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Computer modelling of distributions processes on vacancy nanoclusters depth in the heavy targets irradiated with ions

Abstract. Creation new materials with unique properties is one of priority researches areas, both in physics, and in technique. The study of small metal particles properties from atoms hundreds and thousands is of great interest by their possible usage as materials or surface nanostructures. The fact that nanomaterial properties considerably depend on the particles properties making them is undoubted. The free clusters internal structure research could play a key role in an explanation of their physical or chemical features. Work is assigned to obtaining the regularities arising when modeling radiation processes in the heavy ions irradiated with various ions. The regularities arising when calculating cascade and probabilistic functions depending on particles penetration depth, interactions number are found. Real areas finding the radiation defects concentration result are defined, calculations for various flying particles and heavy targets in the energy range 100 - 1000 keV are made. Calculations results are presented in the schedules and tables form.
Key words: Modeling, ion, heavy target, vacancy nanoclusters, radiation defects concentration, area.

Introduction

Particles interaction problems with substance and radiation defects generation at substance radiation ions have devoted many works [1-5]. Application of the cascade and probabilistic method (CPM) in various fields of physics with usage the simplest cascade and probabilistic function (CPF) is described in works [6, 7]. CPF usage taking into account energy losses of for various charged particles within CPM is shown in work [8]. This work is performed within CPM which essence consists in receiving and further CPM usage. In this work CPF it is used for receiving calculation models on primary beaten-out atoms ranges and vacancy type nanoclusters concentration. Passing ions through substance is a difficult task as during creation physical, and mathematical models. A set of the flying particles types and targets of Mendeleev's Periodic system represents a huge elements number [9-14]. At the same time it is possible to consider various situations when the flying particles mass number are less than a target atomic number, it is commensurable with a target atomic number and a case when the flying particle atomic weight is more or much more target atomic number. Elements are classified by us on easy and heavy by element density. In work interaction process of the flying ions, various on density, with heavy ions is considered [15, 18].

Main results

For receiving calculation models of primary beaten-out atoms ranges and radiation defects concentration it is necessary to receive analytical expression of the cascade and probabilistic functions (CPF) making sense to probability that the particle generated at h' depth, will reach h depth after n impacts number. We have used CPF taking into account energy losses for ions, has the following appearance [8]:

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

where h',h – generation and registration depths of a particle respectively, n– interactions number, E_0 – primary particle initial energy, $l=1/\lambda_0 ak$, λ_0, a, k, E_0 – the approximation parameters entering the following recurrence relation [12-18]:

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

Approximating coefficients selection results are presented in tables 1, 2. Approximations selection results are presented in the figure 1.

Table 1 – Approximating parameters for silicon in silver

E_0	σ_0*10^8	a	E_0`	k	η
1000	0,00084229	0,00028854	1,1432	2440,1	0,999
800	0,28096	0,089117	1,0067	2653,6	0,999
500	0,014611	0,0034919	0,85506	3574,9	0,999
200	0,036748	0,0084184	0,34591	3755,6	0,999
100	0,11412	0,02743	0,16292	3757	0,999

Table 2 – Approximating parameters for silver in silver

E_0	σ_0*10^{10}	a	E_0`	k	η
1000	0,21185	0,16977	1,0087	7528,6	0,998
800	0,59507	0,47916	0,71531	6677,5	0,997
500	0,76419	0,37929	0,7438	11227	0,997
200	2,5751	2,4126	0,13503	4694,8	0,999
100	6,533	10,542	0,035424	2140,5	0,999

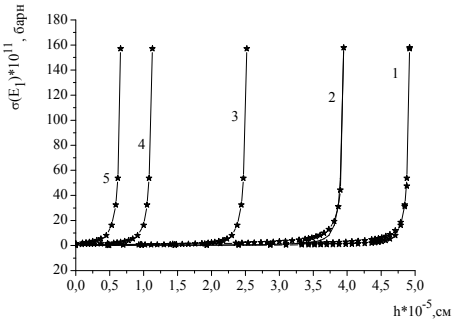

Figure 1 – Approximation of the cascade and probabilistic function modified section for Indian in gold:E_0=1000(1), 800(2), 500(3), 200(4), 100(5) keV. Points – settlement the dependences of section on depth, continuous lines – approximation

CPF Calculations are executed on the following formula:

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

CPF calculations results depending on interactions number and particles penetration depth are presented in figures 2,3.

