

# REFLECTION OF keV LIGHT IONS FROM SOLIDS AT OBLIQUE AND GRAZING INCIDENCE

by

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The particle reflection coefficient of light keV ions backscattered from heavy targets has been determined by two different analytical approaches: by the single collision model in the case of nearly perpendicular incidence and by the small-angle multiple scattering theory in the case of glancing angles of incidence. The obtained analytical formulae are approximately universal functions of the scaled transport cross-section describing the reflection of all light ions from heavy targets. Going from perpendicular to grazing incidence, the transition from pure single to pure multiple scattering type of reflection is observed. For larger values of the scaling parameter the results of these theories cover the whole region of ion incident angles and the present estimates of the particle reflection coefficient are in good agreement with the results obtained from the empirical formula of Tabata *et al.*

*Key words:* light ion, heavy solid, oblique incidence, grazing incidence, particle reflection coefficient

## INTRODUCTION

The reflection of keV light ions from heavy solid targets has been calculated in the multiple scattering theory of ion ranges at relatively low energies [1, 2] and within the single collision approximation at higher energies [3, 4]. The very simple model of ion transport – single scattering and screened Coulomb interaction used in [3, 4] – has been extended to non-zero ion/target mass ratio [5] and recently modified by taking into account the beam attenuation of initial and backscattered ions through the target [6]. All these approaches have predicted that particle and energy reflection coefficients, plotted as functions of Thomas-Fermi reduced energy  $\varepsilon_0$ , give universal curves describing the

total backscattering of a specified light projectile from all heavy targets. Moreover, in many papers based on experimental or computer simulation data, the reduced energy  $\varepsilon_0$  has been utilized as a scaled parameter of the reflection coefficients of ions [7].

However, in several recent papers on this subject [8-10], a new scaled parameter  $\nu$  which represents the mean number of the wide angle collisions of an ion during slowing down has been adopted. For  $\nu \gg 1$ , studies based on the multiple collision model predict universal functions for particle and energy reflection coefficients for all light ions – heavy target combinations. Several procedures have been applied to derive analytical expressions for reflection coefficients: Chandrasekhar's H-function method [8, 11], the  $P_1$ -approximation with the age theory [10], and the DPN method combined with isotropic and anisotropic scattering kernel approximations [12, 13]. In our previous paper [14] we have investigated the validity of the scaling rule in the high energy region, where the single collision model holds and the ion reflection depends strongly on the shape of the scattering cross-section [3, 4]. This analytical study has been done for perpendicular ion incidence.

The purpose of this work is to explore the variation of particle reflection coefficient with the angle of incidence. Since hydrogen hits the first wall of the fusion device with a wide range of angles, analytical estimates in the case of oblique and grazing incidence are of considerable importance. For light ions hitting heavy targets and for not too-oblique incidence, the single collision model

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from [14] can be applied. Conversely, this model fails at glancing incidence since multiple collisions dominate in the reflection, even at very high energies. For grazing incidence, the energy and angular distribution of backscattered particles obtained from the transport theory in the form of analytical solutions is available [15]. By using these results, we shall calculate the reflection coefficient at grazing incidence. These two different analytical approaches, used in [14, 15], give us reflection coefficients in a wide range of incident angles at higher ion energies that correspond to  $\nu > 2$ .

## STOPPING POWER AND SCATTERING LAW

The stopping power and scattering law describing the slowing down of keV light ions in heavy random targets have been specified in refs. [14, 16]:

(1) All energy loss is due to electronic stopping  $dE/d\tau = NS_e(E)$ , which is assumed velocity proportional  $S_e(E) = KE^{1/2}$ . Here,  $N$  is the density of target atoms, and  $K$  is a well defined constant. The ion energy at the path length  $\tau$  is given by

$$E(\tau) = E_0 \left(1 - \frac{\tau}{\tau_0}\right)^2 \quad (1)$$

where  $E_0$  is the initial ion energy, and

$$\tau_0 = \frac{2}{NK} \sqrt{E_0} \quad (2)$$

is the total path length.

