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БИБЛИОТЕКА

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Некоторые эффекты в дифракции нейтронов на идеальных монокристаллах в приближении одномерного периодического потенциала

Приведены новые выражения для амплитуд отражения и прохождения нейтронов при рассеянии на одномерном периодическом потенциале. Рассматривается взаимодействие нейтрона с идеальным кристаллом в случае Лауэ. Показывается, что при учете гравитационного поля и при ограничении падающего пучка на входной поверхности щелью его интенсивность на выходной поверхности можно варьировать с помощью неоднородного магнитного поля, если падающие нейтроны поляризованы, а рассеивающий кристалл - не магнитен. Показывается также, что если нейтрон падает на поверхность кристалла под углом полного отражения, то при вращении кристалла вокруг нормали к входной поверхности можно при определенных условиях наблюдать уменьшение интенсивности отраженного пучка.

Работа выполнена в Лаборатории нейтронной физики ОИЯИ.

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Some Effects in Neutron Diffraction on Ideal Monocrystals in the One-Dimensional Periodic Potential Approximation

New expressions for the amplitudes of reflection and propagation of neutrons scattered on a one-dimensional periodical potential are reported. We consider an interaction of the neutron with an ideal crystal in Laue case. It is shown that taking into account the gravitational field and placing a collimating slit in front of the incident surface the intensity of the beam on the exit surface can be varied by means of a nonhomogeneous magnetic field under condition that the incident neutrons are polarized and the scattering crystal is nonmagnetic. It is shown also that under certain conditions one may observe a decrease of the intensity of reflected beam with rotation of the crystal about a normal to incident surface, if the neutron angle of incidence on the crystal surface is an angle of total reflection.

The investigation has been performed at the Laboratory of Neutron Physics, JINR.

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A one-dimensional periodic potential is used as a model for many problems in solid state physics and optics. Its solution is reduced to a solution of the Matheu [1-2] or Hill equations and is represented by functions satisfying the Bloch theorem [4], known as Floque theorem in mathematics. But in practice it is solved either in the two-wave approximation or with the help of recursion relations [6]. In the latter case a periodic potential is considered to be a multilayer system and the amplitudes of reflection r and transmission t of one layer are supposed to be known. In that way the reflection amplitude from a half-infinite multilayer system [6] and the reflection and transmission amplitude for finite number of layers [7-10] have been found. Nevertheless, the solutions are unknown to most physicists working with periodic potentials due to their rather complicated forms. In the present paper these expressions will be represented in a form that appears to the author to be most simple. This form offers the possibility of predicting some effects in crystal diffraction which have not been pointed out in neutron physics till now. One of them can be easily predicted within the dynamical diffraction Ewald theory, while the other cannot be clearly seen. The reflection amplitude R_n of n similar layers of arbitrary form is expressed with the help of the recursion relation

$$R_n = [r + (t^2 - r^2) \cdot R_{n-1}]/(1 - r \cdot R_{n-1}),$$

where R_{n-1} is the reflection amplitude of $(n-1)$ layers. Here we suppose that every layer is symmetric about the centre. If it is not so, then the amplitudes of reflection from the left and the right, $r^{\pm}$, are not equal to each other, but they can be represented as $r^{\pm} = r \cdot \exp(\pm i\eta)$, where the phase η is equal to zero for symmetrical potentials. The same relation with the same phase holds for the reflection amplitudes $R_n^{\pm}$ /11/. The transmission amplitudes $t^{\pm}$ and $T_n^{\pm}$ (for n layers) are always equal and may be denoted t and T_n, respectively.

For $n \to \infty$ the recursion relation becomes an equation for $R = R_{\infty}$ which is reduced to algebraic second-order equation of the type: $x^2 - 2px + 1 = 0$. The solution of this equation can be represented as

$$R = (\sqrt{a_+} - \sqrt{a_-})/(\sqrt{a_+} + \sqrt{a_-}), \quad a_{\pm} = (r \pm 1)^2 - t^2. \tag{1}$$

The other solution is equal to $1/R$. The expression (1) is very similar to that for the Fresnel coefficient for the reflection of light. In order to determine R_n for finite n it is useful to represent R_n as ratio p_n/q_n and rewrite the recursion relation as a matrix equation for the two-dimensional vector $\xi_n = (p_n, q_n)$. The solution /12/ of this matrix equation is

$$R_n = R[1 - \exp(2iqL)]/[1 - R^2 \exp(2iqL)], \tag{2}$$

where $L = n\ell$, ℓ is the period of the system, and q is the Bloch quasimomentum, which satisfies the equation /13/ $t^2 - r^2 + 1 = 2t\cos q\ell$ in accordance with the Floquet-Bloch theory, and which can also be represented in a form similar to the Fresnel coefficient

$$\exp(iq\ell) = (\sqrt{b_+} - \sqrt{b_-})/(\sqrt{b_+} + \sqrt{b_-}); \quad b_{\pm} = (t \pm 1)^2 - r^2. \tag{3}$$

The expression for R_n is similar to that for the reflection amplitude for a rectangular barrier potential. The same can be said about the transmission amplitude

$$T_n = \exp(iq\ell)(1 - R^2)/[1 - R^2 \exp(2iq\ell)]. \tag{4}$$

The preceding results are applicable to the propagation of arbitrary scalar waves in periodic media.