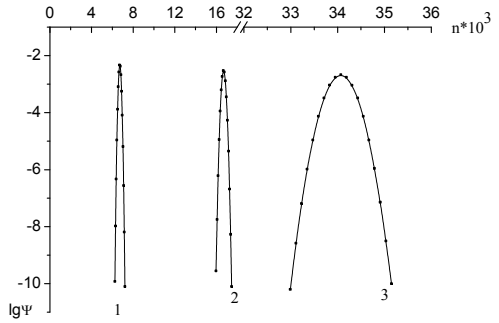

Figure 2 – CPF dependence on interactions number for the titan in iron for E_0=1000 keV h=0,0001; 0,0002; 0,0003 cm (1-3)

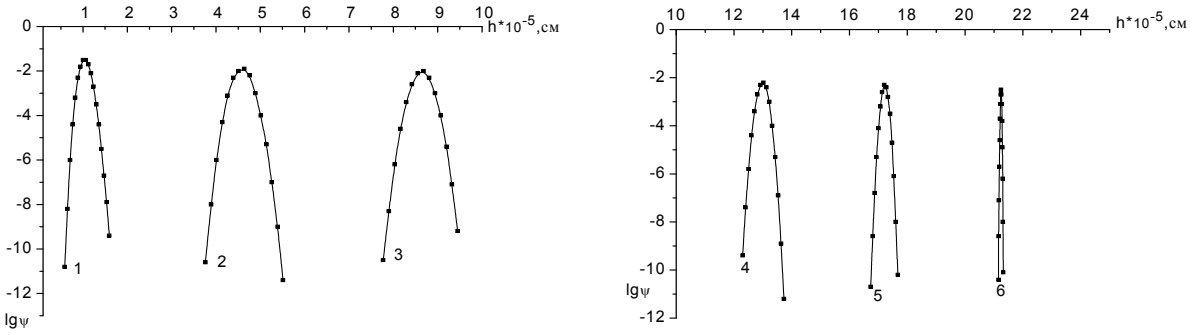

Figure 3 – CPF dependence for aluminum in tungsten from interactions number at E_0= 1000 keV and n=153, 787, 1804, 3496, 6548, 17108 (1-6)

When calculating CPF depending on interactions number and particles penetration depth and also vacancy type nanoclusters concentration needs to find real result finding area. We will note the main regularities when calculating CPF depending on interactions number arising when result finding area for various flying particles and heavy targets [11-15].

1. With initial energy reduction (the flying particle and a target same) with the same penetration depth the area of result is displaced to the small depths area.

2. For heavy targets the area of result is displaced to the small depths area, the area left border decreases more slowly, the right border sharply decreases.

3. With increase in observation depth the area of result is narrowed and displaced to the small depths area.

The regularities arising when calculating CPF depending on penetration depth following [18-21]:

1. With increase in atomic weight of the flying particle the step for calculation increases, reaching several hundred and even thousands.

2. With a big atomic weight of the flying particle and target the counting duration considerably increases and selection of borders becomes complicated.

3. With increase in observation depth the area of result is displaced to the big depths area and narrowed.

4. With initial particle energy reduction the area of result is displaced to the big depths area and narrowed.

Radiation defects concentration at ionic radiation is calculated on the following formula [8]:

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

where E_0 – initial energy of the flying ion, E_d – threshold energy of shift, E_c– energy of the primary beaten-out atom (PBOA) at which the amount of the displaced atoms equals to atoms number N_d, being in a spontaneous recombination zone, E_{2max}– the greatest possible energy acquired by atom, $\psi_n(h')$ – CPF function in modified type, $\lambda_1(h')$ and λ_2 – shift run an ion – and atom - atomic shifts [15, 22].

