REFLECTION COEFFICIENT OF LOW ENERGY LIGHT IONS BASED ON THE THEORY OF ION RANGES

by

Jovan VUKANIĆ

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Multiple collision theory of light ion ranges in an infinite medium has been used to calculate reflection coefficient from penetration profile in the energy region where the electronic stopping is dominating and proportional to the ion velocity. Ion-target atom collisions are determined by the inverse square scattering potential. The Gaussian approximation of a penetration profile as well as reflection coefficient are found in the form of analytic formulas. Corrections for multiple crossings of the surface have been applied. The results are compared with those from our previous calculations on the basis of DP0 solution of the transport equation and with the computer simulation data.

Key words: light ion, heavy target, reflection coefficient, ion range, multiple collision model, scaled parameter

INTRODUCTION

This paper deals with analytical calculations of the range distribution and reflection of light ions (H^+, D^+, T^+, He^+) from heavy targets in the low energy domain (from a few tens of eV to a few tens of keV). Calculations are based on the transport theory. The same technique was used previously [1, 2] and gives the range distribution in an infinite medium as a solution of the transport equation by the moment method. Moment equations were solved numerically and penetration profiles were constructed using the Edgeworth expansion. The reflection coefficient was determined from the penetration profile by assuming that R was the fraction of the ion beam that had negative penetration depths. For more accurate calculations the correction for multiple crossings of the surface (which is possible due to the assumption of an infinite medium) must be done [2].

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Author's address:
VINČA Institute of Nuclear Sciences
P. O. Box 522, 11001 Belgrade, Serbia

Author's e-mail:
vukanic@vin.bg.ac.yu

We follow the approach described in [1] and [2], but we also introduce two simplifying assumptions. Firstly, we deal only with low energies, where multiple scattering plays a dominating role and ions undergo several large angle deflections before coming to rest. In this situation, the penetration profile has the Gaussian shape [1]. Secondly, at low energies ion-target atom scattering potential has a form of the inverse square law [3]. The use of the scattering cross-section for this special power potential allows us to get simple analytic solutions for the Gaussian approximation of the penetration profile and for the reflection coefficient instead of complex numerical treatment used in [1] and [2].

PREVIOUS CALCULATIONS

The basic quantity of interest in light ion transport through heavy targets is the scaling parameter ν. This quantity, called the scaled transport cross-section, is defined as [3-4]

$$\nu \quad N\sigma_1(E_0)\,\tau_0(E_0) \tag{1}$$

where N is the number of target atoms per unit volume, $\sigma_1(E_0)$ is the transport cross-section at the initial ion energy E_0, and $\tau_0(E_0)$ is the total path length. The parameter ν represents the mean number of wide angle collisions of an ion during its slowing down. We take into account sufficiently low ion energies where the parameter ν is large ($\nu \quad 2$) and reflection is determined by multiple collisions.

Analytical transport theory of light ion reflection based on the continuous slowing down approximation already exists [3-7]. The light ion albedo problem has been treated by using Chandrasekhar's H function method [4, 5], the age diffusion theory [3] and double Legendre polynomial approximation (DPN method) [6, 7]. All these approaches use the simplifying assumption that a large number of wide angle deflections produce a nearly isotropic ion distribution inside the target. In [6], the isotropic approximation of the collision integral in the transport equation was utilized. The theoretical model of [6] was improved in [7] by taking into account the anisotropy effects of ion scattering, replacing the isotropic collision integral with the anisotropic P_3 approximation in angular variable. We consider the approach presented in [7] to be the most accurate one and therefore will mention some details of the calculations. Our present results will be compared with those obtained in [7].

The scattering cross-section for light ion-heavy target atom collisions at low ion energies is given by [3]

$$\mathrm{d}\sigma(E,\cos\theta) \quad \frac{1}{2\sqrt{2}}\sigma_1(E)\frac{\mathrm{d}(\quad\cos\theta)}{\sqrt{(1 \quad \cos\theta)^3}} \tag{2}$$

where E is the ion energy, and θ is the laboratory scattering angle. The cross-section (2) describes scattering in the inverse square interaction potential $V(R) \quad R^{-2}$. It appears appropriate for light ions interacting with heavy target atoms in the energy range of some tens of eV to some tens of keV. For the inverse square scattering potential used in [7] the convenient semi-empirical formula for the Laplace transformed DP0 solution of the reflection function was found. That formula allowed the analytic Laplace inversion and led to the simple expressions for the path length distribution of backscattered particles as well as to the particle and energy reflection coefficients.