(2) All scattering is due to nuclear collisions. The Thomas-Fermi interaction is assumed, with the power form approximation for the differential cross-section [14]

$$d\sigma(\tau, \theta) = 2^{m-1} \lambda_m \pi a^2 \varepsilon_0^{2m-1} \frac{\tau}{\tau_0} \frac{d(\cos \theta)}{(1 - \cos \theta)^{m-1}} \quad (3)$$

where  $\theta$  is the laboratory scattering angle and  $\varepsilon_0$  is the initial ion energy in Thomas-Fermi units [17]

$$\varepsilon_0 = \frac{E_0 a \frac{M_2}{M_1}}{Z_1 Z_2 e^2 \left(1 + \frac{M_2}{M_1}\right)} \quad (4)$$

Here,  $M_1$  and  $Z_1$  are the atomic mass and atomic number of the incident ion, while  $M_2$  and  $Z_2$  are the corresponding values of the target atom, and  $a$  is the Thomas-Fermi screening radius. The exponent  $m$  and the matching parameter  $\lambda_m$  are given by

$$m = 0.5 \frac{\varepsilon_0}{\ln(1 + \varepsilon_0)}$$

$$s_n(\varepsilon_0) = (1 - 0.04024 \varepsilon_0^{0.62456}) \frac{0.5}{1 + \varepsilon_0} \quad (5)$$

$$\lambda_m = 2(1 - m) \frac{s_n(\varepsilon_0)}{\varepsilon_0^{1-2m}} \quad (6)$$

In eqs. (5) and (6)  $s_n$  is the reduced nuclear stopping cross-section which is a universal function depending on the details of the screened Coulomb interaction. We have chosen the Kr-C interaction as the best estimate for various ion-target combinations [18].

The reduced nuclear stopping  $s_n(\varepsilon_0)$  for the Kr-C potential has the form

$$s_n(\varepsilon_0) = \frac{0.5 \ln(1 + \varepsilon_0)}{\varepsilon_0^{0.37544} (1.0718 \varepsilon_0^{0.37544})} \quad (7)$$

The exponent  $m$  is the continuous function of the initial energy  $\varepsilon_0$  obtained by matching the reduced stopping cross-section in value and slope. Equations (5) and (6) together match very accurately the Thomas-Fermi cross-section for large scattering angles. The path length dependent cross-section is the key quantity entering the calculations of large-angle scattering events.

Conversely, the small-angle multiple collision process is described by the mean square scattering angle per unit path length  $\langle \theta^2(E) \rangle = N \int \theta^2 d\sigma(E, \theta)$ , rather than by the differential cross-section [15]. By using the relation  $\theta^2 = (M_2/M_1) T/E$ , where  $\theta \ll 1$  and  $T$  is the energy transferred in a single collision, one obtains

$$\langle \theta^2(E) \rangle = N \frac{M_2}{M_1} \frac{S_n(E)}{E} \quad (8)$$

where  $S_n(E)$  is the nuclear stopping cross-section. Moreover, in the case of grazing incidence, most of the backscattered ions emerge with energies close to the initial energy  $E_0$ . Provided the energy loss is small, one can write  $\langle \theta^2(E) \rangle \approx \langle \theta^2(E_0) \rangle = \text{const}$ . Then, the mean square scattering angle at the total path length is given by  $\langle \theta^2(E_0) \rangle \tau_0 = 2(M_2/M_1) S_n(E_0)/S_e(E_0)$ . The total path length is most conveniently expressed in Thomas-Fermi units [17]

$$\rho_0 = 4\pi \tau_0 \frac{M_2}{M_1} \frac{Na^2}{\left(1 + \frac{M_2}{M_1}\right)^2} \frac{2}{k} \sqrt{\varepsilon_0} \quad (9)$$

where for  $M_2 \gg M_1$ ,

$$k = 0.0793 Z_1^{2/3} \frac{1}{\sqrt{A}} \frac{M_2}{M_1} \quad (10)$$

$A_1$  is the mass number of the projectile. Going to reduce units, we obtain

$$\langle \theta^2(E_0) \rangle \tau_0 = \langle \theta^2(\varepsilon_0) \rangle \rho_0 = 2 \frac{M_2}{M_1} \frac{s_n(\varepsilon_0)}{k \sqrt{\varepsilon_0}} \quad (11)$$

## THE SCALED TRANSPORT CROSS-SECTION

As we have mentioned in Introduction, in recent papers on light ion reflection in the low energy region a new scaled parameter has been accepted [8-10]. This

quantity, called the scaled transport cross-section, is defined as

$$\nu = N\sigma_{tr}(E_0)\tau_0(E_0) \quad (12)$$

where  $\sigma_{tr}(E_0)$  is the transport cross-section at the initial ion energy  $E_0$ . The dimensionless parameter represents the mean number of the wide angle collisions of an ion during slowing down. For  $\nu \gg 1$ , studies based on the multiple collision model predict universal functions for particle and energy reflection coefficients for all light ion – heavy target combinations.

