01

Calculation of the average range of charged particles after passing through the finite-thickness target

© A.I. Tolmachev,[1] L. Forlano[2]

Russian New University,
105005 Moscow, Russia
[2] University of Calabria,
87036 Cosenza, Italy
e-mail: tolmachev.alex@rambler.ru, forlano@vegachess.com

Received October 5, 2023
Revised December 2, 2024
Accepted December 12, 2024

Inelatic energy losses in the target are proportional to the average range of the ions, which can essentially differ from the target thickness due to multiple collisions between the ions and the target atoms. The ratio of the average range of the ions L to the target thickness D depends on the energy on the ions, ions and target atoms masses. The ratio L/D has been calculated by the computer simulation method. An elementary analytical theory of the phenomenon has been simulation.

Keywords: ion range, inelastic energy losses, finite-thickness target, computer simulation.

DOI: 10.61011/TP.2025.04.61200.258-24

Introduction

Deceleration capability is traditionally determined by calculating the energy losses of a bombarding particle per a unit range length in the target [1,2]. The work [3] has shown that in case of the hydrogen ions transmitted through the golden film, the average length of the ion path can exceed the film thickness in 2.5 times. The authors explained a large deviation of the path length from the film thickness by an effect of repeated elastic collisions of the ions with the target atoms. The values of the ratio L/D can not be obtained directly from the computer software [4–7]. In the present work, the authors study a dependence of the ratio L/D on the energy and mass of the ions using the PAOLA software [8] as well as by theoretical calculations.

1. Computer modeling

We consider a target located between the planes $x = 0$ and $x = D$. The ions of the energy E_0 and the mass M_1 fall perpendicular to the surface $x = 0$, enter the target and come into elastic collisions with fixed atoms of the target of the mass M_2. As a result of the collisions, some ions return to the surface $x = 0$, come out of the target and are regarded as reflected ones. The other ions go out through the surface $x = D$ and are regarded as ones transmitted through the target. Our aim is to calculate the average ranges of the transmitted ions L, calculate the ratio $L/D \geq 1$ and analyze the dependence of the ratio L/D on the energy of the ions E_0 and the mass ratio $A = M_1/M_2$.

To solve the problem, we have applied the PAOLA software using an atomic potential Mensing [9–12], for which the energy of interaction of two charges at the distance r is

$$U(r) = U_0\left(\frac{r_0}{r} - 1\right) \text{ when } r \leq r_0, \quad (1)$$

$U(r) = 0$ when $r \geq r_0$, r_0 — a radius of potential action.

The works [7,10] regard the magnitudes U_0 and r_0 as adjustable parameters. The values of the parameters were determined from a condition of coincidence of the potential (1) with the values of the true potential and its derivative in a point of maximum approach in a head-on collision of the particles.

Selection of a particular kind of the atomic potential is an important step in creation of any software. The so-called ZBL-potential is superposition of four shielded Coulomb potentials.

$$U_{\mathrm{ZBL}}(r) = \frac{Z_1 Z_2 e^2}{r} \sum_{k=1}^{4} c_k \exp\left(-d_k \frac{r}{a}\right), \quad (2)$$

(Z_1 and Z_2 — the sequence numbers of the ions and the target atoms, e — the electron charge, a — the shielding length) and contains eight parameters c_k and d_k [7]. The recently proposed DFT potential differs from (2) by presence of an attracting multiplier [13,14], which is important for collisions of the low-energy ions. The potential (1) contains only two adjustable parameters and does not possess accuracy of the ZBL potential. But, instead, for the potential (1) all the characteristics of elastic scattering can be expressed analytical formulae both in the classical approximation [10,12] as well as in the quantum-mechanical approximation [9,11]. For example, the differential section of scattering as expressed via the scattering angle in the mass center system ω is as follows

$$d\sigma = \frac{2(1+\epsilon)\sin\omega d\omega}{[2+\epsilon(1-\cos\omega)]^2}, \quad (3)$$

where

$$\epsilon = 4\varepsilon(1+\varepsilon), \quad \varepsilon = E/U_0 \tag{4}$$

— the reduced energy.