The analytic solution for the path length distribution of backscattered projectiles obtained in [7] is of the form

$$G(\mu_0,s)\mathrm{d}s \quad \frac{h\nu}{2\sqrt{\pi(\nu s \quad g)^3}}\,\mathrm{e}^{\quad\frac{h^2}{4(\nu s \quad g)}}\mathrm{d}s \tag{3}$$

where $h = h(\mu_0) = 3.094\mu_0$, $g = g(\mu_0) = -1.72 + 14.44$ $\mu \quad - \quad \mu_0^4 + 11.48\,\mu_0^6$ and $s = \tau/\tau_0$ is the relative path length travelled. The particle reflection coefficient

$$R_N(\mu_0,\nu) \quad \int_0^1 G(\mu_0,s)\mathrm{d}s \quad \mathrm{erfc}\,\frac{h}{2\sqrt{\nu \quad g}} \tag{4}$$

depends on the initial energy and ion-target combination only through the variable ν. For light ions slowing down in heavy targets the parameter can easily be transformed into the form

$$\nu \quad \frac{M_2}{M_1}\frac{S_n(E_0)}{S_e(E_0) \quad S_n(E_0)} \tag{5}$$

PENETRATION PROFILES AND REFLECTION COEFFICIENTS

Transport equation for the penetration profile of light ions in an infinite medium has the form

$$\mu_0\frac{\partial F}{\partial x} \quad N[S_e(E_0) \quad S_n(E_0)]\frac{\partial F}{\partial E_0}$$
$$N \quad \mathrm{d}\sigma(E_0,T,\mathbf{e}_0,\mathbf{e})[F(E_0,\mathbf{e}_0,x)$$
$$F(E_0 \quad T,\mathbf{e},x)] \tag{6}$$

where $F = F(E_0,\mathbf{e}_0,x)$, $\mu_0 = \cos\alpha_0$, and α_0 is the angle between the ion beam and the target surface normal. Moreover, orts $\mathbf{e}_0$ and $\mathbf{e}$ define the directions of the initial and scattered ions and T is the recoil energy. Due to the symmetry, $F(E_0,\mathbf{e}_0,x) = F(E_0,\mu_0,x)$.

The integral eq. (6) with three variables (E_0, μ_0, x) can be replaced by the system of equations of only one variable (E_0). The depth dependence can be removed by introducing the spatial averages over F

$$F^n(E_0,\mu_0) \quad \int_{\infty}^{\infty} x^n F(E_0,\mu_0,x)\mathrm{d}x \quad n \quad 0,1,2\ldots \tag{7}$$

The dependence of the angle of incidence can be eliminated expanding $F^n(E_0,\mu_0)$ in terms of Legendre polynomials $P_l(\mu_0)$

$$F^n(E_0,\mu_0) \quad \sum_{l\quad 0}^{\infty}(2l \quad 1)F_l^n(E_0)P_l(\mu_0) \tag{8}$$

By using eqs. (7) and (8), eq. (6) can be replaced by moment equations. For light ions in heavy targets these equations have the form

$$nlF_{l\quad 1}^{n\quad 1} \quad n(l \quad 1)F_{l\quad 1}^{n\quad 1}$$
$$(2l \quad 1)N(S_e \quad S_n)\frac{\mathrm{d}F_l^n}{\mathrm{d}E_0}$$
$$(2l \quad 1)F_l^n N \quad \mathrm{d}\sigma[1 \quad P_l(\cos\theta)] \tag{9}$$

where $F_l^n \quad F_l^n(E_0)$, $S_e \quad S_e(E_0)$ and $S_n \quad S_n(E_0)$.

In eq. (8) $n = 1, 2, 3, \ldots$ and the normalization condition takes the form $F_l^0(E_0) \quad \delta_{l0}$ The moments $F_l^n(E_0)$ are different from zero only for $l \quad n$ and $l + n$

even. Thus, the expression (7) for $F^n(E_0, \mu_0)$ is always finite.