It is shown in our previous paper [14] that the scaled transport cross-section remains a convenient scaled parameter for light ion reflection in the upper keV energy region where the single collision model can be applied. For light keV ions in heavy targets, the parameter is proportional to the ratio of the nuclear to the electronic stopping cross-section

$$\nu = \frac{M_2}{M_1} \frac{S_n(E_0)}{S_e(E_0)} = \frac{M_2}{M_1} \frac{s_n(\varepsilon_0)}{k\sqrt{\varepsilon_0}} \quad (13)$$

### TOTAL BACKSCATTERING IN SINGLE COLLISION APPROXIMATION

A single collision backscattering event is shown in fig. 1. A light ion with the initial energy  $E_0$  is incident at an angle  $\alpha_0$  with respect to the inward surface normal and penetrates the target. In an elastic collision with a target atom, which occurs at the path length  $\tau_s$ , the ion is scattered through the angle  $\theta$ , and after traveling the path length  $\tau_s \cos \alpha_0 / |\cos \alpha|$  it leaves the solid.  $\alpha$  and  $\phi$  are the polar and azimuthal angles of the exit direction with respect to the inward surface normal.

For  $M_2 \gg M_1$  recoil energy loss can be neglected. Then, the ion energy at the arrival back to the surface is given by

$$E = E_0 \left( 1 + \frac{\cos \alpha_0}{|\cos \alpha|} \right) \left( 1 - \frac{\tau_s}{\tau_0} \right) \left( 1 - \frac{\cos \alpha_0}{|\cos \alpha|} \right) \quad (14)$$

The scattering angle  $\theta$  is connected with the angles of incidence and emergence through

$$\cos \theta = \cos \alpha_0 \cos \alpha + \sin \alpha_0 \sin \alpha \cos \phi \quad (15)$$

Within the single collision model, the probability  $W(E_0, \cos \alpha_0, E, \cos \alpha, \phi) dE d|\cos \alpha| d\phi$  for an ion to be backscattered with the energy ( $E, dE$ ) into the solid angle  $d|\cos \alpha| d\phi$  in  $(\alpha, \phi)$  direction is given by [4]

$$W(E_0, \cos \alpha_0, E, \cos \alpha, \phi) dE d|\cos \alpha| d\phi = N(\tau_s, \theta) \left| \frac{\partial \tau_s}{\partial E} \right| dE d|\cos \alpha| d\phi \quad (16)$$

where

$$N(\tau_s, \theta) = \frac{d\sigma(\tau_s, \theta)}{2\pi \sin \theta d\theta} \quad (17)$$

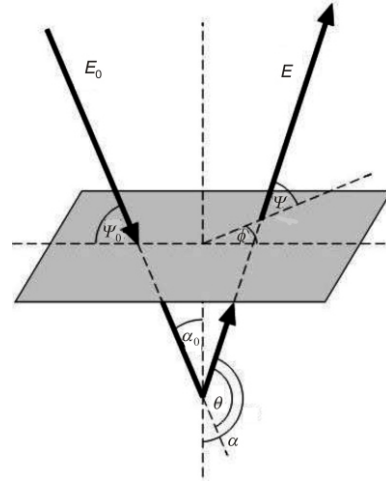


Figure 1. A backscattering event in the single collision geometry

By using eqs. (3), (14), and (15), and going to the reduced units, eq. (16) becomes

$$\begin{aligned} & W(E_0, \cos \alpha_0, E, \cos \alpha, \phi) dE \\ &= w(\varepsilon_0, \cos \alpha_0, \varepsilon, \cos \alpha, \phi) d\varepsilon \\ &= \frac{2^{m-4}}{\pi} \frac{\lambda_m}{k} \frac{M_2}{M_1} \frac{|\cos \alpha|}{\sqrt{\varepsilon}} \\ & \frac{(\cos \alpha_0 |\cos \alpha|)^{4m-1}}{\cos \alpha_0 |\cos \alpha| \sqrt{\frac{\varepsilon}{\varepsilon_0}}^{4m}} d\varepsilon \\ & \frac{1}{(1 - \cos \alpha_0 \cos \alpha + \sin \alpha_0 \sin \alpha \cos \phi)^{m-1}} \end{aligned} \quad (18)$$

where  $\varepsilon$  is the exit energy in Thomas-Fermi units.

Integration of eq. (18) within the hemisphere and over all backscattered energies gives the particle reflection coefficient

$$R_N(E_0, \cos \alpha_0) = \int_0^{E_0} \int_0^1 d|\cos \alpha| \int_0^\pi d\phi W(E_0, \cos \alpha_0, E, \cos \alpha, \phi) \quad (19)$$

By inserting eq. (18) into eq. (19) and integrating, we can obtain

$$\begin{aligned} & R_N(\varepsilon_0, \cos \alpha_0) \\ &= \frac{\lambda_m}{k} \frac{M_2}{M_1} \varepsilon_0^{(2m-1/2)} \cos \alpha_0^{-(4m-1)} \frac{2^m}{4(4m-1)} \\ & \int_0^1 d|\cos \alpha| \frac{(\cos \alpha_0 |\cos \alpha|)^{4m-1} \cos \alpha_0^{4m-1}}{(\cos \alpha_0 |\cos \alpha|)^{m-1}} \\ & P_m \frac{1 - \cos \alpha_0 |\cos \alpha|}{\cos \alpha_0 |\cos \alpha|} \end{aligned} \quad (20)$$

where

$$P_m(x) = \frac{1}{\pi} \frac{\int_0^\pi \frac{d\phi}{(x + \sqrt{x^2 - 1} \cos \phi)^{m+1}} \quad (21)$$

is the Legendre function of the first kind.

