Pis'ma v ZhETF, vol. 85, iss. 1, pp. 90 – 93

Neutron Laue diffraction in a weakly deformed crystal at the Bragg angles close to $\pi/2$

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Submitted 8 November 2006

Resubmitted 4 Desember 2006

An essential magnification of an external force acting on a diffracting neutron for the Bragg angles θ_B close to the right one is observed. Any external action (caused by either crystal deformation or external force affected the neutron) results in a bend of so called "Kato trajectories" inside the crystal and, for the case of finite crystal, gives a considerable variation of the intensities of both diffracted neutron beams (direct and reflected). It is shown that the magnification factor is proportional to $\tan^2(\theta_B)$ and can reach (10^2-10^3) for Bragg angles sufficiently close to 90°.

PACS: 14.20.Dh, 61.12.Gz

1. Introduction. The propagation of neutrons or X-rays in an elastically deformed crystal essentially differs from that in the undeformed one [1 – 3].

There is a well known effect of diffraction enhancement when a small variation of incident beam direction leads to considerable deflection of the neutron trajectory inside the crystal. The neutron in the crystal changes the momentum direction by the angle of $2\theta_B$ (of several tens degrees) while the incident neutron beam deflects by the Bragg width (within a few angle seconds)[4]. Here we propose to utilize this effect for measuring a neutron charge [5] and for investigation of gravitational properties of neutron falling in the Earth field [6].

The influence of a gravity on a neutron diffraction in a deformed single crystal was first observed in the work ref. [3].

Recently the essential slowing down of the neutron passing through the crystal for Bragg angles close to $\pi/2$ was measured [7]. From the general point of view any effect concerning the change of the neutron energy during the diffraction should depend on the time of neutron staying in crystal, so we expect a considerable increasing of diffraction sensitivity to small variations of neutron energy for Bragg angles close to the right one.

It is known, that external field affecting the diffracted neutron is equivalent to some kind of elastic crystal deformation, see [6, 3]. So, at the first stage, we have carried out a simple test, how a small elastic crystal deformation influence a neutron Laue diffraction for the Bragg angles close to $\pi/2$.

2. Neutron trajectories in a deformed crystal. Here we will consider a symmetrical Laue diffraction scheme in a transparent crystal with the system of crystallographic planes described by the reciprocal lattice vector $\mathbf{g}$ normal to the planes (see Fig.1), $g = 2\pi/d$, d is

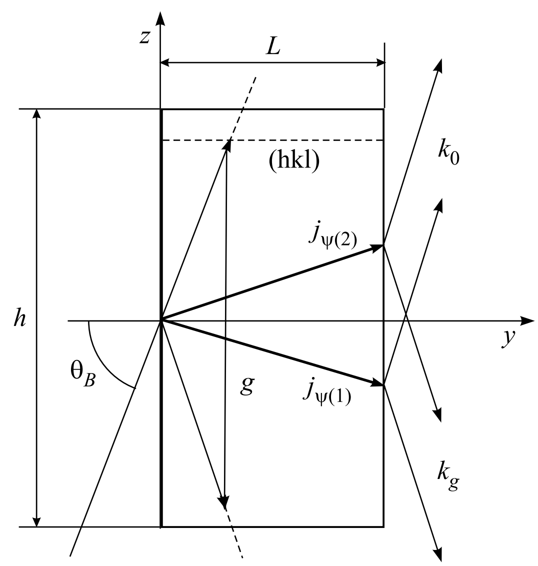

Fig.1. Symmetrical Laue diffraction scheme for finite perfect crystal. $\mathbf{j}_{\psi^{(1)}}$ and $\mathbf{j}_{\psi^{(2)}}$ are the neutron fluxes ("Kato trajectories") for two Bloch waves

the interplanar distance. In this case the neutron wave function in crystal will be a superposition of two Bloch waves $\psi^{(1)}$ and $\psi^{(2)}$ corresponding to two branches of dispersion surface [8].

