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Multiple scattering of protons transmitting through thin films

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A method for calculating multiple scattering of atomic particles passing through thin films is proposed. The angular distribution of protons passing through a thin gold film of different thicknesses is calculated. The use of the atom–solid potential to calculate the differential scattering cross section allows good agreement with experiment to be achieved.

Keywords: multiple scattering, thin films, angular distribution, collision of atoms with a solid.

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Particles passing through thin films undergo multiple scattering and ionization and lose energy. Experimental measurements of the angular and energy distribution of ions and atoms passing through a film are performed in order to determine important parameters, such as electronic stopping losses in matter, obtain data on the potential of interaction of particles with a solid [1], study straggling, and determine the film roughness [2]. The passage of particles through thin films may be used to ionize atomic particle fluxes escaping from plasma, providing an opportunity to analyze the parameters of the ionic component of plasma [3,4].

A review of theoretical studies of multiple scattering may be found in monographs [5,6]. Of note among these works are the papers authored by O.B. Firsov [7,8], where the problem was considered in two approximations: the diffusion approximation, which is valid for near-Coulomb scattering where the main contribution to the mean square of the scattering angle per unit path length is produced by small-angle scattering, and the approximation where the potential of interaction of incident ions with atoms of the medium is regarded as being inversely proportional to the distance squared. Numerical calculations for the Thomas–Fermi–Firsov potential were performed by Meyer [9]. Either the Born approximation or a specific type of potential are used in most published works. Papers [10–14] are worthy of note among the recent research output. The aim of the present study was to develop a method for calculating multiple scattering for arbitrary potential.

Let us consider the case of double scattering (Fig. 1). We assume that the first scattering occurs at angle θ_1 and lies in plane ZX. The second scattering occurs at angle θ_2, and φ is the angle between the planes of the first and second scattering. Let us rotate the coordinate system by angle θ_1 about axis Y. The projections of the velocity vector onto these axes in the $Z'X'Y$ coordinate system are

$$v_{X'} = v\sin\theta_2\cos\varphi, \quad v_Y = v\sin\theta_2\sin\varphi, \quad v_{Z'} = v\cos\theta_2.$$

Applying the matrix of rotation by angle θ_1 about axis Y, we find the magnitude of projection of the velocity vector after the second collision in the initial XYZ coordinate system:

$$v_X = v(\cos\theta_1\sin\theta_2\cos\varphi + \sin\theta_1\cos\theta_2),$$

$$v_Y = v\sin\theta_2\sin\varphi,$$

$$v_Z = v(-\sin\theta_1\sin\theta_2\cos\varphi + \cos\theta_1\cos\theta_2).$$

Thus, the particle escape angle relative to the Z axis after double scattering is

$$\theta_3 = \arccos(-\sin\theta_1\sin\theta_2\cos\varphi + \cos\theta_1\cos\theta_2). \quad (1)$$

It is evident that $\theta_3 = \theta_1 + \theta_2$ when $\varphi = 0$ and $\theta_3 = \theta_1 - \theta_2$ when $\varphi = \pi$.

Let a particle with initial energy E_0 be scattered by angle θ_1. The probability of scattering within the range of angles $\theta - \Delta\theta/2$ and $\theta + \Delta\theta/2$ is written as

$$P(E,\theta) = \frac{d\sigma}{d\theta}(E,\theta)N_t d\Delta\theta, \quad (2)$$

where $d\sigma/d\theta$ is the differential scattering cross section, N_t is the target density, and d is the thickness of the considered layer. In scattering by angle θ_1, energy E_1 of an incident particle is given by

$$\frac{E_1}{E_0} = \left[\frac{M_1}{M_1 + M_2}\right]^2 \times \left(\cos\theta_1 \pm \left\{\left(\frac{M_2}{M_1}\right)^2 - \sin^2\theta_1\right\}^{\frac{1}{2}}\right)^2 = K(\theta_1), \quad (3)$$

where M_1 and M_2 are the masses of an incident ion and a surface atom, respectively.

After the second collision, the particle will have energy $E_2 = E_1K(\theta_2)$. The probability of the second scattering is characterized by function $P(E_1, \theta_2)$.

The resulting distribution of particles over angles θ_3 and energies E_2 is obtained by integrating over all possible angles θ_1, θ_2, and φ.

