QUANTUM AND CLASSICAL EFFECTS IN SCATTERING OF RELATIVISTIC ELECTRONS BY CRYSTAL ATOMIC STRING

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The results of investigation of the relativistic electron scattering by a crystal atomic string at a small incident angle to its axis are presented. The possibility of the particle rainbow scattering and orbiting in this case is shown. It is shown that the Ramsauer-Townsend-type effect of the total cross-section decrease for elastic scattering of relativistic electrons by a crystal atomic string can take place at small values of particle incidence angles.

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1. INTRODUCTION

When fast charged particle is incident on a crystal atomic string under a small angle ψ to its axis (z-axis) a correlation between successive collisions of the particle with string atoms are essential. This correlation leads to the fact that the particle motion in the field of the crystal atomic string is determined mainly by continuous potential of the crystal atoms, i.e. by the crystal atomic string potential, averaged over z coordinate [1]. The component of particle momentum parallel to the z-axis is conserved in such field and the scattering of the particle takes place only along the azimuthal angle φ in the plane (x,y), which is orthogonal to the string axis. As a result, we come to the two-dimensional problem of the particle scattering in the plane orthogonal to the string axis. Such problem was considered in connection with the phenomenon of the axial channeling of fast particles in crystals [1-3]. This phenomenon takes place if the angles of particle motion with respect to one of the crystal axes are of the order of value of the critical axial channeling angle $\psi_c = \sqrt{4Ze^2/\varepsilon d}$, where Z is the atomic number of lattice atoms, ε is the particle energy and d is the distance between atoms of the crystal atomic string and e is the electron charge (see, e. g., [1-3]). The main attention was earlier paid to the peculiarities of the positively charged particles scattered in the field of crystal atomic string.

In the present paper we give a short review of the results of the investigation of relativistic electron scattering by a crystal atomic string when a particle incidence angle ψ with respect to the string axis is less or of the order of the critical angle of axial channeling. The analysis of this problem is done for a number of simplest approximations of the atomic string potential. The possibilities of the particle rainbow scattering and orbiting in this case are shown. It is shown that the process of electron scattering changes essentially with decrease of the angle ψ. It is also shown that for $\psi \ll \psi_c$ the problem of relativistic electron scattering by an atomic string is similar in many respects to the problem of slow electron scattering by an atom. In particular, we show that at the relativistic electron scattering by a crystal atomic string an effect can take place, which is similar to the Ramsauer-Townsend effect of the considerable decrease in the total cross-section of slow electrons scattering by an atom (see, e. g., [4-6]).

We discuss also the validity condition for the application of the semi-classical approximation of quantum mechanics for description of the relativistic electron scattering by an atomic string.

2. DEFLECTION FUNCTION AND CROSS-SECTION OF SCATTERING

The continuous potential $U(\rho)$ of the crystal atomic string is a cylindrically symmetrical function of the transverse coordinates $\rho = \sqrt{x^2 + y^2}$. Let us consider the scattering of relativistic electrons in this field when the beam incidence angle to atomic string ψ is small (see Fig. 1).

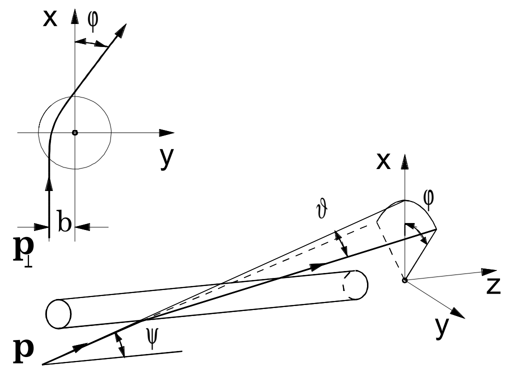


Fig. 1. *Particle scattering in the field of the continuous potential of a single atomic string*