Now let us consider an ideal one-dimensional crystal and a neutron interacting with it. The potential may be taken as

$$v(z) = 2p \sum_n \delta(z - n\ell),$$

where $2p = 4\pi N_s b$, N_s is the density of atoms in a crystal plane, and b is the coherent neutron scattering amplitude for one atom. Then, in the above expression we must put

$$a_+ = k + p \cdot \mathrm{tg}\phi, \quad a_- = k - p\,\mathrm{ctg}\phi,$$
$$b_+ = k\,\mathrm{ctg}\phi + p, \quad b_- = k \cdot \mathrm{tg}\phi - p, \tag{5}$$

where $\phi = k\ell/2$ and k is the z-component of the incident neutron wave vector. The equation for q has a well known form

$$\cos(q\ell) = \cos(k\ell) + (p/k)\sin(k\ell).$$

It follows from this equation that the total or Bragg reflection takes place when $k^2 < u_0$ or $k_n^2 < k^2 < k_n^2 + 2u_0$, where $k_n = \pi n/\ell$, $u_0 = 4\pi N_0 b$ and N_0 is the number of atoms in a unit volume.

It is important to note that the wave function inside the crystal may be written in the form

$$\psi = \sum_n \exp(iqz_n)\psi_n(k, z)\theta(z \in I_n), \tag{6}$$

where θ is the function equal to unity inside the interval $I_n = (z_n - \ell/2, z_n + \ell/2)$, $z_n = (n + 1/2)\ell$, and zero outside it, and

$$\psi_n(k, z) = \exp[ik(z - z_n)] + R(k)\exp[-ik(z - z_n)]. \tag{7}$$

Of course the expression (6) may be represented in the Bloch form: $\exp(iqz)f(z)$, where $f(z)$ is the periodic function with period ℓ, but for us it will be more convenient to handle it as in (6).

Now let us discuss the physical effects mentioned at the beginning of this paper. Let us consider neutron diffraction by an ideal crystal in the Laue case. The interaction of the neutron with the crystal is described by the potential

$$v(\vec{r}) = 2p\theta(0 < z < H) \sum_{n=-\infty}^{\infty} \delta(x - (n + 1/2)\ell),$$

where H is the crystal thickness. The incident neutron may be described by the plane wave $\exp(i\vec{k}\vec{r})$ with k_x approximately equal to $k_1 = \pi/\ell$. It is well known that inside the crystal there appear two waves which we represent in the form

$$A_j \sum_{n=-\infty}^{\infty} \exp(ik_x \cdot x_n)\psi_n(q_{jx}, x)\theta(x \epsilon I_n)\exp(iq_{jz} z); \quad j = 1,2, \quad (8)$$

where A_j are the constants that are determined by the boundary conditions, $I_n = (x_n - \ell/2, x_n + \ell/2), x_n = n\ell$, $\psi_n(q_{jx}, x)$ is given by (7), $q_{jz} = \sqrt{k^2 - q_{jx}^2}$ and q_{jx} satisfies the equation

$$\cos k_x \ell = \cos(q_{jx}\ell) + (p/q_{jx})\sin(q_{jx}\ell). \quad (9)$$

The solutions of this equation lie outside the total reflection interval $(k_n^2, k_n^2 + 2u_0)$ for all k_x^2 as is shown in *fig. 1*. When k_x^2 approaches k_n^2 then q_{jx}^2 tends to the boundaries of this interval from the left and right, respectively. The coefficients A_j are determined from the boundary conditions at $z=0$. The boundary conditions at $z=H$ determine the amplitudes of the transmitted and diffracted transmitted waves to be equal to

$$A_1\exp(iq_{1z}H) + A_2\exp(iq_{2z} \cdot H),$$

$$A_1R_1\exp(iq_{1z}H) + A_2R_2\exp(iq_{2z}H). \quad (10)$$

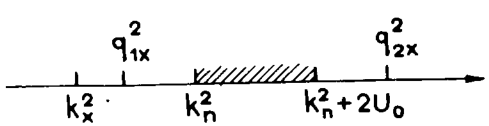

Fig. 1. Relative positions of k_x^2 and q_{jx}^2 in Laue diffraction.

These amplitudes oscillate when H or the total energy of the neutron are varied. Suppose that the x-axis is vertical in the earth's gravitational field.,and area illuminated by the incident neutrons is limited by a slit.

