Computer-based modeling of radiation defect parameters in materials irradiated with charged particles

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Abstract. The paper considers a new approach to approximation expressions for integral sections of interaction and for approximation coefficients included in expressions for cascade-probability functions (CPF), spectra of primary knocked-on atoms (PNA) and the concentration of radiation defects in materials irradiated with charged particles, namely electrons, protons, alpha particles and ions. The obtained approximations made it possible to design the mathematical models of cascade-probability functions taking into account energy losses for electrons, protons, alpha particles and ions. The integral sections of interaction, penetration depths were calculated, the approximation expressions were chosen, and the approximation coefficients for the above particles were found. Recurrence ratios were derived to obtain CPF. The choice of an approximation expression and finding of approximation coefficients was compared with the earlier process using different software packages. It is apparent that that the use of modern algorithms considerably simplifies this process.

1. Introduction

Currently, research related to computer modeling of physical processes has been widely developed. The mathematical process model, numerical algorithm, computer-based calculation program, analysis of results and the object of study allow explaining and describing many phenomena [1–3]. Much attention is paid to the processes of radiation defects in materials irradiated with various charged particles [4–7]. The need for research in this field is related to the problem of controlling the evolution of solid defects in order to ultimately obtain materials with given properties [8–10]. Without research in this direction, solid state radiation physics would remain a fairly academic sphere presenting no interest for practical applications. An example of strong results is ion implantation – introduction of alloying elements using a beam of accelerated ions [11, 12].

Many works are devoted to the problems of interaction of charged particles with substance in the generation of radiation defects in solid bodies irradiated with electrons, protons, alpha-particles, ions [13–16]. During electronic irradiation, defects are formed as Fraenkel pairs, during proton, alpha and ion irradiation in the form of cascade areas of the vacancy type. The work is carried out within the framework of the cascade-probability method, in which the cascade-probability functions are obtained in their analytical form. Then, the models of calculation of spectra of primary knocked-on atoms and the concentration of radiation defects are derived from CPF expressions [16, 17]. The paper discusses the features of computer simulation of radiation defect parameters in solid bodies when irradiating them with various charged particles: electrons, protons, alpha particles and ions. The approximation
expressions for the integral section of the interaction were chosen and the approximation coefficients for the above particles were found using modern methods and algorithms.

2. Calculation methodology

Proceeding from physical reasons, we remove recurrence relations for receiving mathematical models of cascade-probability functions taking into account energy losses for various charged particles. The recurrence relations include the integrated sections of interaction depending on energy, and, therefore, on depth since with the increase in the penetration depth the energy of a projectile decreases. Within the cascade-probability method all expressions are presented analytically, therefore, in order for the expressions to be integrated, we approximate the integrated sections of interaction with various expressions. For electrons the recurrence relation is as follows:

\[
\psi_n(h', h, E_0) = \int_{h'}^h \psi_{n-1}(h', h'', E_0) \psi_0(h'', h, E_0) \frac{1}{\lambda_0} \left( 1 - \frac{1}{a(E_0 - kh'')} \right) dh''
\]  

For protons and alpha particles we have:

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

For ions:

\[
\psi_n(h', h, E_0) = \int_{h'}^h \psi_{n-1}(h', h'', E_0) \psi_0(h'', h, E_0) \frac{1}{\lambda_0} \left( \frac{1}{a(E_0' - kh'')} - 1 \right) dh''
\]  

where \( \psi_n(h', h, E_0) \) – probability of a particle to test \( n \) collisions reaching depth \( h \); \( \psi_{n-1}(h', h'', E_0) \) – probability of a particle to test \( (n-1) \) collisions from the depth \( h' \) to \( h'' \); \( \psi_0(h'', h, E_0) \) – probability that a particle reaches depth \( h \) without experiencing a single collision; \( \frac{dh'}{\lambda(h'')} \) – probability that a particle experiences one collision at depth \( h'' \); \( \lambda_0, a, E_0, k \) – approximation parameters for expressions approximating the values of sections for protons, alpha particles, ions. For electrons, we have 3 approximation parameters – \( \lambda_0, a, k \), the approximation expression is presented as follows:

\[
\frac{1}{\lambda(h)} = \frac{1}{\lambda_0} \left( 1 - \frac{1}{a(E_0 - kh)} \right)
\]  

For protons, alpha particles:

\[
\frac{dh}{\lambda(h)} = \frac{1}{\lambda_0} \left( 1 + \frac{1}{a(E_0' - kh)} \right)
\]  

For ions:

\[
\frac{dh}{\lambda(h)} = \frac{1}{\lambda_0} \left( \frac{1}{a(E_0' - kh)} - 1 \right)
\]  

It is also possible to approximate the integrated sections of interaction with other functions. In our case when choosing the approximation expressions the approximate type of function was defined, the known physical parameters were considered. The approximation expression was chosen so that the expression which it enters was integrated and the theoretical correlation relation was close to 1.
From the recurrence relations (1-3) we receive CPF (transition probabilities) for electrons, protons, alpha particles, ions, $\psi_1(h', h, E_0)$, $\psi_2(h', h, E_0)$, $\psi_3(h', h, E_0)$, ..., $\psi_n(h', h, E_0)$. CPF for electrons is as follows:

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

Here, $\lambda(h) = 1/(\sigma(h) n_0)$ – interaction run depending on the penetration depth, $\sigma(h)$ – integral interaction section depending on the penetration depth, $n_0$ – number of atoms in 1 cm$^3$, $n$ – number of interactions, $\lambda_0 = 1/\sigma_0$, $l = 1/\lambda_0ak$, $h'$, $h$ – generation and registration depths, respectively.

