difficult and diverse phenomena which have important theoretical and practical value for nuclear physics, solid body physics, other science and technology fields are observed. First of all, it belongs to physics of space beams [1-3], radiation physics of a solid body [4-7], and especially recently to radiation manufacturing techniques on materials with the set physical and chemical properties [8, 9].

For understanding and the description the specified phenomena, on the one hand, it is necessary to know what happens to particles (both primary, and secondary, generated in different impacts). One of the main objectives in this case is an establishment of spatial and power and temporary distributions on the falling and secondary particles in the environment. On the other hand, at the moment and also after particles passing through substance practically all properties on the substance change.

At the description these processes there is the choice problem on the research theoretical method. The most known and widely applied theoretical calculation methods is the Monte Carlo [10] method, the Boltzmann kinetic equations [11], Fokker-Planck's equation and various specialized methods and model [12].

Without belittling widely known numerical methods and models, apparently, one may say, at all that an undoubted advantage in comparison with them analytical methods possess even if with their help it is possible to describe any phenomenon only approximately. The analytical calculation method offered by us called cascade and probabilistic (CP) [13, 14] is developed by us in the course of long work in the field of elementary particles physics, physics of space beams, radiation physics of metals

and positron physics and also on the basis on the analysis and these researches generalization. Its correctness is checked on a large number on specific objectives from nuclear physics various fields and physics of a solid body [13-15]. The essence of this method consists in receiving and further usage the cascade and probabilistic functions. The received models allow to track all process in dynamics and further could be used in the industry for receiving materials with beforehand the set properties. Therefore researches in this direction are relevant.

Main results

For protons and alpha particles the approximating function dependence on penetration depth, is presented in the following form [13]:

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

where σ_0, a, E_0, k – the approximation parameters calculated when comparing (1) with calculations of sections for Rutherford's formula.

From Kolmogorov-Chapman's equations we will receive recurrence relations for probabilities of transition:

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

From a ratio (2) we will receive CPF expression for protons and alpha particles in the following look:

$$\psi_n(h', h, E_0) = \frac{1}{n!\lambda_0^n}\left(\frac{E_0 - kh'}{E_0 - kh}\right)^{-l} \times$$
$$\times \exp\left(-\frac{h - h'}{\lambda_0}\right)\left(h - h' + \frac{\ln\left(\frac{E_0 - kh'}{E_0 - kh}\right)}{ak}\right)^n, \qquad (3)$$

where h',h – particle depths on generation and registration respectively, n – number of interactions, E_0 – initial energy of primary particle, σ_0, a, E_0, k – approximation coefficients, $\lambda_0 = 1/\sigma_0$, $l = 1/\lambda_0 ak$.

For CPF calculation for protons it is necessary to calculate interaction section by Rutherford's formula [16]. The sections transformed values calculated on this formula for protons and alpha particles depending on h have an appearance on the increasing curve. For great values of E_1 of section slowly increase, with reduction of E_1 - it is very sharp. Results of selection of approximations are presented in the figure 1. Approximating parameters for alpha particles in molybdenum at various values of initial energy are specified in table 1.

We receive depths of observations for protons, using tables of run and brake abilities for easy ions [17]. The values of sections found on Rutherford's formula are approximated by expression (1). Coefficients σ_0, a, E_0, k are by the smallest squares method, and E_0 here isn't initial energy of primary particle, and there is an approximation coefficient. The theoretical correlation relations fluctuate in an interval 0,97 ÷ 0,9999.

Table 1 – Approximating parameters for alpha particles in molybdenum

E_0	σ_0	α	E_0	k	η
50	13801.11158	89.00812	0.05837	1.60874	0.99786
40	14208.86517	21.31636	0.17366	6.93237	0.99837
29	16103.96377	0.00684	375.16828	25333.17	0.99876
20	19288.56287	0.10035	17.66345	2158.797	0.99931

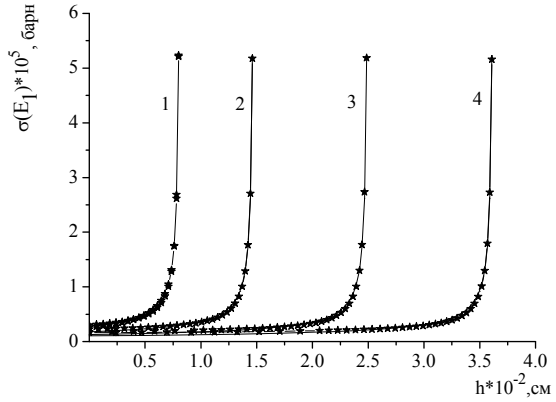

Figure 1 – Dependence σ(h) for alpha particles in wolfram (tungsten) at E_0: 1-20; 2-30;3-40;4-50 (MeV) (1-4)