Let us denote $k_x^2 - k_n^2 = \Delta$, then for $||\Delta| << u_0$, we have

$$k_n^2 - q_{1x}^2 = q_{2x}^2 - k_n^2 - 2u_0 = \sqrt{u_0^2 + \Delta^2} - u_0 \approx \Delta^2/2u_0. \quad (11)$$

The neutrons entering the crystal are accelerated in the gravitational field, and those moving downwards and having q_{1x}^2 will eventually approach the total reflection interval $(k_n^2, k_n^2 + 2u_0)$. Below some limiting level (*fig. 2*) they cannot propagate due to total (Bragg) reflection. The neutrons moving upwards with q_{2x}^2 will be totally reflected at a certain level A, where q_{2x} reaches the interval of total reflection from the right. The effect described here is analogous to the negative resistance in superlattices. Now, since in every direction only one wave can propagate beyond levels A,B the pandellosung effect disappears in the exterior region. It can be

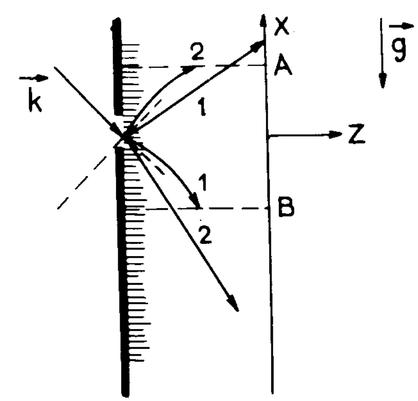

Fig. 2. Propagation of waves inside the crystal, gravitation being taken into account.

restored by an inhomogeneous magnetic field if polarized neutrons are used. If we have a silicon crystal, then u_0 corresponds to ~ 100 *neV*, and if $h^2\Lambda/2m$ is nearly 10 *neV*, then $(\Lambda^2/2u_0)h^2/2m \sim 0.5$ *neV*, and the distance $AB \sim 1$ *cm*, since 1 *neV* is equivalent to ~ 1 *cm* for the neutron in the gravitational field. For compensation it is necessary to give a magnetic field with a gradient of nearly 170 *gauss/cm*. The coefficients $A_{1,2}$ in (8) are found from the matching of (8) with the incident wave on the surface $z = 0$:

$$A_{1,2} = 1/(1 + R^2_{1,2}),$$

where $R_{1,2}$ are the reflection amplitudes in the expression (7) for a wave vector equal to $q_{1,2x}$. The approximate expressions for them are well known:

$$R_{1,2} = \pm u_0/(\sqrt{u_0^2 + \Lambda^2} + \Lambda), \quad R_2 = -1/R_1$$

Now let us consider the other effect: Laue diffraction in combination with total reflection. If a neutron falls on a crystal with $k_z^2 < u_0$, then it will usually be totally reflected. However this is not the case when the crystal is oriented in such a way that k_x^2 is nearly k_n^2. In this case the reflected intensity is smaller than the incident intensity, since some of the intensity can propagate inside the crystal and some is back diffracted. The amplitudes of specular reflection ρ_1, back reflection ρ_2 and the coefficients $A_{1,2}$ are for a crystal semi-infinite in z direction as follows:

$$\begin{aligned}
\rho_1 &= [(k_{2z} + q_{2z})(k_{1z} - q_{1z}) + R^2(k_{2z} + q_{1z})(k_{1z} - q_{2z})]/Q, \\
\rho_2 &= 2Rk_{1z}(q_{2z} - q_{1z})/Q, \\
A_1 &= 2k_{1z}(k_{2z} + q_{2z})/Q, \\
A_2 &= -2R\cdot k_{1z}(k_{2z} + q_{1z})/Q, \\
Q &= (k_{2z} + q_{2z})(k_{1z} + q_{1z}) + R^2(k_{2z} + q_{1z})(k_{1z} + q_{2z}), \\
R &= R_1,
\end{aligned} \tag{12}$$

where $k_{1z} = k_z$, $k_{2z} = \sqrt{k^2 - (k_x - 2k_n)^2}$

and $k_n = \pi/\ell$. When $k_x = k_n$, then $k_{1z} = k_{2z} = q_{1z} = k_z$; $R = 1$; $\rho_1 = r/2$; ; $\rho_2 = -r/2$; ; $A_1 = A_2 = 1/2$; ; and

$$r = (k_z - iq''_{2z})/(k_z + iq''_{2z}), \quad q''_{2z} = \sqrt{2u_0 - k_z^2}.$$

If the crystal is rotated about the normal to the entrance surface, one may observe dips in the reflected intensity. The same effect takes place if k_z^2 lies inside the zone $\tilde{k}_m^2 + u_0 < k_z^2 < \tilde{k}_m^2 + 3u_0$, where $\tilde{k}_m = \pi m/\tilde{\ell}$ and $\tilde{\ell}$ is the distance between the crystalline planes parallel to the entrance surface. It is necessary to note, that the zone of the Bragg reflection is shifted through u_0 due to the existence of crystalline planes perpendicular to the entrance surface. The dip width measured in terms of $\Delta = k_x^2 - k_n^2$ is approximately equal to u_0. The above considerations may be generalized to the case where the crystalline planes are inclined with respect to the entrance surface. The last two effects can be easily found with the help of the ordinary Ewald theory of the dynamical diffraction if one matches the wave function on the interface more carefully than it has been usually done. This matching had been done in paper /14/, but the effects were not pointed out since the authors were interested in the influence of such matching on the pandellosung fringes only.

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