Particle reflection coefficient for perpendicular incidence has been found in [14]. Here, we obtain this result by the integration of eq. (20) for  $\alpha_0 = 0$  and inserting  $\lambda_m$  from eq. (6). This yields

$$R_N(v, 1) = \frac{M_2}{M_1} \frac{s_n(\varepsilon_0)}{s_e(\varepsilon_0)} \psi(m) \quad v\psi(m) \quad (22)$$

where the function  $\psi(m)$  is determined by

$$\psi(m) = (1 - m) \frac{(3m - 1)(4m - 1)2^m - m2^{4m-1}}{2m(4m - 1)(3m - 1)} \quad (23)$$

In order to obtain the reflection coefficient at oblique incidence, we expand eq. (20) in powers  $(1 - \cos \alpha_0)$ . Integration leads to the approximate expression

$$R_N(v, \cos \alpha_0) = R_N(v, 1) [1 - (2m - 1)(1 - \cos \alpha_0) \dots] R_N(v, 1) \cos \alpha_0^{(2m-1)} \quad (24)$$

where the reflection coefficient at perpendicular incidence  $R_N(v, 1)$  is given by eqs. (22) and (23).

## TOTAL BACKSCATTERING AT GRAZING INCIDENCE

At the glancing angles of incidence, ion reflection results from multiple collisions. Our estimates are based on a paper of Remizovich *et al.* [15] who treated reflection from semi-infinite targets. These authors solved the transport equation in diffusion approximation and small-angle limit, with proper boundary conditions at the target surface, and have found the path length and angular distribution of ions backscattered from solids

$$W(E_0, \psi_0, \tau, \psi, \phi) d\tau d\psi d\phi = \frac{2\sqrt{3}\psi}{\pi^{3/2}} \frac{\exp \frac{4(\psi_0^2 - \psi^2 - \psi\psi_0) \phi^2}{\langle \theta^2 \rangle \tau}}{\langle \theta^2 \rangle^{3/2} \tau^{5/2}} \operatorname{erf} 2 \sqrt{\frac{3\psi\psi_0}{\langle \theta^2 \rangle \tau}} d\tau d\psi d\phi \quad (25)$$

where  $\tau$  is the path length traveled,  $\psi_0 = \pi/2 - \alpha_0$  and  $\psi_0 = |\pi/2 - \alpha|$ . The angle of incidence and the ejection angle  $\psi$ , measured from the target surface, have been introduced for convenience. These angles, as well as the azimuthal exit angle  $\phi$  are assumed small ( $\psi, \psi_0$ , and  $\phi \ll 1$ ).

Let us introduce a new dimensionless parameter  $\sigma_0 = \langle \theta^2 \rangle \tau_0 / 4\psi_0^2 = v/2\psi_0^2$  and new dimensionless variables

$$\frac{\tau}{\tau_0} = s, \quad \frac{\psi}{\psi_0} = \zeta, \quad \frac{\phi}{\psi_0} = \chi \quad (26)$$

With these variables we can write eq. (25) in the form

$$W(E_0, \psi_0, \tau, \psi, \phi) d\tau d\psi d\phi = W_1(\sigma_0, s, \zeta, \chi) ds d\zeta d\chi \quad (27)$$

where

$$W_1(\sigma_0, s, \zeta, \chi) = \frac{\sqrt{3}}{4\pi^{3/2}} \frac{\zeta}{\sigma_0^{3/2} s^{5/2}} \exp \frac{\zeta^2 - \zeta - 1}{\sigma_0 s} \operatorname{erf} \sqrt{\frac{3\zeta}{\sigma_0 s}} \quad (28)$$

The particle reflection coefficient can be obtained by integration over all ejection angles and relative path lengths

$$R_N(\sigma_0) = \int_0^1 ds \int_0^\infty d\zeta \int_0^\infty d\chi W_1(\sigma_0, s, \zeta, \chi) \quad (29)$$

Within the small-angle approximation, the distribution (28) peaks strongly at small angles, so the integration limits for relative ejection angles in eq. (29) have been extended to infinity.

