General principles for describing electronic and proton multiple scattering processes in solids

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Abstract. Analytical solution for the reflected light ions Pass Length Distribution Function (PLDF) equation is obtained. Reflected ions energy spectra calculated on the basis of the developed method shows satisfactory agreement with experimental data. The effectiveness of the developed methodology in the procedure for verifying the stopping power value is indicated.

1. Introduction

Consistent and accurate description of the interaction processes of accelerated ion fluxes with the solid surfaces is necessary both for the implementation of technologies for modifying and doping materials, and for signals descriptions from a wide range of ion-scattering spectroscopy techniques.

The most active research in this area was carried out in the 80s of the last century [1-5], which first was associated with the problem of the "first wall" in controlled thermonuclear fusion installations. If we look at the analytical models used to describe the process of ion scattering in solids [1-3], then, due to their extreme simplification, the question arises about the possibility of their use for a qualitative description of the processes of reflection of ions with energies from units to tens of keV.

There are two main characteristics of the scattering of light ions, which are commensurate in the indicated energy range: the transport path \( l_{tr} \) and the residual path \( R_0 = \frac{T_0}{\bar{E}} \) (\( T_0 \) is the initial ion energy, \( \bar{E} \) - stopping power):

\[
R \sim l_{tr}.
\]  

Formula (1) indicates that the use of Strait Line Approximation (SLA), which is traditional for ions energies from 1 to tens keV, is unacceptable. The situation is similar to which is typical for electrons [6-8]. Papers [6, 8] describe the most effective technique for describing electronic spectra.

In this work, we adapt the method presented in [6, 8] to the problems of light ions scattering of in solids.

2. Methods of Reflected Light ions energy spectra calculation

Let us consider the problem of electrons and light ions elastic scattering in solids. Solving the boundary value problem for the elastic transfer equation by the invariant immersion method leads us in azimuthally symmetric situations to the formula:

\[
\left( \frac{1}{\mu} + \frac{1}{\mu_0} \right) \left( 1 + \frac{\alpha}{\gamma} \right) S(\tau, \mu, \mu_0) =
\]  

(2)
where \( S(\tau, \mu, \mu_0) \) is the reflection function determined by (a): the scattering geometry; \( \mu, \mu_0 \) are the cosines of the viewing and probing angles; (b): the dimensionless path length of the ion in the target \( \tau = \frac{z}{l_{el}} \), \( l_{el} \) is the mean free path between the elastic collisions, \( x(\mu, \mu_0) \) is normalized differential elastic scattering cross section.

In the case of conservative scattering, when the channel of inelastic scattering is excluded, it is possible to obtain an analytical solution of equation (2), the solution procedure, justification of the assumptions made based on comparison with the exact numerical solution (2) are presented in [8]. The solution obtained is absolutely the same for both electrons and light ions!

But in the case of light ions, due to the fact that the screening parameter of the process of light ions elementary scattering is orders smaller than electrons, the assumptions made to obtain a series solution in Legendre polynomials. The sections are constructed on the basis of the potential of krypton carbon - KrC [1-3].

**Figure 1.** Part a: PLDF for \( \eta = 10^{-3} \) – red solid line, \( \eta = 5 \cdot 10^{-5} \) – blue dotted line, \( \eta = 5 \cdot 10^{-6} \) – green dashed line, \( \eta = 5 \cdot 10^{-7} \) – purple dashed line. Normal sounding, scattering angle 135°. Part b: PLDF for \( \eta = 10^{-3} \) – red solid line, \( \eta = 5 \cdot 10^{-5} \) – blue dotted line, \( \eta = 5 \cdot 10^{-6} \) – green dashed line, \( \eta = 5 \cdot 10^{-7} \) – brown dashed line. Incidence angle 20°, scattering angle 110°. Rutherford scattering cross section. Horizontal lines coming from PLDF plots obtained on the basis of (3), at point \( s = 0 \), represent the distributions over distances in the Straight Line Approximation (PLDF SLA dependence).

