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INVERSE-SQUARE INTERACTION POTENTIAL IN THE MULTIPLE COLLISION MODEL OF LIGHT ION REFLECTION

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Abstract. The linear Boltzmann transport equation for diffusion and slowing down of low-energy light ions in solids is Laplace transformed in relative path-length and solved by applying the DP0 technique. The ion-target atom interaction potential is assumed to have a form of the inverse-square law and furthermore, the collision integral of the transport equation is replaced by the P_3 approximation in angular variable. The approximative Laplace transformed solution for the reflection function is found and inverted leading to the distribution of backscattered particles in the relative path-length. Analytic expression for the particle reflection coefficient was derived and our result is compared with computer simulation data.

1. INTRODUCTION

In this paper, the energy dependent albedo problem of low energy light ions from heavy targets is considered in a multiple collision model. The ion transport equation is treated with the assumptions that (i) distribution function of reflected ions is almost isotropic and (ii) backscattered particles suffer small energy loss and therefore the transport cross section depends only on initial ion energy. Here we follow the DPN procedure applied in our previous paper (see Simović et al. 1997) improving the model by taking into account the anisotropy effects in ion scattering (Vukanić et al. 2001). This is done by replacing the isotropic approximation of the collision integral in the transport equation with the anisotropic Legendre polynomial approximation of the third order in angular variable.

For ordinary power potentials $V(R) \propto R^{-1/m}$ and the specific case $m = 1/2$, the particle reflection coefficient is found in compact form. The calculated particle reflection coefficient is compared with the results of the Monte Carlo simulations of H, D and He reflection from different targets.

2. PATH-LENGTH DISTRIBUTION OF BACKSCATTERED IONS

In this paper we employ a special power cross section

$$d\sigma(E_0,\hat{\mu}) = \sqrt{2}\,\sigma_1(E_0)\frac{d\hat{\mu}}{(1-\hat{\mu}\,)^{3/2}} \tag{1}$$

which describes scattering in the inverse-square potential $V(R) \propto R^{-2}$. In Eq. (1), $\hat{\mu}$ is the cosine of the scattering angle, E_0 is the ion initial energy and $\sigma_1(E_0)$ is the transport cross section. The scattering cross sections $d\sigma(E_0,\hat{\mu})$ appears appropriate for light ions interacting with heavy target atoms in the energy range of some tens of eV to some tens of keV. The use of Eq. (1) as an input quantity allows simple analytic solutions of the transport equation for the ion reflection.

We have derived the Laplace transformed half space reflection function in DP0 approximation. This procedure gives good results for the reflection function even in the lowest order of approximation (Vukanić et al. 2001)

$$\Re(\mu_0,p) = \frac{1}{1-A}\frac{(\sqrt{1-A\omega(p)}-\sqrt{1-\omega(p)})[\sqrt{1-A\omega(p)}-B(\mu_0)\sqrt{1-\omega(p)}]}{1+2\,\mu_0\,\sqrt{1-A\omega(p)}\sqrt{1-\omega(p)}} \tag{2}$$

Here μ_0 is the cosine of the angle of incidence and p is the Laplace variable. For the inverse-square scattering potential $A = 41/128$, $B(\mu_0) = (3\,\mu_0 + 35\,\mu_0^3)/32$ and the multiplication factor ω is $\omega(p) = 2\nu/(2\nu+p)$. Moreover, $\nu = N\,\sigma_1(E_0)\,\tau_0$, where N is the density of target atoms and τ_0 is the total path length.

The parameter ν represents the mean number of wide-angle collisions that ions suffer before slowing down to rest. For $\nu \gg 11$, because of large number of scattering events, the initially strongly peaked ion beam becomes more and more isotropic. The complete randomization of the direction of motion occurs already at transport path length much less than the total path length: $\lambda_1(E_0) \ll \tau_0 2$. For relative path lengths $s > \lambda_1\,/\,\tau_0 3$, the ion distribution function is almost isotropic.

For not very oblique incidence, we have approximated the Laplace transformed reflection function by an exponential

$$\Re(\mu_0,p) \approx \exp[-h\sqrt{p/\nu} + g(p/\nu)] \tag{3}$$

with $h = h(\mu_0) = 3.094\,\mu_0$ and $g = g(\mu_0) = -1.72 + 14.44\,\mu_0^2 - 24.2\,\mu_0^4 + 11.48\,\mu_0^6$.

The semi-empirical approximation (3) is very accurate except in the tails of the distribution ($p \gg 1$) when deviations occur. However, the approximations used in the derivation of Eq. (2) become questionable for $p \gg 1$ and the theoretical model applied is not very reliable.

Applying Laplace inversion of the approximative $\Re(\mu_0,p)$, we obtained the path-length distribution of backscatered particles

$$R(\mu_0,s) \approx \frac{h}{2\sqrt{\pi}}\frac{\nu}{(\nu s+g\,)^{3/2}}\exp[-\frac{h^2}{4(\nu s+g)}] \tag{4}$$

where s is the relative path-length travelled.

