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Neutrons planar channeling in crystals

K. B. Korotchenko(1)(*) and Yu. P. Kunashenko(1)(2)

(1) *Department of Theoretical and Experimental Physics TPU - Lenin Ave. 30, 634050 Tomsk, Russia*
(2) *Department of Theoretical Physics, TSPU - Kiivskaya Str. 60, 634046 Tomsk, Russia*

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Summary. — The possibility of neutron planar channeling is theoretically investigated. It is shown that stable channeling appears only for relativistic neutrons with relativistic factor greater than 5. The energy bands and its population are calculated for the different neutron energies and entrance angles.

PACS 25.40.Dn – Elastic neutron scattering.
PACS 61.85.+p – Channeling phenomena (blocking, energy loss, etc.).
PACS 03.65.-w – Quantum mechanics.

1. – Introduction

During the passage of relativistic charged particles through an oriented crystal channeled phenomena take place [1-3] and their interaction with a crystal can be described by the continuous (averaged) potential of the crystal plane or axis. It is convenient to divide the motion of a channeled particle into transverse motion (in the direction perpendicular to the crystal plane or axis) and longitudinal motion (in the direction parallel to the crystal plane or axis). When the transverse motion is bounded, then the channeled particle has transverse discrete energy levels.

The neutron does not have an electric charge, but Schwinger [4] predicted that fast neutrons, due to their spin (and anomalous magnetic moment) can be scattered by electric field of the atomic nuclei (atom). The physics of this scattering is explained in the following way: in the neutron rest frame the magnetic field appears and the neutron (anomalous) magnetic moment interacts with it. The electromagnetic Schwinger scattering of fast neutrons was experimentally discovered in 1956 [5].

The velocity of the neutron can be separated into two components: parallel to the crystal plane (transverse) $v_{||}$ and perpendicular to ones (longitudinal) $v_{\perp}$. Ordinary the longitudinal velocity $v_{||}$ is greater than the transverse one $v_{\perp}$. In a frame, which moves

(*) E-mail: korotchenko@tpu.ru

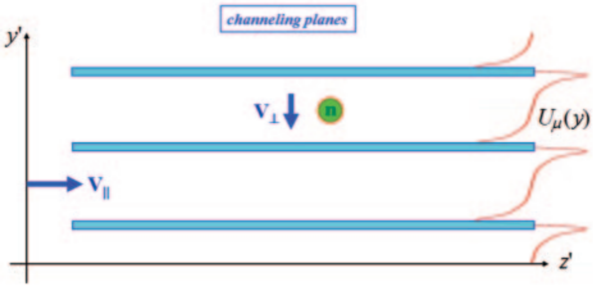

Fig. 1. – Scheme of channeling of neutrons.

with longitudinal neutron velocity $v_{||}$ (comoving frame) the neutron has only transverse velocity $v_\perp$. According to the Lorentz transformation in a comoving frame the magnetic field appears. Due to interaction with the magnetic field the energy of the neutron (in a comoving frame) can be quantized and the neutron is captured into a bounded state in the averaged field of crystal axis or plane. Figure 1 shows the scheme of the neutron channeling. The arrows indicate the transverse velocity $v_{||}$ in the laboratory frame and the longitudinal, $v_\perp$, neutron velocities; $\theta_0 = \mathrm{Arctan}(v_{||}/v_\perp)$ is the initial incidence angle of the neutrons. The thick horizontal lines denote the crystal planes and the thin line is the crystal potential for the neutron in a comoving frame.

Earlier a similar problem was considered in [6, 7], where it was shown that due to the small energy of the neutron interaction with the magnetic field of a crystal in a comoving frame the bound states of neutrons are absent. Later the result of papers [6, 7] were confirmed in the frame of the relativistic quantum theory (based on the Dirac equation) [8]. In the present paper we used a more accurate approximation for the continuous crystal planar potential. In order to have a more brilliant effect we choose (110) Ta, which has the deepest potential well.