Our purpose is to evaluate eq. (29) and thus to obtain the analytic expression for the particle reflection coefficient at grazing incidence. Azimuthal integration can be easily performed. One obtains

$$W_1(\sigma_0, s, \zeta) = \int_0^\infty W_1(\sigma_0, s, \zeta, \chi) d\chi = \frac{\sqrt{3}}{2\pi} \frac{\zeta}{\sigma_0 s^2} \exp \frac{\zeta^2 - \zeta - 1}{\sigma_0 s} \operatorname{erf} \sqrt{\frac{3\zeta}{\sigma_0 s}} \quad (30)$$

The next step in the evaluation of eq. (29) is to integrate eq. (30) over  $\zeta$ . The solution gives the distribution of backscattered ions over relative path lengths in the target

$$W_1(\sigma_0, s) = \int_0^\infty W_1(\sigma_0, s, \zeta) d\zeta = \frac{\sqrt{3}}{2\pi} \frac{\exp \frac{3}{4} \frac{1}{\sigma_0 s}}{\sigma_0 s^2} \int_0^\infty \zeta \exp \frac{(\zeta - 1/2)^2}{\sigma_0 s} \operatorname{erf} \sqrt{\frac{3\zeta}{\sigma_0 s}} d\zeta \quad (31)$$

For small values of  $\sigma_0 s$ , the dominant contribution to the integral in eq. (31) gives the region around  $\zeta = 1/2$  so that using the Laplace method for evaluation of this integral, one obtains

$$W_1(\sigma_0, s) = \frac{\sqrt{3}}{4\sqrt{\pi}\sigma_0} s^{-3/2} \exp \frac{3}{4\sigma_0 s} \quad (32)$$

Integrating the expression (32) over all path lengths, we obtain the asymptotic formula for the reflection coefficient  $R_N(\sigma_0)$ , valid at small values of  $\sigma_0$

$$R_N(\sigma_0) = \int_0^1 W_1(\sigma_0, s) ds = \frac{1}{2} \operatorname{erfc} \sqrt{\frac{3}{4\sigma_0}} \quad (33)$$

We are more interested in the case where the parameter  $\sigma_0$  is large ( $\sigma_0 \gg 1$ ). Following [4], we introduce the new variable  $u = \sqrt{2/\sigma_0} s$ . With this new variable the reflection coefficient  $R_N(\sigma_0)$  can be obtained as

$$R_N(\sigma_0) = \int_0^1 W_1(\sigma_0, s) ds = \int_0^{\sqrt{2/\sigma_0}} W_2(u) du \quad (34)$$

where the distribution  $W_2(u)$  is given by

$$W_2(u) = \frac{\sqrt{3}}{2\pi} \int_0^{\infty} \zeta \exp\left[-\frac{u^2}{2}(\zeta^2 - 1)\right] \operatorname{erf} u \sqrt{\frac{3\zeta}{2}} d\zeta \quad (35)$$

Integration over  $\zeta$  on the right hand side of eq. (35) can be done by using series expansion for the error function

$$\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} e^{-z^2} \sum_{k=0}^{\infty} \frac{z^{2k+1}}{3 \cdots (2k+1)} \quad (36)$$

Inserting eq. (36) with  $z = u\sqrt{3\zeta/2}$  into eq. (35) and integrating over  $z$ , one obtains

$$W_2(u) = \frac{3}{2^{3/2}\pi} \frac{1}{\sqrt{u}} e^{-\frac{u^2}{4}} \sum_{k=0}^{\infty} \frac{3}{2} u^{k+1} D_{k+3/2}(u) \quad (37)$$

where  $D_k(u)$  is a parabolic cylinder function.

The particle reflection coefficient can be written in the form

$$R_N(\sigma_0) = \int_0^{\sqrt{2/\sigma_0}} W_2(u) du = \int_0^{\sqrt{2/\sigma_0}} W_2(u) du \quad (38)$$

and the first integral on the right hand side of eq. (38) can be directly evaluated. This yields

$$\int_0^{\infty} W_2(u) du = \frac{3}{4} \sum_{k=0}^{\infty} \frac{1}{3} \sum_{k=0}^{\infty} \frac{3}{4} \frac{(2k+1)!!}{2^{2k+1}(k+1)!} \left(\frac{3}{4}\right)^{1/2} \quad (39)$$

As we mentioned at the beginning of this chapter, the present approach holds for  $\sigma \gg 1$ . For large

values of  $\sigma_0$ , the second integral in eq. (38) can be evaluated by using the asymptotic formula for the series (37)

$$W_2(u) = \frac{3}{2^{7/4} \Gamma(3/4) \sqrt{\pi}} \frac{1}{\sqrt{u}} \left[ \frac{1}{4} u^2 - \frac{\sqrt{2}}{10} \frac{\Gamma(3/4)}{\Gamma(1/4)} u^3 + \dots \right], u \rightarrow 0 \quad (40)$$