The particle scattering by such field takes place only in the plane orthogonal to the string axis and occurs along the azimuthal angle φ. The total scattering angle ϑ relates to the angle φ by equation

$$\vartheta = 2\psi \sin(\varphi/2) . \tag{1}$$

The quantum differential cross-sections of relativistic electron scattering by a cylindrically symmetrical continuous potential $U(\rho)$ at small angle ψ can be presented as [3]

$$\frac{d\sigma}{d\varphi} = \frac{L\psi}{2\pi\, p_\perp}\left|\sum_{l=-\infty}^{\infty} e^{il\varphi}\left(e^{2i\eta_l} - 1\right)\right|^2 , \qquad (2)$$

where η_l are the scattering phases in the field $U(\rho)$, L is the length of the atomic string and $p_\perp = \varepsilon\psi$ is the transverse component of the particle momentum (we use the system of units where $\hbar = c = 1$). Here the summation is taken over the integer values of the angular momentum in the transverse plane.

The total cross-section of elastic scattering of relativistic electrons by an atomic string is related to the scattering phases η_l by the relation

$$\sigma_t = \frac{4L\psi}{p_\perp}\sum_{l=-\infty}^{\infty} \sin^2\eta_l \, . \qquad (3)$$

In the semi-classical approximation of quantum mechanics the scattering phases η_l are given by [3]

$$\eta_l = \int_{\rho_0}^{\infty} d\rho \sqrt{p_\perp^2 - 2\varepsilon eU(\rho) - l^2\rho^{-2}} - \int_{\rho_0}^{\infty} d\rho \sqrt{p_\perp^2 - l^2\rho^{-2}} \, , \qquad (4)$$

where ρ_0 is the root of the corresponding radical (at l=0 $\rho_0 = 0$).

At $\psi \geq \psi_c$ a large number of terms in Eq. (2) make a comparable contribution to the scattering cross-section. In this case, taking into account the equation $l = p_\perp b$, the summation over l in (2) can be replaced by the corresponding integration over the string impact parameter b (see Fig. 1). In the classical limit ($\hbar \to 0$) Eq. (2) reduces to the corresponding result of the classical scattering theory

$$\frac{d\sigma_{cl}}{d\varphi} = L\psi \sum_n \left|\frac{d\varphi}{db}\right|_n^{-1} , \qquad (5)$$

where $\varphi = \varphi(b)$ is the deflection function of the particle scattering in the field $U(\rho)$ in the plane orthogonal to the string axis. The deflection function $\varphi(b)$ is determined for positive values of b by relation

$$\varphi(b) = \pi - 2b\int_{\rho_0}^{\infty} \frac{d\rho}{\rho^2}\left(1 - \frac{eU(\rho)}{\varepsilon_\perp} - \frac{b^2}{\rho^2}\right)^{-1/2} \qquad (6)$$

and for negative values of b by relation

$$\varphi(b) = -\varphi(|b|) \, . \qquad (7)$$

Here $\varepsilon_\perp = \varepsilon\psi^2/2$ is the energy of a particle transverse motion and ρ_0 is the minimal distance between the particle and the string axis. The summation over n in (5) is taken over single-valued branches of the deflection function with the account of scattering at angles exceeding 180° (see [3,6,7]).

Eqs. (2) and (5) describe the quantum and classical cross-sections of scattering of relativistic particles in the continuous string potential $U(\rho)$. This potential has a rather complicated form. So, approximations of this potential by functions of a simpler form are used to investigate the particle interaction with an atomic string. Let us consider the electron scattering by an atomic string for some approximations of the continuous string potential by the simplest functions.