2. – Neutron motion equation

In order to obtain the equation which describes neutron channeling, we use the standard equation for particle channeling [3], but instead of the continuous potential of the crystal plane we used the interaction energy of the anomalous magnetic moment of the neutron with the magnetic field which appears in a comoving frame. This equation has the same accuracy as the equation used in [8].

In a comoving frame the neutron motion is non-relativistic, and its motion between crystals planes can be described by the Schrödinger equation (the direction of longitudinal neutron velocity is coincident with the OZ-axis)

$$\left[\frac{\hat{p}_\perp^2}{2m_n} + \gamma U_\mu(y)\right]\phi_n(y, k_y) = E_n(k_y)\phi_n(y, k_y), \tag{1}$$

where m_n is the neutron mass, $U_\mu(y)$ is the neutron continuous crystal potential [1-3], $\phi_n(y, k_y)$ is the wave function of the neutron transverse motion, $E_n(k_y)$ is the egenvalue of neutron energy, k_y is the wave vector of the neutron in the first Brilluion zone, $\hat{p}_\perp$ is the momentum operator and γ is the relativistic factor of the neutron longitudinal motion. For the construction of the interaction energy we use the approximation for the single atomic potential [9] in the form

$$eU_{At}(\vec{r}) = -(2\hbar^2/\sqrt{\pi}m_e)\sum\nolimits_j a_j c_j^{-3/2}\exp(-r^2/c_j), \tag{2}$$

where a_j and $b_j = 4\pi^2 c_j$ are coefficients obtained by fitting the electron atomic form factor by 6 points (as opposed to 4 points in the standard model), $r^2 = x^2 + y^2 + z^2$. One can obtain the continuous potential $U_0(y)$ by integration of (2) over the coordinates x and z. The obtained crystal plane potential must be a sum taking into account crystal symmetry.

In a comoving frame due to Lorentz transformation the magnetic field should be written in the form

$$\vec{B}(y,\gamma) = \sqrt{\gamma^2 - 1}\,(-E_y(y), E_x(y), 0)\,, \tag{3}$$

where $\vec{E}(y) = -\vec{\nabla}U_0(y)$ and

$$U_\mu(y,\gamma) = \vec{\mu}_n\vec{B}(y,\gamma), \tag{4}$$

where $\vec{\mu}_n$ is the anomalous magnetic moment of the neutron. Here we wish to stress that in a comoving frame the interaction energy depends on the relativistic factor of the neutron longitudinal motion γ: $\gamma U_\mu(y) \Rightarrow U_\mu(y,\gamma)$. Since the function $U_\mu(y,\gamma)$ is periodical, then one can expand it into Fourier series [10]:

$$U_\mu(y,\gamma) = \sum_m U(g_m,\gamma)\exp\left[ig_m y\right], \tag{5}$$

where g_m is the lattice reciprocal vector perpendicular to the crystal plane (XZ-plane). The transverse wave function $\phi_n(y,k_y)$ should be a Bloch function:

$$\phi_n(y,k_y) = \sum_m C^n(g_m,k_y)\exp\left[i(k_y+g_m)y\right]. \tag{6}$$

Here n is a quantum number which describes the neutron energy in a comoving frame and $C^n(g_m,k_y)$ is the Fourier expansion of the wave function [10]. After substitution of (5), (6) into eq. (1), the differential equation is reduced to the standard algebraic eigensystem problem [11, 12]:

$$\sum_m A_{mn}C^n(g_m,k_y) = E^i(k_y)C^i(g_n,k_y). \tag{7}$$

Here, the following notations are introduced: $A_{mn} = U_{mn} + \delta(m,n)(\hbar^2|g_m + k_y|^2/2m_n)$, $U_{mn} = U(g_m - g_n,\gamma)$ is the Fourier expansion of the interaction energy, and $\delta(a,b)$ is the Kronecker delta.