Before each elastic collision, the code generates three random numbers R_1, R_2, R_3, which are located between zero and unity. These numbers define the average range of the ion between two consecutive collisions as well as the polar and azimuthal angles of scattering in this elastic collision. In accordance with the gas model of binary collisions, the distance passed by the ion between two collisions is

$$\lambda = \lambda_0 \ln(1/R_1), \tag{5}$$

where λ_0 — the mean free path. The scattering angle in the mass center system is determined by the equation

$$\cos\omega = \frac{(2+\epsilon)R_2 - 1}{1+\epsilon R_2}. \tag{6}$$

The angle of scattering in the laboratory system of coordinates Ω is as follows

$$\cos\Omega = \frac{A+\cos\omega}{(1+2A\cos\omega + A^2)^{1/2}}. \tag{7}$$

If we denote the cosines of the angle between the ion velocity and the internal normal to the target surface via μ, then after elastic collision the value of μ_n is converted into the value of μ_{n+1} in accordance with the equation

$$\mu_{n+1} = \mu_n \cos\Omega - (1-\mu_n^2)^{1/2} \sin\Omega \cos(2\pi R_3). \tag{8}$$

When the ion leaves the target, the range is corrected by taking into account a respective geometrical factor.

2. Theoretical research

The function of distribution of the ions in the target $f(x,\mu,t)$ depends on the depth of penetration of the ion into the target x, the angle θ between the ion velocity and the normal to the target surface, $\mu = \cos\theta$ and the range of the ion t. When $A = 0$ (the ion mass is significantly less than the atomic weight of the target) and there is interaction in accordance with the solid spheres law, the transfer equation is as follows

$$\mu \frac{\partial f(x,\mu,t)}{\partial x} + \frac{\partial f(x,\mu,t)}{\partial t} + f(x,\mu,t) = = \frac{1}{2}\int_{-1}^{1} f(x,\mu,t)d\mu. \tag{9}$$

Laplace transform

$$F(x,\mu) = \int_0^\infty f(x,\mu,t)e^{-st}dt \tag{10}$$

gives

$$\mu \frac{\partial F(x,\mu)}{\partial x} + (1+s)F(x,\mu) = \frac{1}{2}\int_{-1}^{1} F(x,\mu)d\mu. \tag{11}$$

The equation (11) is the Chandrasekar problem [15] and the ion reflectance in case of a semi-infinite target can be presented analytically

$$R_N(s) = 1 - H(w_0)(1-w_0)^{1/2}, \ w_0 = 1/(1+s), \tag{12}$$

where H — is the Chandrasekar function. With small s we obtain

$$R_N(s) = 1 - \text{const}\sqrt{s}, \ s \ll 1, \tag{13}$$

and the average range of the reflected ions becomes infinite,

$$L = \lim_{s\to 0} \frac{R_N(0) - R_N(s)}{sR_N(s)} = \infty. \tag{14}$$

This is due to the fact that in the semi-infinite target the reflected ion can intersect the plane $x = D$ several times. In the finite-thickness target, the ion intersects the plane $x = D$ only one, when leaving the target, and the average range becomes finite.

To solve the equation (11), in case of the finite-thickness target we select four discrete values of the angular variable $\mu = 1, 1/3, -1/3, -1$ and designate the respective values of the distribution function F_1, F_2, F_3, F_4. Then the equation (11) is written as a system of four ordinary differential equations.

$$\begin{cases} F_1' + (1+s)F_1 = Q, \\ F_2'/3 + (1+s)F_2 = Q, \\ -F_3'/3 + (1+s)F_3 = Q, \\ -F_4' + (1+s)F_4 = Q, \end{cases} \tag{15}$$

$$Q = \frac{F_1 + 2F_2 + 2F_3 + F_4}{6}, \tag{16}$$

where Q is a trapezoid formula for approximate calculation of the integral on the right-hand side of the equation (11).