The area of zero paths (figure 1) describes protons reflected from the target surface. Setting \( s = 0 \) in (3), we obtain:

\[
S(0, \mu, \mu_0) = \frac{|A| \mu_0}{|\mu| + \mu_0} x_{el} \left( \mu \mu_0 + \sqrt{1 - \mu^2} \sqrt{1 - \mu_0^2} \right),
\]

Formula (4) is of decisive importance in ion backscattering spectroscopy. It describes PLDF in the Straight Line Approximation (SLA):

\[
S_{SLA}(\tau, \mu, \mu_0) = S(0, \mu, \mu_0).
\]
An important result following from calculations based on (3) is the transition to a constant universal form of the PLDF distribution as the screening parameter tends to zero. Moreover, the specified universal form is determined only by the geometry of the experiment! In the case shown in figure 1, the PLDF maximum is observed in the region of the order of one and a half transport paths.

The differences in PLDF obtained on the basis of successive accounting for multiple elastic scattering of ions and in their neglect (SLA approach) is illustrated in figure 1. The possibility of using the SLA approach opens up in cases when the stopping path of a particle is significantly less than its transport path:

\[ R_0 \ll l_{tr}. \]

Attempts to use (3) in the case of lead to absurd results, for which the experimental and calculated in SLA spectra are presented on a logarithmic scale [9].

We will determine the energy spectra of reflected particles in accordance with the formula:

\[ S(\Delta, \mu, \mu_0) = \int_0^\infty dq \cdot S \left( \frac{z}{l_{tr}}, \mu, \mu_0 \right) T \left( \frac{z}{l_{tr}}, \Delta \right). \]  

(7)

\[ T(\tau, \Delta) \] in the case of ion scattering is determined only by two moments of the cross section of inelastic scattering \( \bar{\varepsilon} \) and \( \bar{\varepsilon}^2 \) – the average energy losses per length unit and the mean square of energy losses or straggling, which are dictated by the laws of conservation of energy and momentum, limiting the energies transferred from the ion to the electronic subsystem:

\[ T(\tau, \Delta) = \frac{1}{\sqrt{2\pi}\bar{\varepsilon}z} e^{\left(\frac{(\Delta-\bar{\varepsilon}z)^2}{2\bar{\varepsilon}^2z}\right)}. \]

(8)

Substituting PLDF (3) into the formula for calculating the energy spectra of reflected ions (7), we obtain, in the approximation of continuous deceleration, when \( T(\tau, \Delta) = \delta(\Delta - \bar{\varepsilon}z) \):

\[ S(\Delta, \mu, \mu_0) = \frac{|\mu\mu_0 (1-x_1)(1-\Delta)|}{|\Delta + \mu_0|} e^{-\frac{\Delta}{\bar{\varepsilon}}} \sum_{n=0}^{2\tau+1} P_n(\mu\mu_0 + \sqrt{1 - \mu_0^2}) \left[ e^{-\frac{(\Delta-x_1)(1-\Delta)^2}{2(1-x_1)(1-\Delta)^2}} - e^{-\frac{(\Delta-x_1)(1-\Delta)^2}{2(1-x_1)(1-\Delta)^2}} \right]. \]

(9)

The dimensionless parameter \( \sigma^* \) appeared in formula (9), which is decisive for the analytical description of the process of reflected ions energy spectra formation:

\[ \sigma^* = \frac{E_0}{l_{tr}\bar{\varepsilon}}. \]

(10)

where \( \frac{E_0}{\bar{\varepsilon}} \) makes sense and coincides in order of magnitude with the ion free path until it stops or Residual Range, \( l_{tr} \) - ion transport mileage. For proton energies in the range: 1keV < \( E_0 < 30 \)keV:

\[ \sigma^* \approx 1. \]

(11)

Factors \( (1-\Delta)^{5/2} \) and \( (1-\Delta) \) in (9) take into account the dependence of elastic and inelastic cross sections on energy.