3. ELECTRON SCATTERING IN COULOMB–LIKE FIELD WITH CUTTING

In the channeling theory the Coulomb-like function $|eU(\rho)| = \alpha/\rho$ is often applied (see [1,3]). Here $\alpha = U_0 a$ (a is the Thomas-Fermi screening radius of the atomic potential) and $U_0 = \pi Ze^2/2d$. For this potential the electron deflection function takes the form

$$\varphi(b) = -2\frac{b}{|b|}\arcsin\left(1 + \left(\frac{2\varepsilon_\perp b}{\alpha}\right)^2\right)^{-1/2} . \qquad (8)$$

The deflection function (8) is a single-valued function of the impact parameter b. The module of this function changes from $|\varphi(b)| = \pi$ at $b \to 0$ down to $|\varphi(b)| \to 0$ for $b \to \infty$. The differential cross-section of scattering (5) for the deflection function (8) takes the form

$$\frac{d\sigma_{cl}}{d\varphi} = \left(\frac{\psi_c}{2\psi\,\sin(\varphi/2)}\right)^2 . \qquad (9)$$

So, the deflection function (8) of an electron in the Coulomb-like continuous string potential $eU(\rho) = -\alpha/\rho$ has the same form as the deflection function of the particle scattering in the Coulomb field of a single atom. But the differential cross-section of scattering (9) differs from the Rutherford cross-section of the particle in the field of an atom. This difference is due to the fact that the scattering in the continuous string potential is the two-dimensional problem of scattering, while the Rutherford scattering is the three-dimensional problem of scattering.

At large and small distances from the atomic string the function α/ρ overestimates the potential. At large distances the string potential decreases due to screening by atomic electrons. Beside this, the string potential must be cut at the distance, which is the half of the average distance between the crystal atomic strings. At small distances due to averaging over the thermal oscillations of string atoms the singularity of the string potential is absent. This leads, in particular, to the possibility of electrons passing through the string axis. Let us investigate the influence of each of these factors on the behavior of the electron scattering by an atomic string.

At large distances the string potential must be cut. In the simplest version it may be done by functions

$$eU(\rho) = \begin{cases} -\alpha\left(\dfrac{1}{\rho}-\dfrac{1}{R}\right), & \rho \le R \\ 0, & \rho > R \end{cases}. \qquad (10)$$

and

$$eU(\rho) = \begin{cases} -\dfrac{\alpha}{\rho}, & \rho \le R \\ 0, & \rho > R \end{cases}. \qquad (11)$$

The distance R can be equated to the half of the distance between the crystal atomic strings. Notice that the function of the form (10) but with another values of α and R was also applied in the studies of the slow electron scattering by an atom (see [4,8,9]).

Functions of the forms (10) and (11) permit sometimes to simplify essentially the calculations. So, the electron deflection function in the field (10) takes the form [10]

$$\varphi(b) = 2\arcsin\left[A\left(1-\frac{b^2}{R^2}+A^2\right)^{-1/2}\right] - 2\arcsin\left(\frac{b}{R}\right), \qquad (12)$$

where $A = \dfrac{b}{R} - \dfrac{R}{b}\dfrac{\psi_g^2}{\psi^2}$ and $\psi_g = \sqrt{\alpha/\varepsilon R}$. The potential (11) yields

$$\varphi(b) = 2\arcsin\left[A\left(1+\left(\frac{R\psi_g^2}{b\psi^2}\right)^2\right)^{-1/2}\right] - 2\arcsin\left(\frac{b}{R}\right). \qquad (13)$$

The functions (12) and (13) transform to the function (8) for $R \to \infty$. For the finite R value at $\psi \le \psi_g$ the functions (12) and (13) are essentially different from the deflection function (8).

The plots of the function $\varphi = \varphi(b)$ for potential (10) and (11) for different values of the particle incidence angle ψ are presented in Figs. 2(a) and 2(b).

The presented plots in Fig. 2(a) show that for $\psi > \psi_g$ the deflection function is a monotone decreasing function of the impact parameter b. When $\psi = \psi_g$ for any impact parameter the scattering angle is $|\varphi(b)| = \pi$. This effect is similar to the giant glory effect in the slow electrons scattering by an atom [11]. For $\psi < \psi_g$ the deflection function is a monotone increasing function of the impact parameter from the value $|\varphi(0)| = \pi$ up to maximum value $|\varphi(R)| = 2\pi$.