Using expression (3) for CPF, calculations were made on a formula:

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

CPF calculations results depending on interactions number are presented in the figure 2, from penetration depth in the figure 3. Calculations results shows that CPF for protons behave as follows: at values n=0,1 CPF depending on h decrease, with increase in n CPF increase, reaching a maximum and begin to decrease; at the others n increase. With increase of E_0 the number of the decreasing curves increases, the curves number with a maximum also grows, and the increasing curves number decreases [15, 18]. At small E_0 curves with increase in h already have a maximum, at small h curves have no maximum, at h, approaching to h_{max}, curves increase. At great values of E_0 curves have a maximum already at small h which is displaced with increase in n and h to the right and then disappears. For alpha particles the CPF behavior is similar to CPF behavior for protons except that at the same E_0 values the number of the decreasing curves and curves with maximum increases, but the number on the increasing curves decreases. CPF depending on interactions number for protons and alpha particles behave as follows: at small values of depths CPF decrease, with increase in CPF penetration depth the CPF increase, reaching a maximum, then decrease. With increase E_0 the number of the decreasing curves increases [20-22].

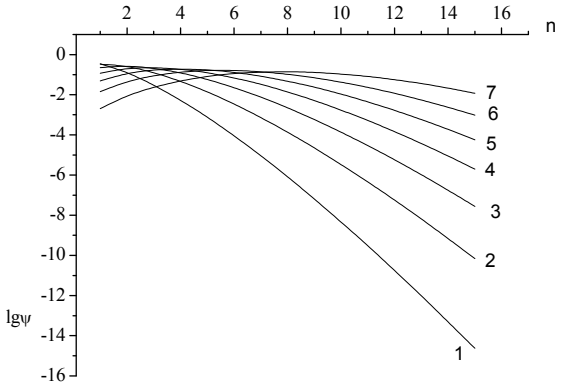

Figure 2 – Dependence $\psi_n(h',h,E_0)$ for protons in copper at E0=5 MeV from number of interactions for h =0,001; 0,002; 0,003; 0,004; 0,005; 0,006; 0,007 cm (1-7)

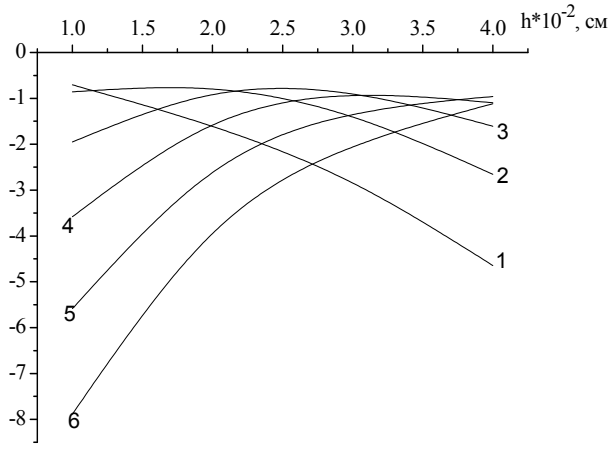

Figure 3 – Dependence $\psi_n(h',h,E_0)$ for protons in copper at E_0=15 MeV from penetration depth for n=1, 4, 7, 10, 13, 16 (1-6)

In the solid bodies irradiated with protons and alpha particles it is necessary for calculation radiation defects concentration in PBOA range $W(E_0,E_2,h)$ to integrate on E_2 to E_c up to E_{2max} [14, 15]. Then:

$$C_k(E_0,h)=\int_{E_c}^{E_{2\max}} W(E_0,E_2,h)dE_2\,, \qquad (5)$$

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

E_2 – energy of primary beaten-out atom, E_c – threshold energy, E_{2max} – the maximum energy transferred to atom, m_1c^2 – energy of rest of a proton or alpha particle, m_2c^2 – energy of rest of a target, E_1 – energy of a particle after losses.