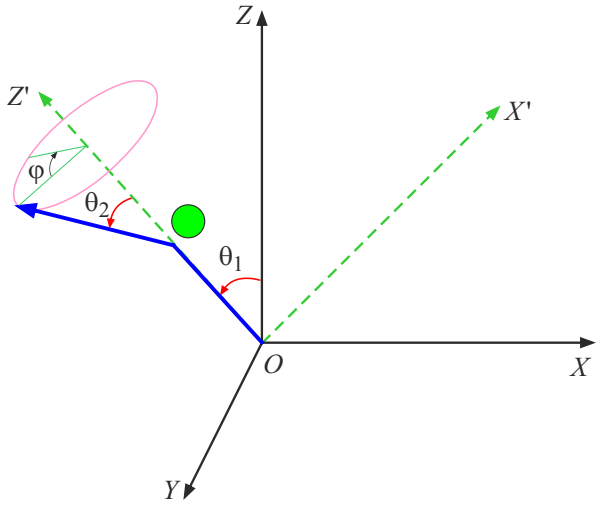

Figure 1. Geometry of double scattering.

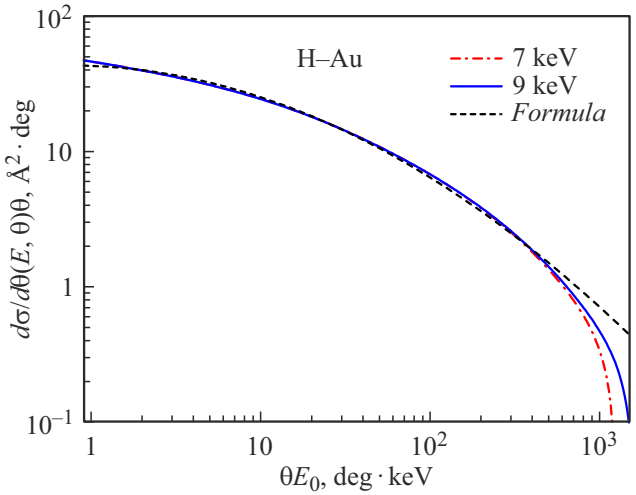

Figure 2. Dependence of the differential scattering cross section in universal coordinates in comparison with approximation formula (7).

Let us write the solution in implicit form

$$F(E_2, \theta_3) = \int_0^{\pi} d\theta_1 \int_0^{\pi} d\theta_2 \int_0^{2\pi} d\varphi P(E_0, \theta_1) P(E_1, \theta_2), \quad (4)$$

with angle θ_3 calculated using formula (1), $E_1 = E_0 K(\theta_1)$, and $E_2 = E_1 K(\theta_2)$.

It is convenient to solve these equations by discretizing the values of θ_3 and E_2 and summing up all the cases when these parameters are realized. This solution may be generalized to the case of multiple scattering. The solution for collision multiplicity m is derived from the solution for $m-1$. It is taken into account that a particle scattered at angle θ_{m-1} may have different energies E_{m-1},

$$F_m(E_m, \theta_m) = \int_0^{E_0} dE_{m-1} \int_0^{\pi} d\theta_{m-1} \int_0^{\pi} d\theta_2 \times \int_0^{2\pi} d\varphi F(E_{m-1}, \theta_{m-1}) P(E_{m-1}, \theta_2), \quad (5)$$

where

$$\theta_m = \arccos(-\sin\theta_{m-1} \sin\theta_2 \cos\varphi + \cos\theta_{m-1} \cos\theta_2),$$

$$E_m = E_{m-1} K(\theta_2). \quad (6)$$

The angular distribution of particles passing through a thin gold film was simulated in [2] in our proprietary program using the Monte Carlo method. It was demonstrated that an agreement with experimental data cannot be achieved with traditional pair potentials. Formulae introducing the screening of interaction of colliding particles passing through a metal were proposed in [15]. These formulae made it possible to obtain a satisfactory agreement with the experiment and were used in the present calculation.

As an example, let us consider multiple scattering in passage of hydrogen atoms with an energy of 9 keV through a thin gold film with a thickness of 143 Å. The corresponding experimental data are available [16].

The energy range of 7–9 keV and scattering angles smaller than 45° are of interest to us in this case. It is convenient to use universal coordinates to characterize the cross section: $\tau = E\theta$ and $\rho = (d\sigma/d\Omega)\sin\theta \cdot \theta$, where E and θ are the collision energy and the scattering angle. Figure 2 shows the calculated differential scattering cross sections for energies of 7 and 9 keV in universal coordinates. It is evident that the obtained results for angles smaller than 45° are approximated well by dependence

$$\frac{d\sigma}{d\theta}(E, \theta)\left[\frac{\text{Å}^2}{\text{sr}}\right] = \frac{43.04}{\theta}(\theta E)^{-0.05099 - 0.18106 \lg(\theta E)}. \quad (7)$$

This formula has a problem in that the cross section diverges at small angles. In the case of a solid target, this problem is solved due to the fact that the maximum impact parameter is limited to $d/2$, where d is the average distance between target atoms. The integration step in our calculations was 0.1°, and the same interval was chosen for angle θ_3 discretization. The energy spectrum discretization interval was $0.01E_0$. The obtained results remained the same at smaller discretization intervals.