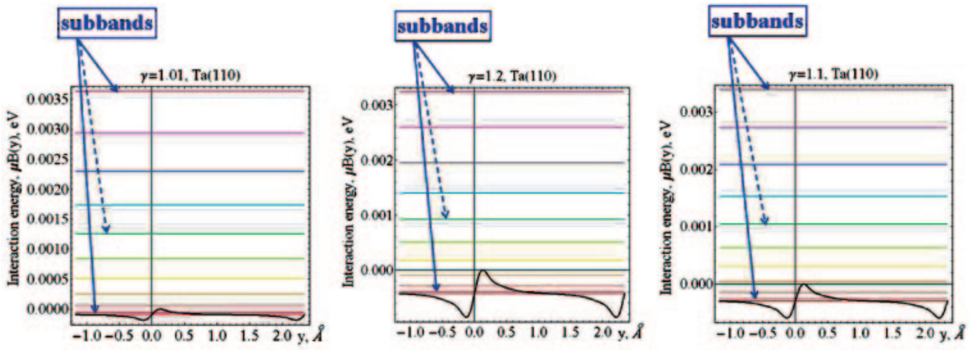

Fig. 2. – Positions of the energy sub-bands of the first energy band for (110) neutron channelling in Ta.

3. – Results of calculations

Equation (7) was solved with the help of the Mathematica© 7.0 package, as a result we obtained the allowed transverse neutron energies, the corresponding wave functions and the initial populations. The transverse neutron energies are the energy bands, as it should be for any periodic potential. In order to have more detailed information about the energy bands, during the calculation the wave vector k_y in the first Brillouin zone was divided into 10 equal parts. Therefore, a neutron energy band was divided into 11 sub-bands.

In the calculations (in analogy with the case of charged-particles channeling) for neutrons we introduce the critical angle of channeling $\theta_L = \sqrt{\Delta U_\mu(y,\gamma)|_{\max}/E_n}$, where $\Delta U_\mu(y,\gamma)|_{\max}$ is the maximal interaction energy, E_n is the total neutron energy.

In fig. 2, the positions of the energy sub-bands of the 1st energy band for (110) channeling in Ta are shown for three values of the neutron relativistic factor γ.

One can see that only few sub-bands of this first energy band are the sub-barrier ones. These bellow-barrier sub-bands are the channeled states of the neutron. With a small increase of the relativistic factor, the number of sub-barrier sub-bands increases from 2 for $\gamma = 1.05$ up to 4 for $\gamma = 1.2$, with a total number of sub-bands 11 equal to.

The probability of neutron capture in this energy states determines the possibility of the channeling of fast neutrons. The results of the calculation the initial populations for (100) channeling in Ta is shown on fig. 3. The probability of neutron capture on any of the first of the sub-bands does not exceed 0.04% and remains virtually unchanged up to the critical angle of channeling $\theta_0 = \theta_L$ (therefore, the populations are normalized to each initial angle independently).

The calculations show that up to a neutron relativistic factor $\gamma \approx 5$ the probability of neutron capture into the channeling regime remains the same.

This picture changes with further increase of the relativistic factor γ. In fig. 4, the energy bands $E^i(k_y)$ of the relativistic neutrons transverse motion for the (110) channeling in Ta are shown for two values of the neutron relativistic factors: $\gamma = 10$ and $\gamma = 50$. At $\gamma = 10$, only the first energy band and three sub-bands of the second band are the sub-barrier ones, while at $\gamma = 50$ there appear three sub-barrier bands. One may that a well-pronounced isolated sub-barrier energy appears at $\gamma = 50$. In both cases, remarkable gaps between bands are seen.

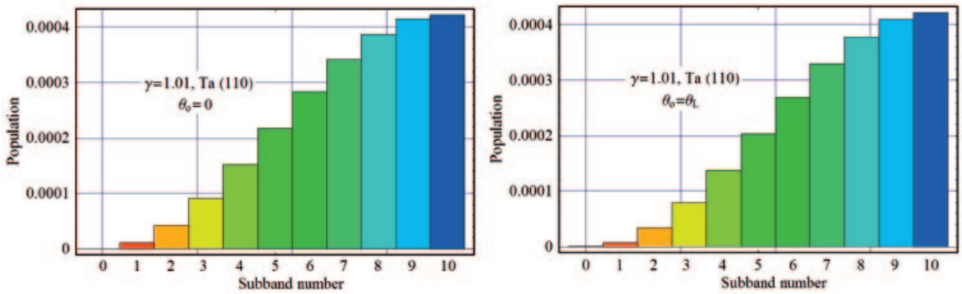

Fig. 3. – Population of the sub-bands of the first energy band for the neutron channelling in (110) Ta, for $\gamma = 1.01$ and for two values of angle of incidence: $\theta_0 = 0$ (left) and $\theta_0 = \theta_L$ (right).