Fig. 2(b) shows that in the case of the potential (11) the function $|\varphi(b)|$ has a minimum for $\psi \ge 0.2\psi_c$. It means that the effect of the rainbow scattering takes place in the field (11) for such angles. For $\psi < 0.2\psi_c$ the deflection function is a monotone increasing function of the impact parameter b from the value $|\varphi(0)| = \pi$ up to some maximum value $\varphi_{max}(R) < 2\pi$. Note also that for $\psi \approx 0.2\psi_c$ the function $\varphi(b)$ is close to the constant value $|\varphi(b)| \approx \pi$ in a wide range of impact parameters ($b \le 0.8R$). In other words, in this case for a wide range of impact parameters b particles scatter into the angle $\varphi \approx \pi$.

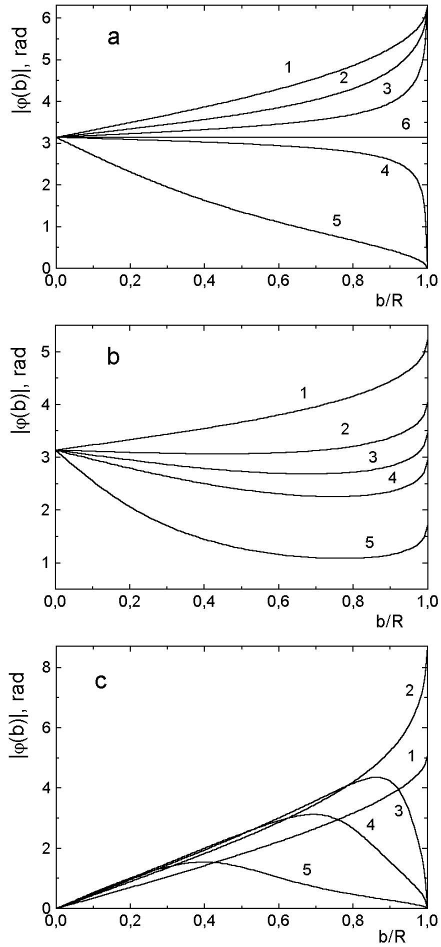


Fig. 2. *Deflection functions $\varphi = \varphi(b/R)$ of electrons, which are scattered on the <100> silicon crystal string in the field (10) (a), in the field (11) (b) and in the field (14) (c) for different values of the angle ψ:*

1 – $\psi = 0.1\psi_c$, 2 – $\psi = 0.2\psi_c$, 3 – $\psi = 0.25\psi_c$, 4 – $\psi = 0.3\psi_c$, 5 – $\psi = 0.5\psi_c$, 6 – $\psi = \psi_g$

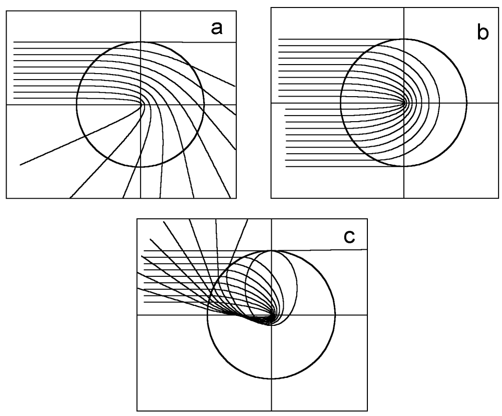


Fig. 3. *Electron trajectories in the plane orthogonal to the <100> silicon crystal string in the field (10) for $\psi = 0.5\psi_c$ (a), $\psi = \psi_g \approx 0.28\psi_c$ (b) and $\psi = 0.2\psi_c$ (c)*

To illustrate the obtained results the typical electron trajectories in the fields (10) and (11) in the plane orthogonal to the string axis for different ψ values are presented in Figs. 3 and 4.