The energy spectrum was calculated with a correction for electronic stopping

$$E_2 = E_1 K(\theta_2) - \Delta E_e = E_1 K(\theta_2) - \left(\frac{dE}{dx}\right)_e \frac{d}{\cos\theta_2}. \quad (8)$$

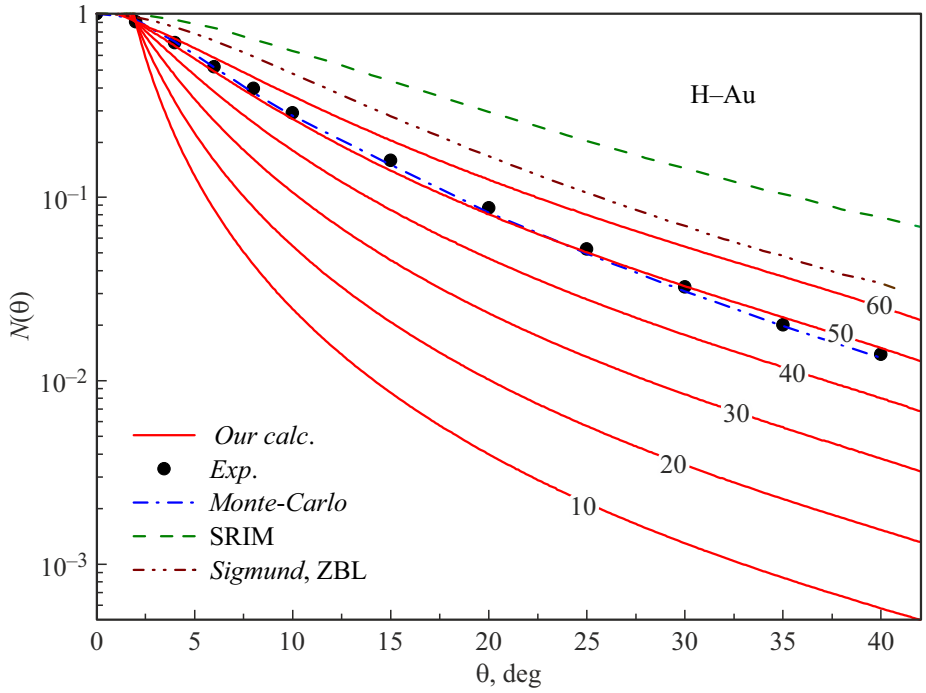

Figure 3. Variation of the angular distribution in passage through m layers with thickness d. Number m of layers is indicated next to the curves. Experimental data (dots) [16] and data calculated using the Monte Carlo method [2] and the SRIM code are presented for comparison. The results of calculations by the analytical formula of Sigmund from [18], where the ZBL potential was used, are also shown.

The value of electronic stopping power $(dE/dx)_e$ was taken from [17] and approximated as

$$\left(\frac{dE}{dx}\right)_e \left[\frac{\text{eV}}{\text{Å}}\right] = 1.6E[\text{keV}]^{0.722}. \qquad (9)$$

In formula (8), $\cos\theta_2$ introduces extension of the trajectory in passing through a layer with thickness d.

The calculation results are shown in Fig. 3. The calculated curves were normalized to the experimental data at an angle of 2° with account for the angular resolution of the detector (0.58°). Figure 3 presents the variation of angular distribution in passage through m successive target layers with thickness d.

It can be seen in Fig. 3 that the calculated angular distribution for a film thickness of 143 Å($\sim$ 50 layers) agrees well both with the experimental data [16] and with the results of Monte Carlo simulations in our program [2].

It is worth emphasizing that the values calculated by the proposed method agree with the results of Monte Carlo calculations in our program performed using the same potential. The complexity of iterative numerical integration is comparable to the use of the Monte Carlo method for calculating the passage of particles through thin films. The considered method offers the advantages of a simpler adjustment of modeling parameters (interaction potential, stopping energy losses) and automatic tracking of their influence on the passage through films of different thicknesses.

The use of the atom–solid potential proposed in [15] provides a fine agreement with experimental data.

For comparison purposes, Fig. 3 also presents the SRIM code data and the results of calculation by the analytical formula from [18]. The ZBL potential was used in both cases. This potential is known to be ill-suited for characterizing the collisions of light particles with a target, since it was obtained by averaging data on potentials for a large number of collisions of atoms of medium masses.

In our view, the difference between the results obtained using the analytical formula and the SRIM calculation is attributable to the approximate nature of this formula. Since the data of these calculations do not fit the experiment, it was needed to correct the interaction potential and introduce the variation of screening in the event of particle collisions in metal [15].

Conflict of interest

The authors declare that they have no conflict of interest.

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