PBOA range $W(E_0,E_2,h)$ is defined by a formula:

$$W(E_0,E_2,h)=$$
$$=\sum_{n=0}^{n_1}\int_{h-k\lambda_2}^{h}\psi_n(h')\exp\left(-\frac{h-h'}{\lambda_2}\right)\frac{\omega(E_1,E_2,h')}{\lambda_1(h')}\frac{dh'}{\lambda_2}\,, \quad (6)$$

where n_1 – maximum number of elastic collisions, $\psi_n(h')$ – cascade and probabilistic function taking into account losses of energy for protons and alpha particles later for n-number interactions at generation depth h'.

$$\lambda_1(h')=\frac{1}{\sigma_0 n\left(1+\frac{1}{a(E_0-kh')}\right)}*10^{24}\,(\text{cm}). \quad (7)$$

For λ_2 calculations on σ_2 on Rutherford's formula at z_1=1 for protons, z_1=2 for alpha particles, z_2=z (z – atomic number of the considered element). A PBOA range in the elementary act $\omega(E_1,E_2,h')$ at h' depth is defined as the relation of differential Rutherford section $\frac{d\sigma(E_1,E_2,h)}{dE_2}$ to integrated [14,15]. Calculations results are presented in the Figure 4.

From results of calculations it is visible that concentration distributions curves defects on depth increase, reaching a maximum, then decrease to zero. With increase in initial energy on a particle curves are displaced to the right and defects concentration values decrease. With increase in threshold energy on the E_c concentration value decrease, and curves pass much below, transition through a maximum is carried out more smoothly.

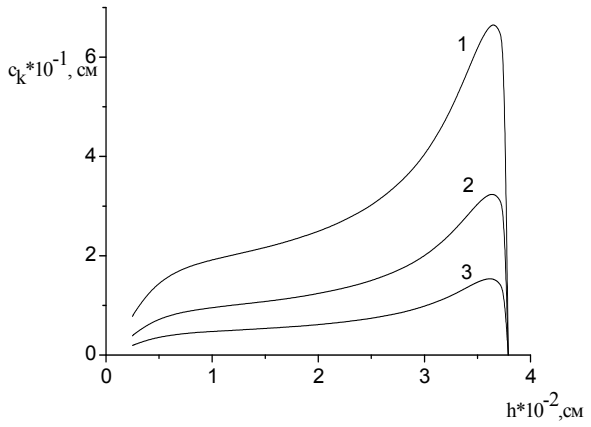

Figure 4 – Dependence of radiation defects concentration on depth at radiation by aluminum alpha particles at E_0=30 MeV E_c=50 KeV(1), E_c=100 KeV(2), E_c=200 KeV(3)

Conclusion

Thus, mathematical models of cascade and probabilistic functions taking into account energy losses for protons and alpha particles are received. With usage the received models, the calculation models of primary beaten-out atoms ranges and radiation defects concentration are received. The CPF calculation algorithm depending on interactions number and particles penetration depth is presented. Approximating expression selection is made for protons and alpha particles, approximation coefficients for various targets are found. CPF Calculations depending on interactions number and particles penetration depth , concentration of radiation defects in the materials irradiated with protons and alpha particles are made. Results of the received researches can be used by experts in the area to radiation physics of a solid body, space physics.

References

1. Yanossi L. Space beams. – M.: Foreign literature, 1949. – P. 463.

2. Rossi B., Greisen K. Interaction of space beams with substance. – M.: Foreign literature, 1948. – P. 132.

3. Dobrotin N.A. Space beams. – M.: Gostekhizdat, 1954. – P. 320.

4. Dins J., Vinyard J. Radiation effects in solid bodies. – M.: Foreign literature, 1960. – P. 243.

5. Damask A., Dins J. Dot defects in metals. – M.: World, 1966. – P. 291.

6. Czarnacka, K., Komarov, F.F., Romanov, I.A., Zukowski, P., Parkhomenko, I.N. AC measurements and dielectric properties of nitrogen-rich silicon nitride thin films. // Proceedings of the 2017 IEEE 7th International Conference on Nanomaterials: Applications and Properties, NAP 2017. – No. 5. – P. 657-669.

7. Komarov, F.F., Milchanin, O.V., Parfimovich, I.D., Tkachev, A.G., Bychanok, D.S. Absorption and Reflectance Spectra of Microwave Radiation by an Epoxy Resin Composite with Multi-Walled Carbon Nanotubes. //Journal of Applied Spectroscopy. – 2017. – Vol. 84. – No. 4. – P. 570-577.