The boundary conditions for the system of equations (15):

$$F_1(0) = 1, \quad F_2(0) = 0, \tag{17}$$

$$F_3(D) = 0, \quad F_4(D) = 0, \tag{18}$$

correspond to the normal fall of the ions to the surface $x = 0$ and absence of the ions entering the target through the surface $x = D$.

The system of equations (15) is solved as follows

$$F_k(x) = \sum_{m=1}^{4} C_m Y_{km} \exp(-\lambda_m x), \quad k = 1, 2, 3, 4, \tag{19}$$

where Y_{km} — the eigen vectors, λ_m — eigenvalues obtained from the biquadratic equation

$$3\lambda^4 - (1+s)(11+30s)\lambda^2 + 27s(1+s)^3 = 0. \tag{20}$$

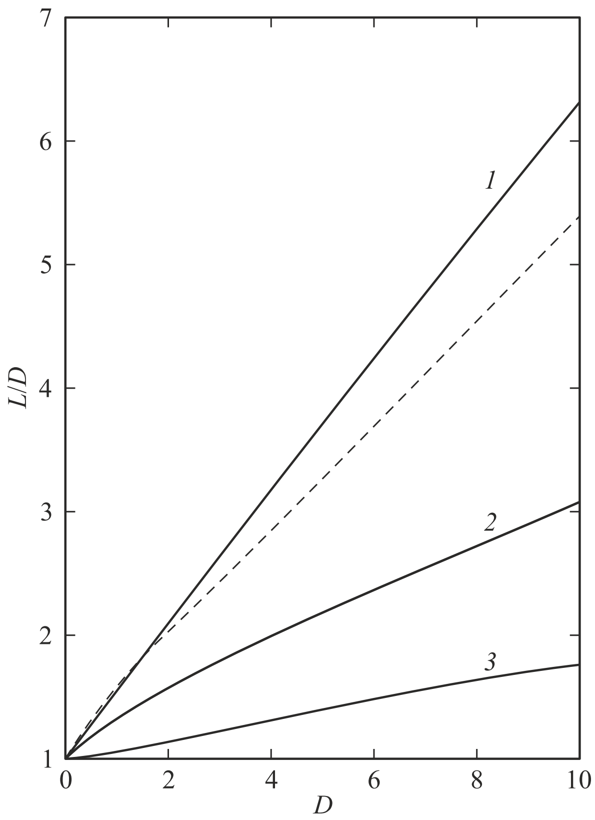

Figure 1. Dependences of the ratio L/D on the target thickness D for the potential of solid spheres and the various mass ratios: $A = 0$ (the curve *1*), 1 (*2*), 2 (*3*). The dashed line — the formula (23).

The coefficients C_m are determined from the boundary conditions (17), (18). The ion transmission ratio is

$$T_N(D, s) = \int_0^1 \mu F(D, \mu) d\mu = F_1(D) + \frac{2}{3} F_2(D), \qquad (21)$$

and the average range of the transmitted ions is calculated as a limit

$$L = \lim_{s \to 0} \frac{T_N(0) - T_N(s)}{s T_N(s)}. \qquad (22)$$

The solution of the problem (15)−(18) for the four discrete flows has been obtained in an analytical form, but it is rather cumbersome. Approximately, the final result with the accuracy of 1% can be written as a formula

$$\frac{L}{D} = 1 + \frac{5D(D+1)}{12D+5}. \qquad (23)$$

3. Results

Fig. 1 show the dependence of the ratio of the average ion range to the target thickness on the mass ratio and the target thickness at small ion energies (interaction according to the solid spheres law). The ratio L/D increased with the target thickness and with decrease on the ion mass. In case of the heavy ions ($A \gg 1$), the elastic scattering occurs only to the small angles and the curves L/D tend to unity. The dashed line depicts the function (23) belonging to the case when $A = 0$. It can be shown that with further increase of the numbers of the discrete flows divergence between the theoretical result and the computer modeling results decreases and does not exceed the error of the Monte Carlo method.