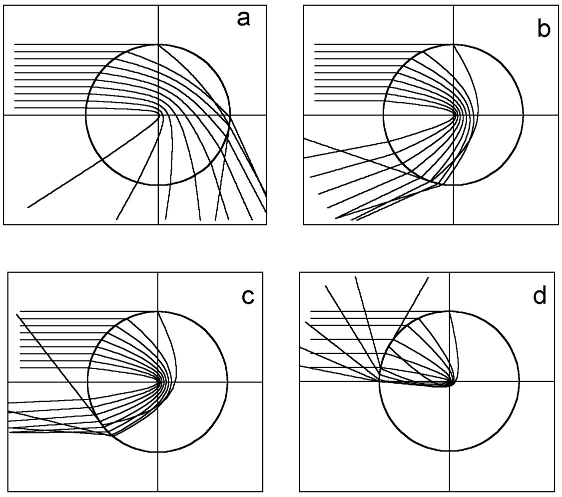


Fig. 4. *Electron trajectories in the plane orthogonal to the <100> silicon crystal string in the field (11) for* $\psi = 0.5\psi_c$ *(a),* $\psi = 0.25\psi_c$ *(b),* $\psi = 0.2\psi_c$ *(c) and* $\psi = 0.1\psi_c$ *(d)*

The obtained results show that the cutoff of the potential α/ρ at large distances from the string axis leads to essential change of the electron scattering pattern for $\psi < \psi_g$ as compared with the case $\psi > \psi_g$. Notice that the value of the angle $\psi_g = \sqrt{\pi a/8R}\psi_c$ is small in comparison with the critical angle of the axial channeling. Besides, the character of the scattering depends not only on the angle ψ but on the form of the atomic string potential also.

4. RAINBOW SCATTERING AND ORBITING

The more exact approximation of the crystal atomic string potential at small and large distances from the string axis is given by the following function [3]

$$eU(\rho) = \begin{cases} U_1 \ln\left(1 + \dfrac{\alpha_1 a^2}{\Delta^2 + \rho^2}\right) - U_2, & \rho \le R \\ 0, & \rho \ge R \end{cases}, \quad (14)$$

where U_1, α_1, Δ and U_0 are determined from the condition of the best approximation of the real crystal atomic string potential by the function (14). For instance, for the silicon crystal atomic string directed along the <100> axis, a good approximation is achieved at U_1 =51.5 eV, U_2 =4.05 eV, α_1=2.035 and Δ=0.119 Å.

Next, consider the characteristic properties of the electron scattering in such field and compare it with some properties of the particle scattering in the fields (10) and (11).

The numerically calculated deflection functions and the typical electron trajectories in the field (14) are shown in Fig. 2(c) and Fig. 5 for different values of the ψ angle.

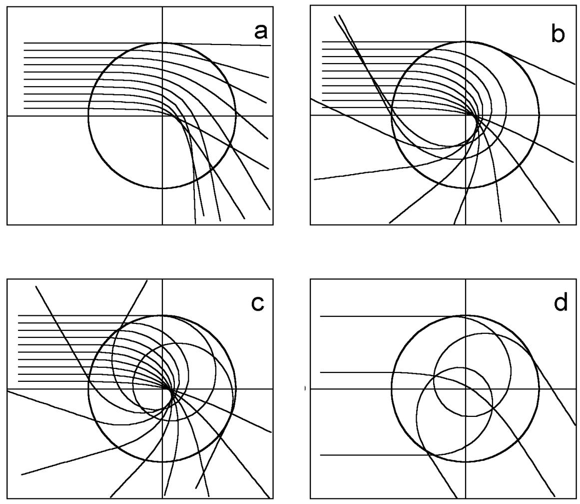
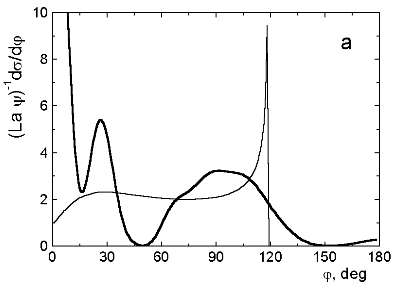


Fig. 5. *Electron trajectories in the plane orthogonal to the <100> silicon crystal string in the field (14) for* $\psi = 0.5\psi_c$ *(a),* $\psi = 0.25\psi_c$ *(b) and* $\psi = 0.2\psi_c$ *(c and d)*