Inserting eqs. (39) and (40) into eq. (38) and integrating, we obtain the particle reflection coefficient

$$R_N(\sigma_0) = 1 - \frac{0.977}{\sigma_0^{1/4}} - \frac{0.0977}{\sigma_0^{5/4}} \quad (41)$$

Since the angle of incidence  $\psi_0$  is small, the dimensionless parameter  $\sigma_0$  can be expressed via the angle of incidence  $\alpha_0$  measured from the target surface normal

$$\sigma_0 = \frac{v}{2\psi_0^2} = \frac{v}{2\sin^2\psi_0} = \frac{v}{2\cos^2\alpha_0} \quad (42)$$

The asymptotic formula (33) becomes

$$R_N(v/\cos^2\alpha_0) = \frac{1}{2} \operatorname{erfc} \sqrt{\frac{3}{2v} \cos^2\alpha_0} \quad (43)$$

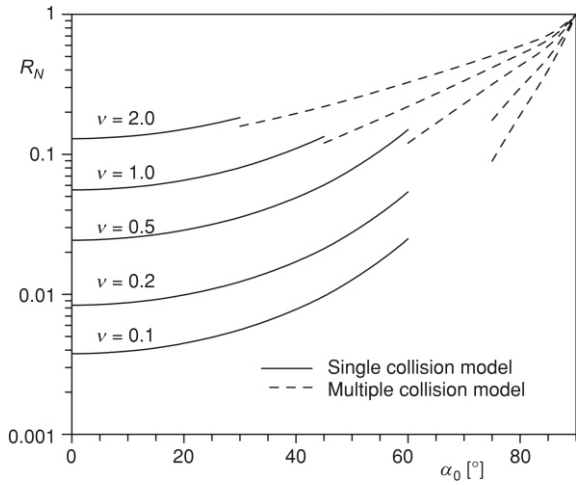
This expression is very accurate for  $v/\cos^2\alpha_0 \geq 2$  and for  $v/\cos^2\alpha_0 \geq 4$  underestimates the reflection coefficient by about 10%. For  $v/\cos^2\alpha_0 \geq 2$ , the particle reflection coefficient can be calculated by the asymptotic formula (41) written over  $v/\cos^2\alpha_0$

$$R_N(v/\cos^2\alpha_0) = 1 - 1.162 \frac{\cos^2\alpha_0}{v}^{1/4} - 0.232 \frac{\cos^2\alpha_0}{v}^{5/4} \quad (44)$$

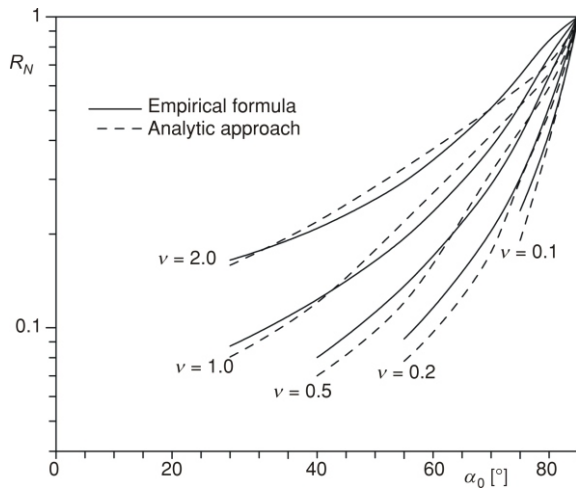
with in a few percent of accuracy.

## RESULTS AND DISCUSSION

Figure 2 shows the particle reflection coefficient  $R_N(v, \cos \alpha_0)$  for light ions backscattered from heavy targets as a function of an angle of incidence (degrees from surface normal), for several values of the scaled transport cross-section  $v$ . Solid lines are calculated from eqs. (22)-(24) of the single collision theory. Dashed lines follow from eq. (44) from the small-angle multiple scattering theory. For a given scaling parameter  $v$ , going from perpendicular to grazing incidence one can observe the transition from the pure single to pure multiple scattering type of reflection. For the large values of parameter  $v$  the results of single and multiple collision theories cover the whole region



**Figure 2.** The particle reflection coefficient for light ions backscattered from heavy targets as a function of angle of incidence  $\alpha_0$  for several values of the scaling parameter  $\nu$ , obtained from the single collision model and small angle multiple scattering theory