Calculations results on distributions at the vacancy nanoclusters depth are presented in figures 4-6.

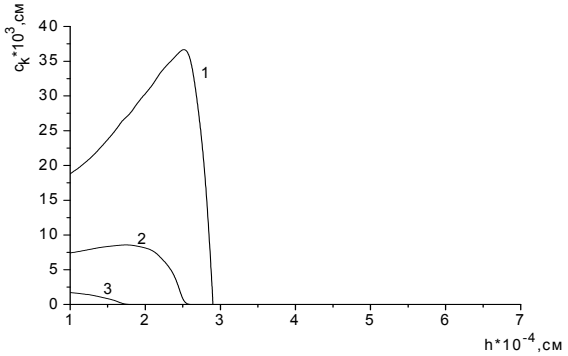

Figure 4 – Dependence on concentration of cascade areas on depth at copper radiation by aluminum ions: E_0= 500 keV, E_c= 50 (1), 100 (2), 200 (3) eV

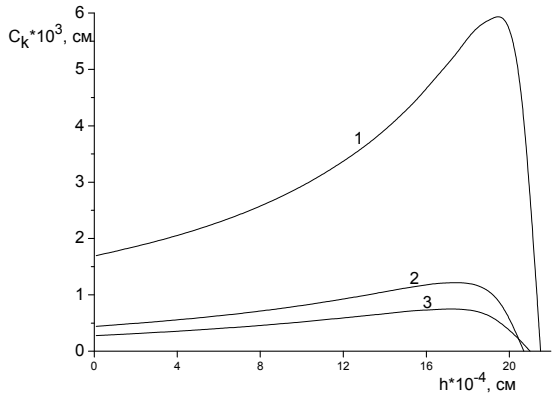

Figure 5 – Dependence of radiation defects concentration on depth at ionic radiation for carbon in Germanium (1), boron in Germanium (2) and fluorine in Germanium (3); E_c=50 keV; E_0= 1000 keV

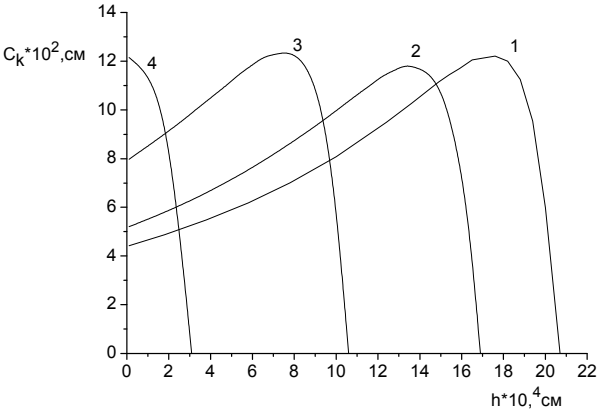

Figure 6 – Dependence of the radiation defects concentration on the depth at ion irradiation for nitrogen in germanium at E_c=50 keV; E_0= 1000 (1), 800 (2), 500 (3) keV

Conclusion

Thus, in the work an approximation expression for the interaction cross-section is selected and the approximation coefficients are found. Cascade-probability functions are calculated as a function of the interactions number and the particles penetration depth, the defects concentration in heavy targets. The regularities in the result domain behavior for calculating cascade-probability functions, the spectrum on primary-knocked-out atoms, and the radiation defects concentration of in heavy targets irradiated by ions are obtained. It could be seen that as the atomic number of the target increases for the same incident particle, the value of the function at the maximum point increases insignificantly, the depth values decrease, that is, in the heavier target of the vacancy clusters, more is formed, especially in the near-surface region.

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