Fig. 2 shows the dependence of the ratio L/D on the ion energy at the fixed target thickness. The ratio gets to the largest values with the small energies. With the high energies, the scattering is close to the Rutherford scattering, all the ions move almost along the straight line and their ranges are equal to the target thickness. At the same time, all the curves tend to the straight line $L/D = 1$.

Fig. 3 shows the results of calculation of the dependence of the ratio L/d on the energy of hydrogen ions bombarding the golden film of the thickness of $d = 200$ Å. The average range between two subsequent collisions and the cut-off radius are selected to be equal to each other: $\lambda_0 = r_0 = 4$ Å. With this selection, the normalized thickness of the target and the atomic energy unit turn out to be $D = d/\lambda_0 = 50$ and $U_0 = 284$ eV, thereby enabling use of the formulae (4) and (6) in the computer calculation. Compliance of our calculations with the calculations [3] may be considered to be satisfactory. Noticeable difference of the results with

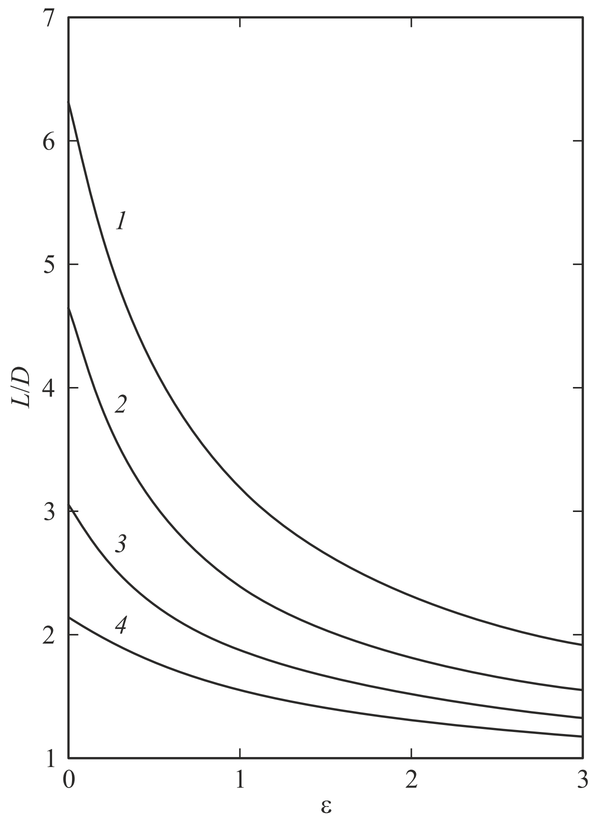

Figure 2. Dependences of the ratio L/D on the reduced energy ε for the normalized thickness of the target $D = 10$ at the various mass ratios: $A = 0$ (the curve *1*), 0.5 (*2*), 1 (*3*), 1.5 (*4*).