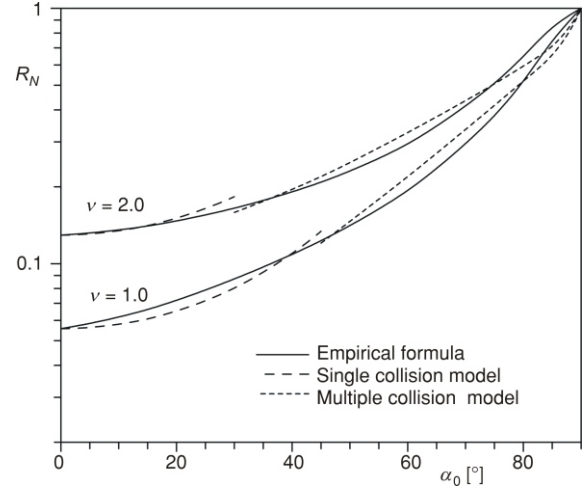


**Figure 3.** The comparison of the particle reflection coefficient calculated by the empirical formula of Tabata *et al.*, and by the multiple collision model

of incident angles  $\alpha_0$ . For small  $\nu$  ( $\nu = 0.2$ ) the approximations used in the present estimates do not describe well the light ion reflection in the region of incident angles between  $60^\circ$  and  $75^\circ$ , and the results for  $R_N$  are omitted in fig. 2.

Figure 3 compares the particle reflection coefficients calculated from empirical formula of Tabata *et al.* [19] and from the present multiple collision theory. The empirical formula gives the dependence of the reflection coefficient  $R_N$  on the angle of incidence

$$R_N(\varepsilon_0, \alpha_0) = R_N(\varepsilon_0, 0) \frac{1 - R_N(\varepsilon_0, 0)}{1 - a_1 \text{ctg}^{2a_2} \alpha_0} \quad (45)$$



**Figure 4.** The comparison of the particle reflection coefficient calculated by the empirical formula, single collision model and multiple collision theory, for large values of the scaling parameter  $\nu$

where  $R_N(\varepsilon_0, 0)$  is the value of the reflection coefficient at normal incidence, and  $\varepsilon_0$  is the reduced energy of the incident ion. The values of the empirical coefficients are given as:  $a_1 = 7.38\varepsilon_0^{0.359}$  and  $a_2 = 0.836/\varepsilon_0^{0.087}$ .

The agreement of the analytic approach with the empiric formula is good for the large values of the reflection coefficient  $R_N$  ( $R_N > 0.1$ ). The applied multiple scattering model is formulated for grazing incidence and small angle collisions, but surprisingly it gives good results for oblique incidence whenever reflection coefficients are large.

Having in mind that the empirical formula is derived for the low energies of initial ions ( $\varepsilon_0 < 5$ ), in fig. 4 we compare the particle reflection coefficients as a function of the angle of incidence for large values of the scaling parameter  $\nu$ . The results obtained by the analytical approaches agree well with the empirical formula in the whole range of angles of ion incidence. We expect that the applied analytical single and multiple collision models hold better at higher ion energies.

## CONCLUSIONS

For keV light ions backscattered from heavy solids, the particle reflection coefficient has been calculated by two approaches: within the single collision model for oblique ion incidence, eqs. (22)-(24), and on the basis of the small angle multiple collision theory for glancing incidence, eq. (44). The obtained formulae for the reflection coefficient are approximately universal functions of the scaled transport cross-section. The analytical expressions derived from the single and multiple collision theories cover the whole region of incident angles for the larger values of  $\nu$ . For small  $\nu$ , the applied approximations used in the present

analysis give the less accurate results for the particle reflection coefficient in the region of initial angles between  $60^\circ$  and  $75^\circ$  (fig. 2).

The present results are compared with the empirical formula of Tabata *et al.*, which gives the dependence of the reflection coefficient  $R_N$  on the angle of incidence for low energies of initial ions. The multiple collision theory gives results for grazing and even oblique incidence in good agreement with the empirical formula whenever the reflection coefficients  $R_N$  are larger than 0.1 (fig. 3). Moreover, for the initial ion energies that correspond to the scaling parameter  $\nu = 1$ , the agreement of the theories and empirical formula is very good in the whole range of angles of ion incidence (fig. 4).

