A SCAT program is developed for calculation of the angular distribution of multiply scattered ions in the case of various interaction potentials. The accuracy attained is higher than that obtained with the well-known Meyer and Sigmund programs. The influence of the interaction potential on the angular distribution of multiply scattered ions is analyzed. A good agreement between the angular distribution calculated by the SCAT program and the experimental data and the results of simulation by the Monte Carlo method is observed.

In recent years, in connection with the creation of powerful high-energy implanters, the method of high-energy implantation of heavy and intermediate ions with energies between 0.5 and 100 MeV is finding ever-increasing application [1]. When the models designed earlier for low-energy implantation [2] are applied to high-energy implantation, a substantial discrepancy between theory and experiment is found [3]. One cause of this is that multiple scattering of the incident particles was not taken into account.

In the present investigation we have developed a program for calculating the angular distribution of ions undergoing multiple scattering. The program can be used to simulate high-energy implantation as well as to analyze the experimental data.

Multiple scattering of ions can be described by the integrodifferential transport equation [4] whose formal solution for the multiple scattering function obtained in [5] has the form

\[ F(S, \theta) = \frac{1}{2} \int_0^\infty k \, \kappa \, J_0(\kappa \theta) \exp\left(-\frac{\psi(\kappa)}{\kappa}\right) \, d\kappa, \tag{1} \]

where \( F(S, \theta) \) is the probability (normalized to unity) for scattering of particles into an angle interval \( \theta, \theta + d\theta \) after traversing a layer of matter of thickness \( S \); \( \theta \) is the resultant deflection angle, \( \kappa \) the integration variable, and \( J_0 \) the Bessel function. It should be noted that expression (1) can be derived from the Boltzmann kinetic equation [6] as well as by the collision summation method [7].

The function in the index of the exponential function in (1) is defined as

\[ \psi(\kappa) = \pi S \int_0^\infty d\sigma(\eta \Phi) \left[ 1 - J_0(\kappa \Phi) \right] \tag{2} \]

where \( d\sigma(\Phi) \) is the differential scattering cross section, \( \Phi \) is the scattering angle and \( n \) the concentration of the target atoms.

In the case of implantation of heavy particles or of low-energy particles [Born parameter \( \alpha = (z_1 z_2)/(137 \beta) > 1 \), where \( \beta \) is the ratio of the incident particle velocity \( v_0 \) to that of light \( c \)], the scattering cross section can be calculated on the basis of the laws of classical mechanics. The differential scattering cross section obtained in [8] in the form

\[ \frac{d\sigma}{d\eta} = \pi a^2 \frac{\sigma(\eta)}{\eta^2}, \tag{3} \]

has found wide application. Here \( a \) is the Thomas—Fermi (TF) screening radius, \( \sigma(\eta) \) is the scattering function determined by the interaction potential; \( \eta = \varepsilon \sin(\theta/2) \), \( \varepsilon = (\mu A_2)/(z_1 z_2 e^2(A_1 + A_2)) \) is the reduced energy; \( A_1, A_2, z_1, \) and \( z_2 \) are the masses and charges of the incident ion and of the target atom respectively; \( e \) is the electron charge.

In [7] the cross section, as written down in (3), was used to transform expression (1) for the multiple scattering function to the form
\begin{equation}
F(\theta, S) = \left(1/2\pi\right) \left( f_0(x, \theta) - a^2/r_0^2 f_2(x, \theta) \right),
\end{equation}

\begin{equation}
f_1(x, \theta) = \int_0^\infty e^{-\lambda} \left[-\tau \Delta(x)\right] J_0(\hat{\theta} x) x \cdot dx,
\end{equation}

\begin{equation}
f_2(x, \theta) = 0.5 \int_0^\infty e^{-\lambda} \left[-\tau \Delta(x)\right] J_0(\hat{\theta} x) \Delta^2(x) x \cdot dx,
\end{equation}

\begin{equation}
\Delta(x) = \int_0^\infty \eta J_0(\eta \tilde{\theta} x) x \cdot d\eta,
\end{equation}

where \( r_0 = 0.5 n^{-1/3} \), \( \tau = \pi a^2 n S \) and \( \tilde{\theta} = E a \theta/(2z_1 z_2 e^2) \) are the reduced thickness of the layer of matter and the reduced scattering angle respectively.