8. Komarov F.F. Nano- and microstructuring of solids by swift heavy ions//Physics-Uspekhi. -2017. – Vol. 187. – No. 5. –P. 465-504.

9. Komarov, F.F., Romanov, I.A., Vlasukova, L.A., Mudryi, A.V., Wendler, E. Optical and Structural Properties of Silicon with Ion-Beam Synthesized InSb Nanocrystals.// Spectroscopy.-2017. – Vol. 120. – No. 1. –P. 204-207.

10. Komarov, F.F., Konstantinov, S.V., Strel'nitskij, V.E., Pilko, V.V. Effect of Helium ion irradiation on the structure, the phase stability, and the microhardness of TiN, TiAlN, and TiAlYN nanostructured coatings. //Technical Physics. – 2016. – Vol. 61. – No. 5. – P. 696-702.

11. Al'zhanova, A., Dauletbekova, A., Komarov, F., Akilbekov, A., Zdorovets, M. Peculiarities of latent track etching in SiO2/Si structures irradiated with Ar, Kr and Xe ions.-2016. – Vol. 374. – No. 1. –P. 121-124.// Nuclear Instruments and Methods in Physics Research, Section B: Beam Interactions with Materials and Atoms.-2016. – Vol. 426. – No. 1. – P. 1-56.

12. Komarov, F.F., Zayats, G.M., Komarov, A.F.,Michailov, V.V., Komsta, H.Simulation of radiation effects in SiO2/Si Structures.// Acta Physica Polonica A. –2015. – Vol. 3. – No. 1. – P. 854-860.

13. Komarov, F., Uglov, V., Vlasukova, L., Zlotski, S., Yuvchenko, V.Drastic structure changes in pre-damaged GaAs crystals irradiated with swift heavy ions.// Nuclear Instruments and Methods in Physics Research, Section B: Beam Interactions with Materials and Atoms. – 2015. – Vol. 360. – No. 4. – P. 150-155.

14. 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, Scientific Research Institute for New Chemical Technologies and Materials under al-Farabi KazNU, 2015. – P. 388.

15. Kodanova, S.K., Ramazanov, T.S., Issanova, M.K., Golyatina, R.I., Maiorov, S.A Calculation of ion stopping in dense plasma by the Monte-Carlo method.// Journal of Physics: Conference Series. – 2018. – Vol. 946. – No. 1. – P. 148-154.

16. Smyrnova, K.V., Pogrebnjak, A.D., Beresnev, V.M., Kravchenko, Y.O., Bondar, O.V. Microstructure and Physical–Mechanical Properties of (TiAlSiY)N Nanostructured Coatings Under Different Energy Conditions.// Metals and Materials International. – 2018. – Vol. 24. – No. 2. – P. 241-439.

17. Kozhamkulov, B.A., Kupchishin, A.I., Bitibaeva, Z.M., Tamuzs, V.P. Radiation-Induced Defect Formation in Composite Materials and Their Destruction Under Electron Irradiation // Mechanics of Composite Materials. – 2017. – Vol. 53. – No. 1. – P. 59-64.

18. Kupchishin, A.I. On positrons irradiation in the defects of vacancy type.// IOP Conference Series: Materials Science and Engineering. – 2017. – Vol. 184. – No. 1. – P. 234-248.

19. Kupchishin, A.I., Niyazov, M.N., Voronova, N.A., Kirdiashkin, V.I., Abdukhairova, A.T.The effect of temperature, static load and electron beam irradiation on the deformation of linear polymers.// IOP Conference Series: Materials Science and Engineering. – 2017. – Vol. 168. – No. 1. – P. 229-274.

20. Kupchishin, A.I., Kupchishin, A.A., Voronova, N.A. Cascade-probabilistic methods and solution of Boltzman type of equations for particle flow// IOP Conference Series: Materials Science and Engineering. -2016. – Vol. 110. – No. 1. – P. 123-129.

21. Kupchishin, A.I., Kupchishin, A.A., Voronova, N.A., Kirdyashkin, V.I.Positron sensing of distribution of defects in depth materials. // IOP Conference Series: Materials Science and Engineering. – 2016. – Vol. 110. – No. 4. – P. 248-258.