Computer simulation of the energy spectra of PKA in materials irradiated by protons in the framework of the Cascade-Probabilistic method

T A Shmygaleva¹, A I Kupchishin¹,², A A Kupchishin² and C A Shafi³
¹Kazakh National University named after al-Farabi, al-Farabi av 71, Almaty, Kazakhstan
²Kazakh National Pedagogical University named after Abai, Dostyk 13, Almaty, Kazakhstan

E-mail: ankupchishin@mail.ru

Abstract. The work is performed within the framework of a cascade-probabilistic method, the relevance of which is beyond doubt, since the models obtained make it possible to trace the entire process in dynamics and can later be used in industry to obtain materials with predefined properties. Algorithms for calculating the spectra of primary knocked-on atoms for protons have been developed. The features of the selection of approximate expressions and approximation coefficients for proton irradiation are considered. Calculations have been made for the concentrations of vacancy clusters in copper irradiated by protons.

1. Introduction
Modeling the radiation damage of solids irradiated with charged particles is one of the important problems of solid-state radiation physics [1, 2]. Studies in the field of radiation influence on the physical properties of materials are of great interest both for studying the structure of a solid body and for the practical use of substances with new properties obtained as a result of irradiation [3, 4]. In the interaction of charged particles with matter, primary, secondary, knocked-off atoms, etc., are generated. As a result, the structure of a solid is disturbed and radiation defects are formed. [5 – 11]. During proton irradiation, defects are generated in the form of cascade regions of the vacancy type. The main characteristic of the damaged material is the energy spectrum of the primary knocked-on atoms at different depths of the irradiated material, the knowledge of which makes it possible to calculate the number of defects formed, and also to model their distributions in depth and in dimensions, i.e. it is possible to trace quite effectively the entire process in dynamics at any depth of the irradiated material.

In this paper, models of the PKA spectra and cluster concentrations were obtained, and their depth calculations were made in materials irradiated with protons. A comparison with the previously obtained results was made. The work was performed within the framework of a cascade-probabilistic method.

2. Method of calculation
To calculate the spectra of primary knocked-on atoms in materials irradiated with protons, it is first necessary to find analytic expressions for cascade-probability functions (CPF). To calculate the CPF
it is necessary to obtain an approximate expression that describes the cross section of the interaction that enters into the recurrence relation, from which the expressions for the CPF are obtained. For protons, the dependence of the approximation function on energy, which in turn depends on the depth of penetration, is represented in the following form [8]:

$$\sigma(h) = \sigma_0 \left( \frac{1}{a(E_0 - kh)} + 1 \right).$$  \hspace{1cm} (1)

where \(\sigma_0, a, E_0, h, k\) are the approximation coefficients, \(h\) is the penetration depth of the particle. 

The cascade-probability function with allowance for energy losses for protons is represented in the following form [8]:

$$\psi_n(h', h, E_0) = \frac{1}{n! \lambda_0^n} \left( \frac{E_0 - kh'}{E_0 - kh} \right)^{-l} \exp \left( - \frac{h - h'}{\lambda_0} \right) \left[ \ln \left( \frac{E_0 - kh'}{E_0 - kh} \right) \right]^{n},$$  \hspace{1cm} (2)

where \(l = 1/(\lambda_0 ak)\), \(\lambda_0 = 1/\sigma_0\), \(h', h\) are the generation and registration depths of the proton, respectively, \(n\) is the number of interactions, \(E_0\) is the initial energy of the proton.

The spectrum of primary knocked-on atoms is determined by the formula:

$$W(E_0, E_2, h) = \frac{E_{d}E_{2\max}}{E_2^2 (E_{2\max} - E_{d})} \sum_{n=0}^{m} \int \exp(-n! - n \ln \lambda_0) - \frac{1}{\lambda_0 ak} \ln \left( \frac{E_0 - kh'}{E_0 - kh} \right) - \frac{h'}{\lambda_0} + \ln \left( \frac{E_0 - kh'}{ak} \right) - \frac{h - h'}{\lambda_2} - \ln \lambda_1(h') - \ln \lambda_2(h') dh''.$$  \hspace{1cm} (3)

where \(E_d\) is the threshold energy of displacement, \(E_{2\max}\) is the maximum possible energy acquired by the atom, \(\lambda_1(h')\) and \(\lambda_2\) are the ranges of displacement of the proton and atom-atom displacements, \(n_1\) is the maximum number of collisions during proton irradiation. The concentration of radiation clusters during proton irradiation is calculated by the formula:

$$C_K(E_0, h) = \int_{E_c}^{E_{2\max}} W(E_0, E_2, h) dE_2.$$  \hspace{1cm} (4)

\(E_2\) is the energy of the primary knocked-on atom, and \(E_c\) is the threshold energy for cluster formation.