It can be seen that for potential (14), unlike the potentials (10) and (11), $|\varphi(b)| \to 0$ for any value of the ψ angle when $b \to 0$. For $\psi \sim \psi_c$ the electron deflection function in the field (14) has the maximum for some value of the impact parameter. It means that the phenomenon of the electron rainbow scattering by the crystal atomic string takes place in this case, being absent for the potential (10). As shown in Fig. 2(c), the rainbow scattering angle increases with the decrease of ψ, and exceeds 180° for $\psi < 0.3\psi_c$. For the angles $\psi < 0.2\psi_c$ the electron deflection function is a single-valued function of the impact parameter. In this case the deflection angle can exceed 2π (see Fig. 5(c)). It means that the phenomenon of orbiting is possible in this case. (The possibility of the rainbow scattering and orbiting in scattering of fast particle by the atomic string was pointed out in papers [12,13]).

The classical and quantum differential cross-sections of the electron scattering in the field (14) for $\psi = 0.4\psi_c$ and $\psi = 0.2\psi_c$ are presented in Fig. 6 by thin and thick lines respectively. (The differential cross-sections of the electron scattering in the field of the cut Coulomb potential (10) are presented in [10].)

The obtained results show that at $\psi = 0.4\psi_c$ the phenomenon of the particle rainbow scattering takes place. In this case there exists the maximal scattering angle value $\varphi = \varphi_r$, above which the electron scattering according to the classical theory is absent. In the region of the scattering angles $\varphi < \varphi_r$ the deflection function is two-valued. According to this, the particle scattering at the angle φ can take place along the two classical trajectories determined by two different values of the impact parameter. For $\varphi \to \varphi_r$ the classical cross-section of scattering increases infinitely, because the function $d\varphi / db$ tends to zero at $\varphi \to \varphi_r$. The quantum cross-section oscillates with respect to the classical one in the region $\varphi < \varphi_r$ and in the region $\varphi > \varphi_r$ decreases rapidly when φ increases.



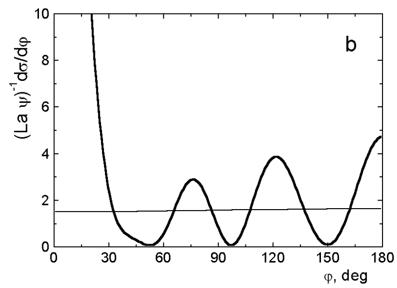


Fig. 6. *Scattering differential cross-section for 20 MeV electron, incident on the silicon crystal string <100> at the angle $\psi = 0.4\psi_c$ (a) and $\psi = 0.2\psi_c$ (b). Thin line corresponds to calculation using the equation (5) of the classical theory of particle scattering, thick line corresponds to calculation using the equation (2) of the quantum theory of particle scattering*

The phenomenon of the rainbow scattering is absent for $\psi = 0.2\psi_c$. In this case the particle can be deflected by the atomic string at the angle φ, exceeding 180°. The scattering angle φ for electron can change, however, in the range $\pi \geq \varphi \geq -\pi$. Therefore, for $|\varphi(b)| > \pi$ there exist several trajectories, leading to the scattering at the given angle φ. In this case the situation similar to the one considered in [6] for slow electron scattering by an atom may arise when the impact parameter *b* of the trajectories leading to the scattering at the given angle φ could be both positive and negative (see Fig. 5(d)). In this case the quantum scattering cross-section oscillates with respect to the classical one. These oscillations are similar to the oscillations observed in the generalized Ramsauer-Townsend effect for slow electron scattering by an atom at large angles [4-6]. They are due to the fact that at small ψ the main contribution to the cross-section (2) comes from several first terms with low index values *l*.

