COMPUTER MODELING OF CASCADE PROBABILISTIC FUNCTIONS, ENERGY SPECTRA OF PKA AND CONCENTRATION OF VACANCY CLUSTERS IN MATERIALS IRRADIATED WITH LIGHT IONS

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I. INTRODUCTION

As is known, the main cause of changes in the structure and physicochemical properties of materials during radiation exposure is the formation of defects [1 - 4]. In contrast to light particles (electrons, photons, etc.), the interaction of ions with matter forms cascade regions, vacancies, clusters of interstitial atoms (and not Frenkel pairs, as is considered in many papers), etc.

Thus, when considering the passage of ions (including light ions: protons and alpha particles) through the matter, it is necessary to solve the cycle of physical and mathematical problems. Most of our work in this direction will be carried out in the framework of the cascade-probability method [5].

II. RESULTS AND DISCUSSIONS

As the calculations show, approximation describes the modified cross sections quite well with a correlation coefficient above 0.99, in particular for molybdenum (Table 1).

Table 1. Approximation values and theoretical correlations for protons in Mo

E_0, [MeV]	σ_0	a	E_0'	K	η
1	17176	0.22	4.39	5600	0.999
5	2919	0.0249	31.35	3719	0.9999
10	2123	1.45	1.06	42.1	0.999
15	1694	2.68	0.84	16.92	0.999
20	1413	2.33	1.23	15.19	0.997
25	1227	1.89	1.85	15.64	0.99
30	1067	1.60	2.43	15.01	0.996
40	912.2	0.13	37.98	142.36	0.996
50	790.3	0.11	53.77	136.92	0.99

The software package for calculating CP-functions and selecting the type of theoretical curves is implemented in Visualbasic 6.0, C ++ Builder 6.0, Delphi 6.0. Calculations are made for protons and α-particles in various targets. As an example, Figures 1 and 2 show the dependences of CPF on the number of interactions and the penetration depth for alpha particles in Mo at E_0 = 10 MeV. The calculation results show that with values of n = 0.1 CPF decrease, depending on h, with increasing n, they increase, reaching a maximum and begin to decrease. As E_0 grows, the curves shift to the right.

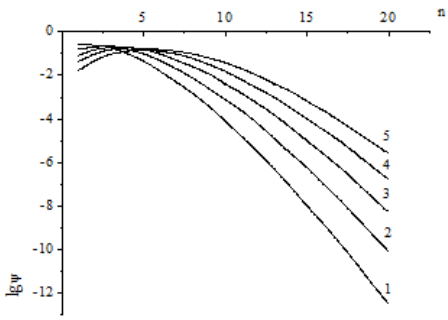

Figure 1. Dependence of CPF on the number of interactions for alpha particles in molybdenum at E_0 = 10 MeV, h = 0.006; 0.008; 0.01; 0.012; 0.014 cm (1-5)

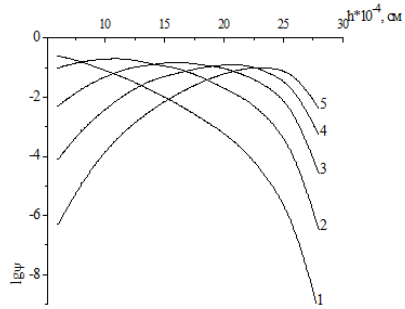

Figure 2. Dependence of CPF on the depth of penetration for alpha particles in molybdenum at E_0 = 10 MeV; n = 1, 4, 7, 10, 13 (1-5)

Further, the energy spectra of PKA were calculated, in particular, for α-particles in Mo. It can be seen that these are decreasing functions. In a good approximation, W (E_2) ~ 1/E_2. The concentrations of vacancy clusters were calculated at E_0 = 10, 50 MeV. With increasing depth h, C_k increases, and at the end of the run it drops sharply to zero. With increasing E_c, the concentration of clusters decreases.

III. CONCLUSIONS

1. The analysis of modified sections and the calculation of cascade-probability functions for alpha particles were carried out. It was shown that the correlation coefficients η > 0.99 (calculated and modified values), which is a good approximation.

2. CPF were analyzed and its main properties were established. When k = 0, this function goes to the simplest CPF. There are inflection points and maxima. With increasing n, CPF increases, reaches a maximum, and further decreases. As h increases, the maxima of the curves shift to the right.

3. The energy spectra of PKA in Mo were calculated. In a good approximation, W(E_2) ~ 1/E_2. With increasing depth, Ck increases slowly, reaches a maximum near the end of the path, and drops sharply to zero. With increasing E_c, C_k decreases.

ACKNOWLEGMENTS

This research has been/was/is funded by the Science Committee of the Ministry of Education and Science of the Republic of Kazakhstan (Grant No. AP08855701).

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