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## REFERENCES

- [1] Weissmann, R., Sigmund, P., Sputtering and Backscattering of Light Ions Bombarding Random Targets, *Radiat. Eff.* 19 (1973), 1, pp. 7-14
- [2] Vukanić, J., Reflection Coefficient of Low Energy Light Ions Based on the Theory of Ion Ranges, *Nuclear Technology & Radiation Protection*, 22 (2007), 1, pp. 54-57
- [3] Vukanić, J., Sigmund, P., Total Backscattering of keV Light Ions from Solid Targets in Single-Collision Approximation, *Appl. Phys.*, 11 (1976), 3, pp. 265-272
- [4] Vukanić, J., Janev, R. K., Heifetz, D., Total Backscattering of keV Light Ions from Solids at Oblique and Grazing Incidence, *Nucl. Instr. and Meth. B*, 18 (1987), 1-6, pp. 131-141
- [5] Wedell, R., Total Backscattering and Energy Reflection of Light Ions from Solids in the Single-Collision Approximation, *Appl. Phys. A* 35 (1984), 2, pp. 91-97
- [6] Tolmachev, A. I., Energy Distribution of Light Ions Backscattered from a Solid in the Single-Collision Approximation, *Nucl. Instr. and Meth.*, B 155 (1999), 1-2, pp. 36-42
- [7] Eckstein, W., Verbeek, H., Data on Light Ion Reflection, Max Planck Inst., *Plasma Phys. Rep.*, IPP 9/32, 1979
- [8] Tilinin, I. S., Reflection of Low Energy Atomic Particles from Solid Surface, *Phys. Chem. Mech. Surf.*, 2 (1984), pp. 640-660
- [9] Luo, Z. M., A New Parameter for Describing the Reflection Coefficient of Light Ions Scaled Transport Cross Section, *Nucl. Instr. and Meth.*, B 48 (1990), 1-4, pp. 444-447
- [10] Vicanek, M., Urbassek, N. M., Reflection Coefficient of Low-Energy Light Ions, *Phys. Rev. B*, 44 (1991), 14, pp. 7234-7242
- [11] Vukanić, J., Simović, R., Analytical Solutions of the Boltzmann Transport Equation for Light Ion Reflection, *Fus. Technol.*, 30 (1996), 2, part 1, pp. 372-382
- [12] Simović, R., Vukanić, J., The Albedo Problem of Low-Energy Light Ions Treated Analytically in the DP0 Flux Approximation, *J. Phys. D: Appl. Phys.*, 30 (1997), 16, pp. 2331-2337
- [13] Vukanić, J., Simović, R., Reflection Coefficients of Light Ions for the Inverse-Square Interaction Potential, *Nucl. Instr. and Meth.*, B 179 (2001), 4, pp. 497-502
- [14] Vukanić, J., Simović, R., Scaling Properties in Single Collision Model of Light Ion Reflection, *Nucl. Instr. and Meth.*, B 215 (2004), 3-4, pp. 337-344
- [15] Remizovich, V. S., Ryazanov, M. I., Tilinin, I. S., Energy and Angular Distribution of Reflected Particles from a Beam Incident on a Surface at Glancing Angles, *JETP* 52a (1980), pp. 225-235
- [16] Schiott, H. E., Range-Energy Relations for Low-Energy Ions, *Mat. Fys. Medd. Dan. Vid. Selsk.*, 35 (1966), p. 9
- [17] Lindhard, J., Scharff, M., Schiott, H. E., Range Concepts and Heavy Ion Ranges, *Mat. Fys. Medd. Dan. Vid. Selsk.*, 33 (1963), 14, pp. 1-42
- [18] Willson, W. D., Haggmark, L. G., Biersack, J. P., Calculations of Nuclear Stopping, Ranges, and Straggling in the Low-Energy Region, *Phys. Rev.*, B 15 (1977), 5, pp. 2458-2468
- [19] Tabata, T., Ito, R., Itikawa, Y., Itoh, W., Morita, K., Tawara, H., Dependence of Backscattering Coefficients of Light Ions upon Angle of Incidence, Rep. IPPJ-AM-34, Institute of Plasma Physics, Nagoya, Japan, 1984

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## РЕФЛЕКСИЈА ЛАКИХ ЈОНА keV-СКИХ ЕНЕРГИЈА ОД ТЕШКИХ МЕТА ПРИ КОСОМ УПАДУ ЈОНСКОГ СНОПА

Коефицијент рефлексije лаких јона keV-ских енергија рефлектованих од тешких мета одређен је употребом два аналитичка поступка: моделом једног судара у случају приближно нормалног упада јонског снопа и на основу теорије вишеструког расејања у случају малог угла упада према површини мете. Изведене аналитичке формуле, изражене средњим бројем расејања јона током успоравања, приближно су универзалне функције које описују рефлексiju свих лаких јона од тешких мета. Променом угла упада јонског снопа од нормалног ка малом углу према површини мете, региструје се прелаз у механизму рефлексije – од чисто једноструког расејања до вишеструког расејања. У случају већег броја судара јона током успоравања, резултати ових теорија покривају читаву област упадних углова јонског снопа и израчунате вредности честичног коефицијента рефлексije добро се слажу са резултатима емпиријске формула Табате и сарадника.

*Кључне речи:* лаки јон, тешка мета, кос упад, упад под малим углом на површину мете, честични коефицијент рефлексije