Following [1], the evaluation is done in reduced Thomas Fermi units

$$\varepsilon_o = \frac{E_0 a \dfrac{M_2}{M_1}}{Z_1 Z_2 e^2 \left(1 + \dfrac{M_2}{M_1}\right)}; \quad \rho = xN\pi a^2 4 \frac{\dfrac{M_2}{M_1}}{\left(1 + \dfrac{M_2}{M_1}\right)^2} \tag{10}$$

With the notation

$$f_l^n(\varepsilon_0) = \left(\frac{\rho}{x}\right)^n F_l^n(E_0) \tag{11}$$

the moment equations for the inverse square scattering potential have the form

$$nl f_{l-1}^{n-1}(\varepsilon_0) - n(l+1) f_{l+1}^{n-1}(\varepsilon_0) = (2l+1)[k\sqrt{\varepsilon_0} + s_n(\varepsilon_0)] \frac{\mathrm{d}f_l^n(\varepsilon_0)}{\mathrm{d}\varepsilon_0} + (2l+1) l \frac{M_2}{2M_1} \frac{s_n(\varepsilon_0)}{\varepsilon_0} f_l^n(\varepsilon_0) \tag{12}$$

Here, $k\varepsilon_0^{1/2}$ and $s_n(\varepsilon_0)$ are the electronic and nuclear stopping cross-sections expressed in Thomas Fermi units. One assumes that the electronic stopping is dominating thus the total stopping cross-section $k\varepsilon_0^{1/2} + s_n(\varepsilon_0)$ remains approximately proportional to $\varepsilon_0^{1/2}$.

It is important to mention that at low ion energies one obtains the Gaussian shape of the range profile since the great number of large angle collisions ($\nu \gg 1$) removes the "skewness" of the distribution. Reversely, for $\nu \le 2$, with decreasing ν the increasing deviation of the Gaussian shape of the penetration profile occurs because single collision events become important. Thus, at higher energies, the range distribution must be constructed from several moments by applying a suitable Edgeworth method [1].

Using eq. (2) as an input quantity, moments of the first and second order were evaluated analytically, leading for $\nu \ge 2$ to the Gaussian approximation of the penetration profile

$$f(\varepsilon_0, \rho) = \frac{1}{\sqrt{2\pi\langle\Delta\rho^2\rangle}} \mathrm{e}^{-\frac{(\rho - \langle\rho\rangle)^2}{2\langle\Delta\rho^2\rangle}} \tag{13}$$

where ρ is the penetration depth, $\langle\rho\rangle$ is the mean penetration depth, and $\langle\Delta\rho^2\rangle$ is the variance. These quantities (for normal ion incidence) are determined by the approximate formulas

$$\frac{\langle\rho\rangle}{\rho_0} = \frac{3f_1^1(\varepsilon_0)}{\rho_0} = 1 - \nu e^{\nu} E_1(\nu) \approx \frac{1}{\nu}\left(1 - \frac{2!}{\nu} + \frac{3!}{\nu^2}\right) \tag{14}$$

$$\frac{\Delta\rho^2}{\rho_0^2} = \frac{f_0^2(\varepsilon_0) + 5f_2^2(\varepsilon_0) - [(3f_1^1(\varepsilon_0)]^2}{\rho_0^2} \approx \frac{2}{9\nu}\left(1 - \frac{3}{\nu} + \frac{11}{\nu^2}\right) \tag{15}$$

where $\rho_0(\varepsilon_0)$ is the total path length in Thomas Fermi units and $E_1(\nu) = \int_\nu^\infty (e^{-t}/t)\mathrm{d}t$ is the exponential integral.

Integrating eq. (5) over all negative penetration depths we obtain the "Gaussian" value of the reflection coefficient

$$R(\nu) = \frac{1}{2}\mathrm{erfc}\left(\frac{\langle\rho\rangle}{\sqrt{2\Delta\rho^2}}\right) \approx \frac{1}{2}\mathrm{erfc}\sqrt{\frac{2.25}{\nu\left(1 - \dfrac{1}{\nu}\right)}} \tag{16}$$

For large values of the reflection coefficients, $R \ge 0.1 - 0.15$, a correction for multiple crossing of the surface must be done. We use the result of [2] where this correction has been estimated. The reflection coefficient for semi-infinite target R_N is connected with R through the integral equation

$$R_N(\mu_0, E_0) = R(\mu_0, E_0) + \int_0^1 G(\mu_0, s) \frac{2R(E)\ln 2R(E) - 2R(E) + 1}{[\ln 2R(E)]^2} \mathrm{d}s \tag{17}$$

where $R(\mu_0, E_0) = 2^{\mu_0 - 1} R(E_0)^{\mu_0}$. In our approach, one has the path length distribution of reflected particles.