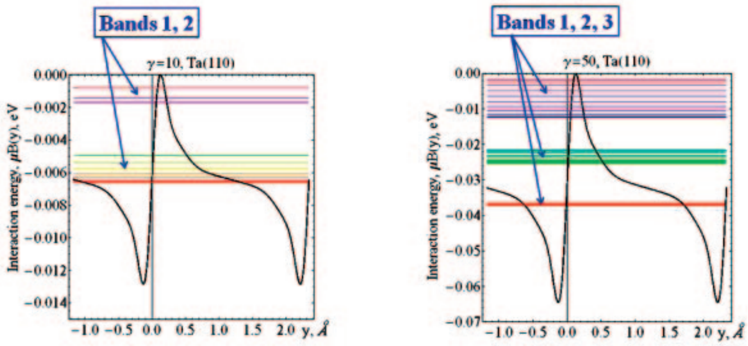

Fig. 4. – Relativistic neutrons channeling in (110) Ta: potential and schematic of transverse energy bands for $\gamma = 10$ (left) and $\gamma = 50$ (right).

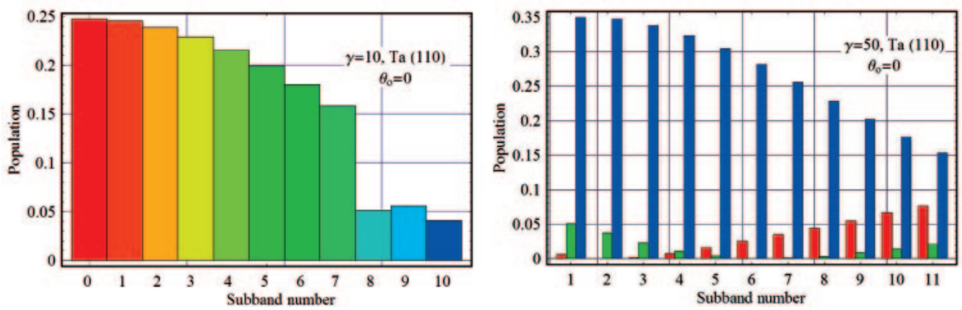

Fig. 5. – Population of the sub-bands of the sub-barrier energy bands for the neutron channelling in (110) Ta, for $\gamma = 10$ (1 sub-barrier band) and $\gamma = 50$ (3 sub-barrier bands).

Figure 5 shows the calculated results for initial populations of sub-bands for relativistic neutrons for $\gamma = 10$ and $\gamma = 50$ (populations are normalized to all sub-barrier bands for all initials angles $\theta_0 \in (0, \theta_L)$). The total population (average) for each of the sub-barrier bands equals:

– $\gamma = 10 : 0.954078$, the 1st band;

– $\gamma = 50 : 0.443245$, the 1st; 0.123699, the 2nd and 0.43221, the 3rd band.

4. – Conclusion

The results of the numerical calculations presented in this paper can be summarized as follows:

– The transverse energies of planar channeled neutrons are energy bands.

– In the crystal, the channeling of the neutrons can occur only for relativistic energies, *e.g.* in a Ta crystal for relativistic factor $\gamma \geq 1$. The probability of the neutrons capture into the channeling state in this case is close to unity, if the angle of incidence $= 0$.

– In the case of non-relativistic neutrons with $\gamma \approx 1$ only a small part of the neutrons transverse energy bands are sub-barrier ones. The probability of the neutrons capture into the channeling states in this case is negligibly small.

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