3. Results and discussion

The integrated cross-section of the interaction was calculated by Rutherford’s formula [12], the penetration depths were obtained from the tables of ranges and braking powers for light ions [13]. For the calculated cross-section of the interaction, the approximate expression was chosen by formula (1) depending on the depth of observation, and the approximation parameters included in the expression for CPF and PKA spectra were found. The results of the approximation coefficients are given in Table 1 and in Figure 1.
Table 1. Approximation values and theoretical correlation ratios for protons in Cu

| $E_0$ (MeV) | $\sigma_0$ | $a$ | $E_0'$ | $K$ | $\eta$ |
|-------------|------------|-----|--------|-----|--------|
| 5           | 3341       | 0.17 | 4.11   | 500.4 | 0.9997 |
| 10          | 1810       | 0.0445 | 18.45  | 704.4 | 0.9998 |
| 15          | 1973       | 2.8  | 0.74   | 15.01 | 0.999 |
| 20          | 1087       | 0.55 | 2.08   | 24.64 | 0.999 |
| 25          | 821        | 0.0954 | 10.77  | 85.47 | 0.9997 |
| 30          | 779        | 0.24 | 5.51   | 32.39 | 0.999 |
| 40          | 1097       | 0.14 | 34.34  | 126.6 | 0.999 |
| 50          | 947.7      | 0.12 | 49.13  | 122.6 | 0.9999 |

The points are the calculated data, the solid line is the approximation (curves 1–5, respectively)

Figure 1. Dependences of the modified CPF cross section for protons in copper from $h$.

Figure 2. Dependence of CPF on the number of interactions for protons in Cu.

The coefficients $\sigma_0$, $a$, $E_0'$, $k$ are found by the method of least squares, where $E_0'$ is not the initial energy of the primary particle, but is the approximation coefficient. The theoretical correlation ratio for all elements and energies in the range from 5 to 50 MeV ranges from 0.99 to 0.999, which indicates a very good selection of approximations. When choosing approximation curves for protons according to formula (1), difficulties arise that involve a specific analysis of each curve. The choice of optimal values depends on the initial data, for protons we have 4 approximation parameters. In addition, there are situations when the step in $h$ fluctuates strongly, it is small, then large, and then the approximation formula is even harder to pick up. In this case, you need to use techniques to eliminate emerging features. In the region of small initial particle energies for protons, the process of selecting the type of approximation curves is also complicated by the fact that the step in $h$ and the depths themselves are small, while the values of the cross sections are large. Compared with light, for heavy elements, for example Mo, the approximation curve is chosen somewhat easier. With increasing initial energy, the selection of curves is better.
Calculation of CPFs taking into account the energy losses for protons was carried out according to formula (2). The results of the calculations are shown in Figure 2. Depending on $n$, for different $h$, the CPFs first increase, then reach a maximum and then decrease.

The calculation of PKA spectra was carried out according to the formula (3). The results of the calculations are shown in Figures 3 – 5.

The results of the calculations show that the dependence of PKA spectra on PKA energy is a decreasing function. It can be seen that as the initial proton energy increases (Figure 3), the values of the PKA concentration decrease, with increasing penetration depths increase (Figure 4).

\[ E_0 = 10(1); 15(2); 20(3); 30(4) \text{ MeV} \]

**Figure 3.** Dependence of $w (E_0, E_2, h)$ on $E_2$ for protons in Cu at a depth of $h = 10 \mu m$

\[ E_0 = 10 \text{ MeV}; h = 20(1), 110(2), 181(3), 226(4) \mu m \]

**Figure 4.** Dependence of $w (E_0, E_2, h)$ on $E_2$ for protons in Cu

The results of PKA spectra calculated using formula (3) are compared with the results obtained earlier in [14] and shown in Figure 5 with a dashed line. We see a good agreement. The small difference is due to the fact that in [14] the average value of the mean free path length for the formation of PKA was taken to calculate PKA spectrum, and in this paper we used a range that takes into account the energy loss for ionization and excitation during PKA generation. To compare the results of calculations, in addition to protons in copper and molybdenum, alpha particles were taken in molybdenum, presented in Figure 5. There is a slight difference. Calculation of the concentration of radiation defects during proton irradiation was carried out according to formula (4). The results are shown in Figure 6. For light targets, the curves increase, reaching a maximum, then decrease to zero. With an increase in the initial energy of the particle, the values of the concentration of radiation clusters increase, the maximum is more pronounced. With increasing atomic number of the target, the behavior is similar. With an increase in the threshold energy $E_c$, the values of the concentration decrease, and the curves pass much lower, the transition through the maximum is made smooth.
4. Conclusions
The energy spectra of PKA and the concentration of vacancy clusters in materials irradiated with protons were simulated. The approximation of the expression was performed and the approximation parameters for various values of the initial energy were found. Calculations of cascade-probability functions were performed. Algorithms are presented and calculations of the spectra of primary knocked-on atoms were performed as a function of PKA energy for different values of the initial energy and depths. The results of calculations were compared with calculations made earlier. There is a good agreement. Calculations of the concentration of defects at various values of the threshold energy were made. \( C_k \) as a function of \( h \), first it increases, then, reaches a maximum and then decreases.

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