Function \( e^{-\frac{\Delta}{\bar{\varepsilon}}} \) in (9) is related to the phenomenon of charge exchange of reflected hydrogen ions [3,4], the constant \( A \) is an adjustable parameter.

Formula (9) was obtained under the assumption that there are no fluctuations in energy losses or other factors leading to a broadening of the energy spectrum. Since all broadening mechanisms: Doppler broadening, broadening associated with the non-monochromaticity of the probing beam and taking into account the instrumental function of the energy analyzer have a Gaussian profile, then taking into account all factors leading to the spread of energy losses can be determined on the basis of convolution:

\[ S_{\text{full}}(\Delta, \mu, \mu_0) = \int_0^\infty d\varepsilon \cdot S(\Delta - \varepsilon, \mu, \mu_0) \frac{1}{\sqrt{2\pi}\sigma_\varepsilon} e^{-\frac{\varepsilon^2}{2\sigma_\varepsilon^2}}, \]

(12)

where \( \sigma_\varepsilon = \bar{\varepsilon}^2 + \sigma_{\text{Dop}} + \sigma_{\text{beam}} + \sigma_{\text{en},\varepsilon} \) - total broadening factor.
Figure 2. Energy spectra of protons with an initial energy of 25 keV, reflected from tungsten. Probing at an angle of 710, viewing angle - 1090, A = 1. Calculation – blue solid line based on formulas (7), (9) and (10), experiment – red circles [10].

Figure 2 shows the experimental [10] and calculated energy spectra of protons reflected from the tungsten array. As mentioned above, the elastic scattering parameters were determined on the basis of the KrC potential [1-3]. The protons stopping power is taken from the NIST tables. The change in stopping power from the value $\bar{\varepsilon} = 137.6$ eV/nm, presented in the NIST data, to the value $\bar{\varepsilon} = 110.1$ eV/nm, leads to the coincidence of the maxima of the calculated and experimental spectra.

The largest number of experimental data on the reflected ions energy spectra falls on the 80s and 90s of the last century [1–3, 10, 11]. Let us consider the results of experiments showing the dependence of the spectral width and the maximum on the target material.

Figure 3 illustrates the qualitative agreement between experimental data and calculations based on formulas (7) and (9). However an exact quantitative agreement is not achieved. The experimental maxima are shifted to the region of high energy losses. The main parameter influencing the position of the maximum is the stopping power $\bar{\varepsilon}$. Calculating the spectra in figure 3, we used $\bar{\varepsilon}$ data on taken from NIST. In order to achieve quantitative agreement with the data of [12], it is necessary to increase the value of $\bar{\varepsilon}$.

3. Conclusions and main results
Calculations based on the method presented in [6, 8] make it possible to describe Reflected Electron Energy Loss Spectrometry (REELS), Elastic Peak Electron Spectroscopy (EPES) and Reflected
Electron Spectra (RES) signals with satisfactory accuracy. The solution of the boundary problem for the elastic transport equation allows us to find the equation for the distribution of reflected atomic particles - Pass Length Distribution Function of reflected ions. Equation (2) obtained for PLDF has a universal and has the same form for both electrons and light ions, the difference concerns only the form of differential cross sections $\chi(\mu, \mu_0)$. It is shown that the maximum of the PLDF function (figure 2) is determined by the scattering geometry and weakly depends on the proton energy. In this work, the method presented in [6, 8] is used to solve (2) and describe the energy spectra of reflected light ions. It is shown that formulas (7) and (9) give a satisfactory description of the energy spectra of reflected protons. It is pointed out that it is inadmissible to use the SLA approximation to describe the energy spectra of reflected protons. Relying on the fact that the elastic scattering cross sections of light ions are much better studied than inelastic, then taking into account the sensitivity of the energy spectrum to the parameter $\sigma^*$, we obtain a technique that allows us to refine the values of $\bar{\varepsilon}$. Verification of the value $\bar{\varepsilon}$ is one of the most important problems in the physics of the light ions interaction with a surface.

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