Obviously, the second function under the integral sign in eq. (17) varies slowly compared to the path length distribution $G(\mu_0, s)$. In that case, the reflection coefficient from a semi-infinite target is connected with R by the approximate relation

$$R_N(\mu_0, \nu) = \frac{R(\mu_0, \nu)}{1 - \bar{\delta}} \tag{18}$$

where the function $\bar{\delta}$ depends on the mean relative path length of reflected ions $\bar{s} = \int_0^1 sG(\nu, s)\mathrm{d}s / \int_0^1 G(\nu, s)\mathrm{d}s$ through the relation

$$\bar{\delta} = \frac{2R(\bar{\nu})\ln 2R(\bar{\nu}) - 2R(\bar{\nu}) + 1}{[\ln 2R(\bar{\nu})]^2} \tag{19}$$

with $\bar{\nu} = \nu/(1 - \bar{s})$. The mean path length has been calculated by using eq. (3).

Figure 1 compares our present result for the reflection coefficient, eq. (18), with the one obtained by DP0 method, eq. (4). Since our present and previous results have been obtained by different transport approaches, an agreement of 10% is satisfactory. Good

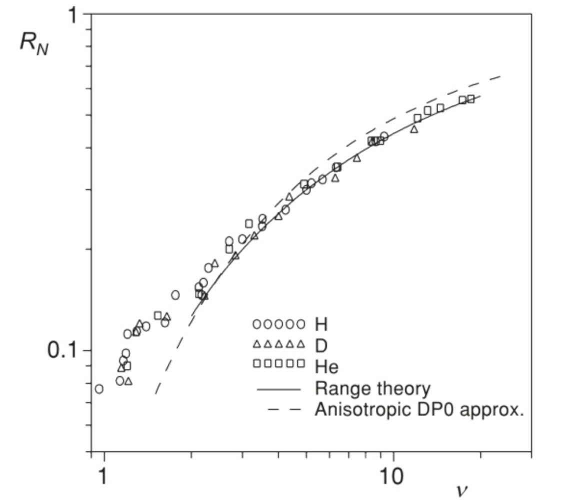

Figure 1. Reflection coefficient for light ions incident normally on heavy targets as a function of parameter ν. Solid line: pesent work, eq. (18). Dashed line: our previous result [7], eq. (4). Computer simulation data from [3]

agreement of the calculated $R_N(\nu)$ with Monte Carlo simulation data of [3] is obtained for ν *i. e.* in the multiple collision region.

CONCLUSION

Reflection coefficient of low energy light ions backscattered from heavy solid targets has been calculated within transport theory of ion ranges in an infinite medium. The technique applied gives the range distribution in an infinite medium as a solution of the transport equation by the moment method. The reflection coefficient was determined from the penetration profile by assuming that R is the fraction of the ion beam that has negative penetration depths. To obtain more accurate results, corrections for multiple crossings of the surface have been applied. The Gaussian approximation of the penetration profile as well as reflection coefficient are found in the form of analytic formulas. The results are compared with our previous calculations on the basis of DP0 solution of the transport equation and with computer simulation data. Good agreement is found in the multiple collision region.

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Јован ВУКАНИЋ

ИЗРАЧУНАВАЊЕ КОЕФИЦИЈЕНАТА РЕФЛЕКСИЈЕ НИСКОЕНЕРГЕТСКИХ ЛАКИХ ЈОНА ПРИМЕНОМ ТЕОРИЈЕ ДОМЕТА ЈОНА

Теорија вишеструког расејања домета лаких јона у неограниченој средини коришћена је за израчунавање коефицијента рефлексије из пенетрационог профила у нискоенергетској области где је електронско заустављање доминантан процес успоравања јона. Електронско заустављање је пропорционално брзини пројектила, а судари између јона и атома мете одређени су потенцијалом који је обрнуто пропорционалан квадрату растојања. Гаусова апроксимација пенетрационог профила као и коефицијент рефлексије нађени су у облику аналитичких формула. Извршена је корекција на вишеструко пресецање површине мете. Добијени резултати упоређени су са нашим претходним израчунавањима добијеним на бази DP0 решења транспортне једначине, као и са резултатима рачунарских симулација.

Кључне речи: лаки јон, тешка мета, коефицијент рефлексије, домет јона, модел вишеструког расејања, универзални параметар