At normal incidence $\mu_0 = 1$, $g = 0$ and $R(\mu_0,s)$ is the exact inversion of $\Re(\mu_0,p)$. For $\mu < 1$, $g > 0$, but small, and $R(\mu_0,s)$ is the very good approximate inversion of

$\Re(\mu_0, p)$. $R(\mu_0, s)$ is the peak shaped distribution with a sharp peak at $\nu_{S_m} \approx 1.6\,\mu_0^2$, where S_m is the most probable relative path-length.

Figures 1 (a) and (b) compare the universal function $R(\mu_0, s)/\nu$ obtained from the simple expression (4) with the exact solution accomplished by numerical inversion of the original DP0 Laplace transformed solution (2). One can see that the analytical solution is a very good overall approximation of the numerical result for both normal and oblique incidence.

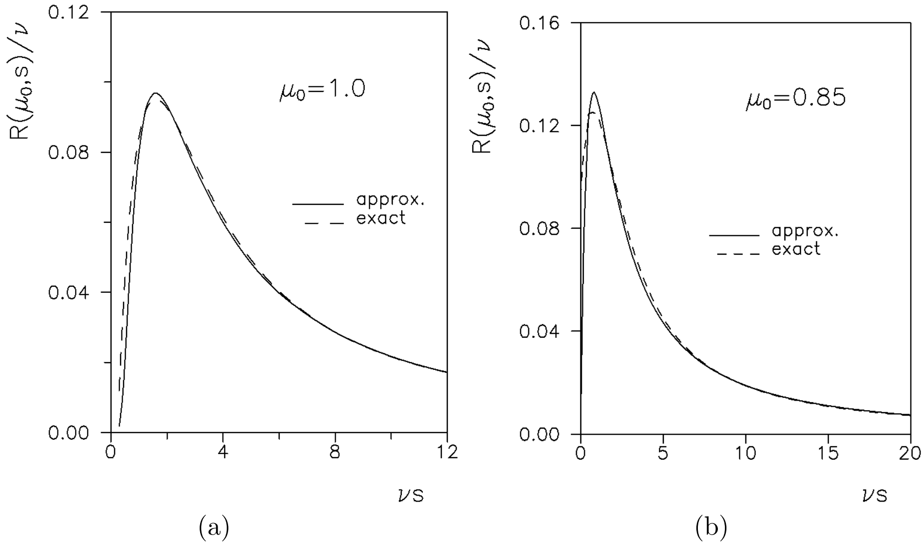

Figure 1: Path-length distributions of backscattered ions calculated for (a) perpendicular incidence and (b) oblique incidence.

3. RESULTS AND DISCUSSION

Thanks to the simplicity of the approximate expression (4) for $R(\mu_0, s)$, we obtained in analytic and condensed form the particle reflection coefficient $R_N(\mu_0, \nu)$

$$R_N(\mu_0, \nu) = \int_0^1 R(\mu_0, s)ds = erfc(u) \tag{5}$$

with $u = 3.094\,\mu_0\,/[2\sqrt{(\nu + g)}]$.

One can see from Eq. (5) that particle reflection coefficient depends on initial energy and ion-target combination through the variable ν which represents the mean number of wide-angle collisions that ions suffer before slowing down to rest. The scaling holds at low ion energies ($\nu > 14$) when reflection is determined by multiple collisions, as well as at high energies ($\nu < 15$) when single collisions dominate. It was found recently that the reflection coefficient of heavy ions from solids also scales with the parameter ν6.

Fig. 2 gives the particle reflection coefficient for light ions incident normally on heavy targets as a function of the parameter ν. The present work is compared with the Monte Carlo simulations of H, D and He reflection from different targets for a wide range of initial energies (Vicanek et al. 1991).One can see that the agreement of our results with simulated data is good for $\nu > 2$.

Good agreement of our theoretical estimates with computer simulation data suggests that the obtained analytical universal formula describes correctly the low-energy light ion reflection from solids.

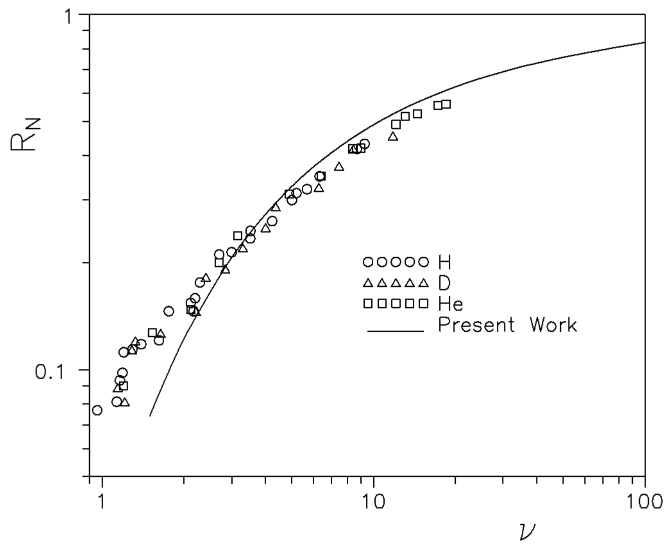

Figure 2: Particle reflection coefficient for light ions incident normally on heavy targets. Comparison of the present work with the computer simulation data of Vicanek et. al.

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