The scattering function \( f(\eta) \) for the Thomas–Fermi potential calculated in [7] on the basis of the scattering integral tables presented in [9] was used in [7] for calculation of tables of the multiple scattering function. Formulas (4)-(7) for calculation of the multiple scattering function tables were also applied in [6] in which, however, the function \( f(\eta) \) for the Thomas–Fermi and Lenz–Jensen (LJ) potentials was specified by the approximation formula given in [10]. The problem involved in the use of the tables presented in [6, 7, 11] is connected with the insufficient accuracy of the computations as well as with the limited choice of the interatomic interaction potential.

For calculation of the angular distribution during multiple scattering, we have developed a SCAT program based on a numerical solution of Eqs. (4)-(7).

It should be noted that the form of functions \( f_1 \) in (5) and \( f_2 \) in (6) depends strongly on the values of \( \theta \) and \( \tau \) and may change from an almost Gaussian shape for \( \tau \geq 2 \) to a strongly oscillating function for \( \tau \leq 0.1 \). The integration of such functions is a difficult mathematical problem. Therefore the QUANC8 procedure [12], designed for the integration of complex periodic functions, was used in the SCAT program.

In order to enhance the computation efficiency, and this is particularly important when the SCAT program is employed for Monte Carlo calculations, it is necessary to approximate the function \( \Delta(x) \). Approximation of \( \Delta(x) \), for example, was carried out in the computation of the tables in [6, 7]. For this purpose in the SCAT program the \( x \) scale was divided into nine intervals with a sufficiently smooth variation of \( \Delta(x) \). In each interval \( \Delta(x) \) was approximated by a ninth-degree polynomial with a relative error \( \delta \) of less than 5% in the region 0-0.3 and of less than 1% for other values of \( x \). The polynomial coefficients for each of the intervals have been presented in [13].

As a whole, good agreement was observed on comparing the results of test calculations carried out by the SCAT program for the Thomas–Fermi potential and the theoretical data of other authors [6, 7]. For small values of \( \tilde{\theta} \) and large values of \( \tau \) there is a small discrepancy in the results of [7] and of our data as well as those in [6], which agree with our data. It was suggested in [6] that the discrepancy could be due to an insufficient accuracy of the computation procedure employed in [7]. The SCAT calculations showed that it is not the inaccuracy of the computation schemes but rather the insufficient accuracy in approximating the scattering function \( f(\eta) \) for the Thomas–Fermi potential in [6] as a result of using the expression in [10].

Large relative discrepancies between the calculation results of [6, 7] and SCAT were observed for large values of \( \tilde{\theta} \). Since the principle difference between the calculation procedures in [6, 7] and SCAT consists only in the representation of the function \( \Delta(x) \), we calculated the multiple scattering function for various approximations of \( \Delta(x) \). The dependence of function \( f_1 \) on the relative error of approximation (\( \delta \)) of \( \Delta(x) \) is shown in Fig. 1 for \( \tilde{\theta} = 2 \) and \( \tau = 0.2 \). It can be seen that the \( f_1 \) values converge for \( \delta \leq 3 \times 10^{-3} \) which has been chosen as the most effective value in the SCAT. The values of \( f_1 \) calculated in [6, 7] are not sufficiently accurate due to the unreliable approximation of \( \Delta(x) \).

Computation of the tables of the multiple scattering functions for the Thomas–Fermi, Lenz–Jensen, and Kalbitzer–Oetzmann potentials were performed in the 1970s and beginning of the 1980s. At present the Ziegler–Biersack–Littmark (ZBL) potential [14] is regarded as the most realistic interaction potential. We have calculated tables of the angular distribution during multiple scattering of ions in the 0.01 \( \leq \tau \leq 1400 \) range; the calculations were carried out in accordance with the SCAT program by using the ZBL potential and the differential cross section from [15]. The tables have been published in [13]. The relative error of evaluation of integrals (5)-(7) is \( 10^{-5} - 10^{-6} \).

The characteristic dependences of \( f_1 \) on \( \tilde{\theta} \) for fixed values of \( \tau \) and various potentials are shown in Fig. 2. In the region of small \( \tau \) (Fig. 2a) the values of the scattering functions for the ZBL potential are intermediate between the values for the TF and LJ potentials. With increasing \( \tau \) (Fig. 2b) the distribution of the multiple scattering function for the ZBL potential becomes the widest. The explanation of this is that for small target thicknesses the number of collisions a high-energy ion undergoes