5. RAMSAUER-TOWNSEND-TYPE EFFECT FOR TOTAL CROSS-SECTION OF ELECTRON SCATTERING BY ATOMIC STRING

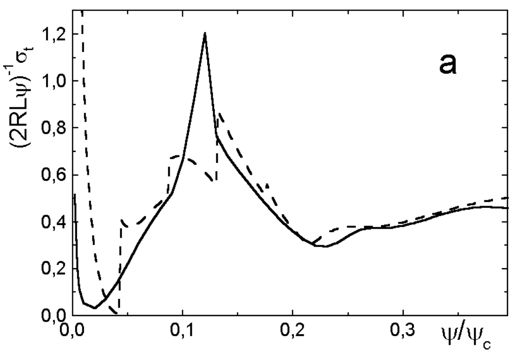
Let us discuss the orientation dependence of the total cross-section of elastic electron scattering by the atomic string.

In the classical theory the total cross-section of elastic electron scattering by the field of the atomic string, the potential of which $U(\rho)$ is cut at distances $\rho \geq R$, is determined by the relation

$$\sigma_{cl} = 2RL\psi . \qquad (15)$$

This magnitude is the square of the atomic string potential projection on the orthogonal to the incidence particle momentum plane.

According to Eq. (3) for determination of the total quantum cross-section of elastic scattering one has to know the scattering phases η_l. In the semi-classical approximation of quantum mechanics the scattering phases are determined by relation (4). The semi-classical dependence of the total cross-section on incident angle for electron scattering by atomic string is presented in Fig. 7 by dashed line. The calculations were done for 15 MeV and 25 MeV electrons.



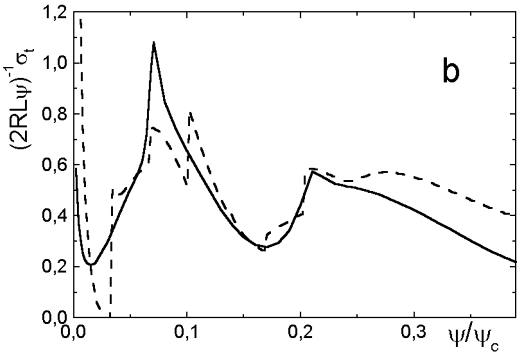


Fig. 7. *Total elastic scattering cross-section for electron energy 15 MeV (a) and 25 MeV (b) by the silicon crystal string <100> as function of the incident angle ψ*

The results of calculation show that the cross-section has a very complicated structure in the range of small ψ. The sharp changes of the cross-section are caused by successive dropping out of the individual terms from the sum over *l* in (3) with decreasing ψ. For $\psi \to 0$ the term only with $l = 0$ contributes to the cross-section.

However, the semi-classical formula (4) for scattering phases η_l becomes inconsistent at small l values. For determination the phases of scattering in this case the method of phase function for cylindrically symmetric potential may be used [14,15]. The corresponding calculations of the total cross-section, based on the phase function method, are presented in Fig. 7 by solid line.

The obtained results show that the total cross-section has a deep minimum in the range of small ψ values. This effect is similar to the Ramsauer-Townsend effect of the total cross-section decreasing of slow electron scattering by an atom in a certain range of particle energies [4,5]. In the considered case the effect takes place for relativistic electrons and depends not only on the electron energy (see Fig. 7) but also on the angle of particle incidence on the atomic string as well.

Notice in conclusion that the results that are presented in Fig. 6 by thick line and by dashed line in Fig. 7 are obtained in the quasi-classical approximation of the quantum scattering theory when the scattering phases are determined by Eq.(4). Unlike the case of slow electrons scattering from an atom, these scattering phases contain the relativistic particle energy instead of electron mass. Therefore, the condition imposed by the quasi-classical approximation can be written in our case as [16]

$$\frac{\varepsilon F}{p_\perp^3} << 1 \ , \qquad (16)$$

where F is the force acting on the particle in the atomic string field. Estimating that $F \sim U_0 4a/d^2$, the inequality (16) can be rewritten in the form

$$\frac{U_0}{\varepsilon_\perp}\frac{1}{p_\perp d}\frac{a}{d} << 1 \qquad (17)$$

For ε=10 MeV this inequality is satisfied for the crystal atomic string of silicon even for $\psi \sim 0.2\psi_c$.

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