INTRODUCTION

Reflection of ions from solids is one of the most important processes of charged particle interaction with a solid and can be used as an effective surface analysis method [1]. Angular ion distribution is one of the most important characteristics of reflection. When ions with average energies fall obliquely on a solid surface, their angular distribution exhibits a characteristic regularity. When a primary beam is observed in an incidence plane and all particles are recorded independent of their charge state, a sharp maximum is observed at the angular distribution for oblique incidence angles at an angle of reflection, which is approximately equal to a grazing angle. When the grazing angle is increased the maximum is moved toward large angles. The largest number of reflected ions head out in the direction perpendicular to the target surface starting from a certain glancing angle [1, 2].

The angular distribution at glancing angles of incidence was theoretically investigated in [3, 4] based on two simplified assumptions: the diffusion approximation, to describe ion scattering from target atoms, and the small-angle approximation, to determine the range of considered angles. In [5], the diffusion approximation was taken into consideration, but the small-angle approximation was not used, making it possible to generalize the results [3, 4] over the entire range of incidence angles. The present work represents further development of the theory in [5] and uses the analytic method of solution expansion in terms of eigenfunctions; as a result, the angular distribution is determined by the method of moments. In addition, a parameter taking into account inelastic energy losses was added to the theory. However, as a result of the large number of collisions, particles gradually turn and leave the target.

THEORETICAL ANALYSIS

The integro-differential Boltzmann equation for the particle distribution function in a target, \( f(x, \mu, \varphi) \) is transformed in the diffusion approximation to the partial differential equation [3–5]

\[
\frac{\partial f}{\partial x} + pf = \frac{\partial}{\partial \mu} \left[ (1 - \mu^2) \frac{\partial f}{\partial \mu} \right] + \frac{1}{1 - \mu^2} \frac{\partial^2 f}{\partial \varphi^2},
\]

where \( x \geq 0 \) is the normalized coordinate, \( \mu = \cos \theta \) is the angle cosine between the particle velocity and the positive direction of the \( x \) axis, \( \varphi \) is an azimuthal angle, and \( p \geq 0 \) is the inelastic energy loss parameter. The left-hand side of Eq. (1) describes the variation in the number of particles with target depth. The right-hand side of Eq. (1) is a collision integral written in the diffusion approximation and represents the angular part of the Laplace operator in spherical coordinates. Equation (1) is solved when the boundary condition on the target surface is

\[
f(x = 0, \mu, \varphi) = \begin{cases} \delta(\mu_0 - \mu)\delta(\varphi) & \text{for } 0 < \mu \leq 1, \\ R(-\mu, \varphi) & \text{for } -1 \leq \mu < 0, \end{cases}
\]

where \( \mu_0 = \cos \theta_0 \), \( \theta_0 \) is the incidence angle of the primary beam counted from the normal to the target surface, and \( R(-\mu, \varphi) \) is the reflected particle angular distribution function to be determined.

We will solve Eq. (1) in the form of a series

\[
f(x, \mu, \varphi) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} Y_{mn}(\mu) \cos(m\varphi) \exp(-\lambda_{mn}x),
\]
where $\lambda_{mn}$ and $Y_{mn}(\mu)$ are the eigenvalues and eigenfunctions of a standard differential equation

$$\frac{d}{d\mu} \left[ (1 - \mu^2) \frac{dY_{mn}}{d\mu} \right] + \left( \lambda_{mn} \mu - \frac{m^2}{1 - \mu^2} \right) Y_{mn} = 0. \quad (4)$$

The eigenfunctions of Eq. (4) can be expanded into a series of adjoined Legendre polynomials [6]

$$Y_{mn}(\mu) = \sum_{k=m}^{\infty} B_k P^m_k(\mu), \quad (5)$$

in which the $B_k$ coefficients are determined from the recurrent formula

$$[k(k + 1) + p] B_k = \lambda_{mn} \left( \frac{k - m}{2k - 1} B_{k-1} + \frac{k + m + 1}{2k + 3} B_{k+1} \right), \quad (6)$$

in this case the eigenvalues and eigenfunctions are determined from the condition $B_k \to 0$ for $k \to \infty$.

If the angular distribution $R(\mu, \varphi)$ is represented in the form of a Fourier series

$$R(\mu, \varphi) = R_0(\mu) + \sum_{m=1}^{\infty} R_m(\mu) \cos(m\varphi), \quad (7)$$

then using Eqs. (2), (3), (7), and eigenfunction orthogonality it is possible to obtain a set of integral equations for determining the unknown $R_m(\mu)$ functions by their known moments

$$\int_0^1 \mu Y_{mn}(\mu) R_m(\mu) d\mu = \int_0^1 \mu Y_{mn}(-\mu) d\mu, \quad n \geq m. \quad (8)$$

The reflection coefficient is determined by the first term in (7)

$$R_N(p, \mu_0) = \int_0^1 \mu R_0(\mu) d\mu. \quad (9)$$

If inelastic energy losses are absent, then the parameter $p$ is zero and the reflection coefficient is unity for any angles of ion incidence.

To solve the set of Eqs. (8), we approximated the unknown $R_m(\mu)$ functions by the polynomials with indefinite coefficients. The values of the coefficients were determined by solving a set of linear equations. In this case to obtain solutions with four correct significant figures, it was sufficient to be limited to the first ten equations when particles normally fall on a target surface. The number of equations increases at oblique incidence.

**RESULTS AND DISCUSSION**

The calculated dependences of the angular distributions, measured in the incidence plane of a primary beam, on the observation angle counted from a target surface are shown in Fig. 1 for a case when there are no inelastic energy losses ($p = 0$). When ions fall normally ($\theta_0 = 0^\circ$), the angular distribution has a maximum at the observation angle $90^\circ$, i.e., in the direction perpendicular to the target surface. When the angles of incidence are $\theta_0 = 60^\circ$ and $75^\circ$, the maximum is shifted to $150^\circ$ and $167^\circ$, respectively. In this case, the half-width of the maximum decreases with increasing angle of incidence. One can show that the results of the present work turn into the results of the small-angle theory [3, 4] for the limiting case of grazing incidence angles ($\theta_0 \to 90^\circ$).

The angular dependences of the reflection coefficient for different values of the inelastic energy loss parameter $p$ obtained by Eq. (9) are presented in Fig. 2. The angular dependences calculated by the TRIM Program [7] for an argon–copper combination at the ion energy 30 keV are denoted by markers. It follows from the figure that it should take the value of the inelastic energy loss parameter $p = 2$.

Comparison of the theoretical angular distributions obtained from Eq. (7) for $p = 2$ with the experimental data [2] for 30 keV argon ions reflected from a copper target at the grazing angles $\alpha_0 = 8^\circ - 16^\circ$ (i.e., at the angles of incidence $\theta_0 = 90^\circ - \alpha_0 = 74^\circ - 82^\circ$) is shown in Fig. 3. The angular distributions are presented in the form of a function of the ion scattering angle counted from the direction of primary beam incidence and normalized to the value of the maximum at $\alpha_0 = 8^\circ$. Good agreement between the heights of the theoretical and experimental maxima follows from the figure; however, the positions of the