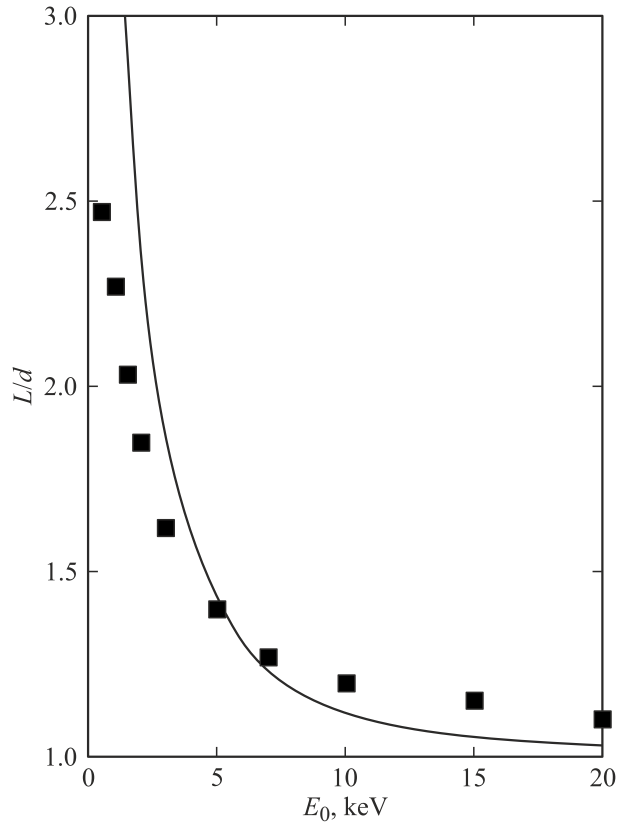

Figure 3. Dependence of the ratio L/d on the ion energy E_0 for the combination H−Au with the thickness of the golden film $d = 200$ A. The solid line — the PAOLA software, the markers — the results of calculation [3].

the small energies may be related to either the negative attracting area in the DFT potential or different values of energy sublimation.

Conclusion

The computer modeling method has shown that the average range of the ions transmitted through the finite-thickness target can exceed the target thickness in several times. The effect turns out to be especially noticeable for the low energies of the ions, when the ion mass is significantly less than the atomic weight of the target. The results substantially depend on the value of the average range of the ion λ_0 between two subsequent collisions. It is different from scattering of the ions in the semi-infinite target, when the obtained results sometimes do not depend on λ_0 at all. The theory of the phenomenon is built based on approximation of the solution of the integro-differential transfer equation by the discrete flow method. The deviations of the value of L/D from unit shall be taken into account when experimentally measuring the deceleration capability of the substance.

Conflict of interest

The authors declare that they have no conflict of interest.

References

[1] P. Sigmund. *Particle Penetration and Radiation Effects* (Springer, Berlin, 2014), 603 p.
[2] Yu.A. Belova, N.V. Novikov, Ya.A. Teplova. *Expreimental'nye i teoreticheskie issledovaniya protsessov vzaimodeistviya ionov s veshchestvom* (Universitetskaya kniga, M., 2019), 234 s. (in Russian)
[3] A.N. Zinoviev, P.Yu. Babenko. JETP Lett., **115** (9), 560 (2022).
[4] SRIM. *The Stopping and Range of Ions in Matter.* http://srim.org
[5] J.F. Ziegler. Nucl. Instr. Methods Phys. Res., Sect. B, **136–138**, 141 (1998).
[6] V.I. Shulga. Appl. Surf. Sci., **439**, 456 (2018).
[7] W. Eckstein. *Computer Simulation of Ion–Solid Interactions* (Springer, Berlin, 1991), 296 p.
[8] A.I. Tolmachev, L. Forlano. J. Surf. Invest., **11** (6), 1313 (2017).
[9] L. Mensing. Zeitshcrift fur Physik, **45** (9−10), 603 (1927).
[10] G. Leibfreid, O.M. Oen. J. Appl. Phys., **33** (7), 2257 (1962).
[11] V.V. Rumyantsev, Yu.A. Morozov, B.N. Libenson. Soviet Phys. JETP, **36** (4), 643 (1973).
[12] A.V. Tolmachev. Poverkhnost', **8**, 27 (1992). (in Russian)
[13] A.N. Zinoviev, P.Yu. Babenko. Tech. Phys. Lett., **46**, 909 (2020).
[14] P.Yu. Babenko, A.N. Zinoviev. Tech. Phys., **67** (12), 1 (2022).
[15] S. Chandrasekhar. *Radiative Transfer* (Clarendon Press, Oxford, 1950), 393 p.

Translated by M.Shevelev