CPF for protons and alpha particles is presented in the form of formula (1) from [16], for ions – (3.8) from [17]. Modified CPF expressions for further calculations are included in the expressions for the spectra of CPF and radiation defect concentrations.

3. Results and discussion
The sections for electrons are calculated using McKinley-Feshbach formula [17], for protons, alpha particles, ions – using the Rutherford formula [17]. The depths of observations for electrons are found using the Bethe-Bloch formula [17], for protons, alpha particles – also using the Bethe-Bloch formula intended for protons and alpha particles [18], for ions – from tables of parameters of spatial distribution of the ion-implanted impurities [19]. The calculated sections were approximated by expressions (4–6). Earlier, special software packages, in particular Origin 7.0 and above, were used to choose the approximation expressions and find the approximation coefficients. At the same time, the selection of approximation coefficients strongly depended on initial data, and the selection process sometimes had a large number of iterations and took a lot of time. If initial data are set unsuccessfully, then it was not always possible to perform approximation and to find coefficients. This study suggests a new approach: use of the Levenberg-Marquardt algorithm [20, 21], advanced and useful version of the Gauss-Newton method [22]. The Gauss-Newton method is used for the solution of tasks by a nonlinear least square method. The Levenberg-Marquardt algorithm represents a combination of two methods: the method of the fastest descent (or gradient) and parabolic extrapolation. The Levenberg-Marquardt algorithm is based on heuristic reasons, minimization of functionality is carried out, a function may be set in any form, and the number of coefficients may change. The advantages of this algorithm compared to the Gauss-Newton method as the following: high speed of convergence, higher chances to find a global extremum, well works with a curve-fitting problem [20, 21]. The selection of function does not depend on initial data, it is enough for our functions to set data once, for example, ranging from –1 to 1. The calculation results show that the values found using formulas and approximation parameters (4–6) will be well coordinated. The theoretical correlation relations characterizing the narrowness of communication for any dependence for all elements vary in the range of 0.9–0.9999. The program complex was developed in the Microsoft Visual Studio in the C# programming language.

The choice of the approximation expression in the Python language on django framework is also performed. This is a full Web application, which calculates the integrated sections of interaction, depths of penetration, CPF. In Python there is a scipy computing module, which includes the most known and applied mathematical functions. The scipy.optimize package includes a set of optimization procedures. The most often used methods include the minimization via the least square method, adjustment of curves, minimization of multidimensional scalar functions, etc. [23]. As the parameters $\sigma_0, c=aE_0, b=ak$ are found by the least square method, the curve_fit function was used [21]. The values of theoretical correlation relations are also in the range from 0.9 to 0.9999. The calculations are
performed for charged particles in Al, for electrons – in the range from 1 to 10 MeV, for protons – from 5 to 30 MeV, alpha particles – from 5 to 50 MeV, ions – from 100 to 1000 KeV. The calculation results of the interaction sections and the selection of approximating curves are given in Tables 1–3 and in Figures 1–4 where the points designate calculation data of section dependence on depth, solid lines – approximations.

**Figure 1.** Dependence of the approximation function of the interaction section on the penetration depth for electrons in Al for various $E_0$: 1 – 10; 2 – 8; 3 – 6; 4 – 4; 5 – 2 MeV

**Figure 2.** Relationship of the approximation function of the interaction section on the penetration depth for protons in Al at $E_0 = 30(1), 25(2), 20(3), 15(4), 10(5), 5(6)$ MeV

**Figure 3.** Dependence of the approximation function of the interaction section on the penetration depth for electrons in Al at $E_0 = 50(1), 30(2), 20(3), 10(4), 5(5)$ KeV

**Figure 4.** Dependence of the approximation function of the interaction section on the penetration depth for Al ions in Al at $E_0 = 1000(1), 800(2), 500(3), 200(4), 100(5)$ KeV

| $E_0$, MeV | $\sigma_0$ | $c$ | $b$ | $\eta$ |
|------------|------------|-----|-----|-------|
| 1          | 26.18      | 5.9 | 26.2 | 0.999 |
| 2          | 29.6       | 7.2 | 13.3 | 0.9999|
| 4          | 29.4       | 14.2| 14.4 | 0.9999|
| 6          | 29.2       | 21.3| 14.9 | 0.999 |
| 8          | 29.1       | 29.06| 15.8 | 0.999 |
| 10         | 28.8       | 37.7| 16.8 | 0.999 |
The figures and tables show high degree of relation between estimated and approximating dependences.

4. Conclusion

Thus, the study suggests a new approach to the selection of approximation expressions for interaction sections and finding of the approximation coefficients using the Levenberg-Marquardt algorithm. Integrated interaction sections, penetration depths for electrons, protons, alpha particles and ions were calculated. The analytical expressions of CPF taking into account the energy losses for electrons, protons, alpha particles and ions were received from recurrence relations, which include the received approximation expressions for various charged particles. The software complex for the selection of approximations using the Levenberg-Marquardt algorithm in Microsoft Visual Studio in the C# programming language is developed and a full Web application using modern django framework via the python language was created. The approximations for electrons, protons, alpha particles, aluminum ions in aluminum for various values of particle initial energy were performed.

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