The deformation of crystal means that the value and direction of vector $\mathbf{g}$ are different for the different points of crystal, i.e. $\mathbf{g}$ depends on the spacial coordinates Y and Z. A weak crystal deformation for a neutron Laue diffraction can be described by so called "Kato forces"

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[9], which are directed along the reciprocal lattice vector **g** and their values are determined by the value of crystal deformation [3]:

$$f_k(y,z) = -\frac{k_0}{4\cos\theta_B}\left(\frac{\partial}{\partial z} + \frac{1}{c}\frac{\partial}{\partial y}\right)\alpha(y,z), \quad (1)$$

where k_0 is the neutron wave vector in the crystal, θ_B is the Bragg angle,

$$\alpha(y,z) = \frac{g^2 + 2(\mathbf{k_0}\cdot\mathbf{g})}{\mathbf{k_0^2}} \quad (2)$$

is a parameter of deviation from the exact Bragg condition. Eq. (1) is valid for crystal deformations small as compared with the diffraction Bragg width.

A neutron "Kato trajectories" for two kinds of Bloch waves in the crystal (describing a behaviour of the neutron flux density) are determined by the equation

$$\frac{\partial^2 z}{\partial y^2} = \pm\frac{c}{m_0} f_k(y,z), \quad (3)$$

here $c = \tan\theta_B$, and $m_0 = 2F_g d/V$ is the so called "mass Kato", F_g is the neutron structure amplitude, V is the volume of unit cell. The sign $\pm$ in equation (3) corresponds to different Bloch waves.

Let's consider a most simple case of the crystal deformation. So let the gradient of the interplanar distance will be a constant $d = d_0(1+\xi z)$, see Fig.1. For this case the "Kato force" will be equal to

$$f_k(y,z) = \frac{1}{2}cg\xi \quad (4)$$

and the corresponding equation of neutron trajectories will be

$$\frac{\partial^2 z}{\partial y^2} = \pm\frac{c^2 g\xi}{2m_0}. \quad (5)$$

The right part of Eq. (5) is proportional to the square of $c = \tan\theta_B$. So for the Bragg angles $\theta_B \approx (84-88)^\circ$ the influence of a deformation can be intensified by a factor $\sim 100-1000$ as compared with the Bragg angle $\sim 45^\circ$.

3. Experiment. Experiment was carried out at the WWR-M reactor (PNPI, Gatchina). The scheme of the experiment is shown in Fig.2. The neutron diffraction at the (110) plane ($d = 2.45$ Å) of quartz crystal with the sizes $140\times140\times35$ mm^3 was studied. We used developed in our laboratory method to deform the crystal by applying the temperature gradient. The coefficient of thermal expansion for the quartz crystal along the direction perpendicular to the (110) plane is $\chi_{(110)} = 1.3\cdot10^{-5}$/K. Therefore, the parameter of deformation will be

$$\xi = \chi_{(110)}\Delta T/h = 0.93\cdot10^{-6}\Delta T, \quad (6)$$

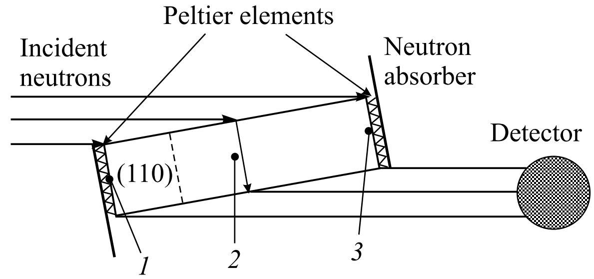

Fig.2. Scheme of the experiment. *1*, *2*, *3* are the positions of the temperature probes

where ΔT is the crystal temperature difference between points (1) and (3), see Fig.2, $h = 14$ cm is the crystal height, Fig.1. The Peltier elements were used to control the crystal temperature gradient. An increase of the crystal deformation will result in decreasing the diffraction beam intensity because some part of neutrons will not reach the exit surface of crystal due to strong bending of the Kato trajectories.

An example of the calculated neutron trajectory configurations in the crystal for Bragg angle equal to 86° and parameter of deformation $\xi = 6\cdot10^{-8}$/cm, that corresponds to the $\Delta T = 0.07\,°$C, is shown in Fig.3. The

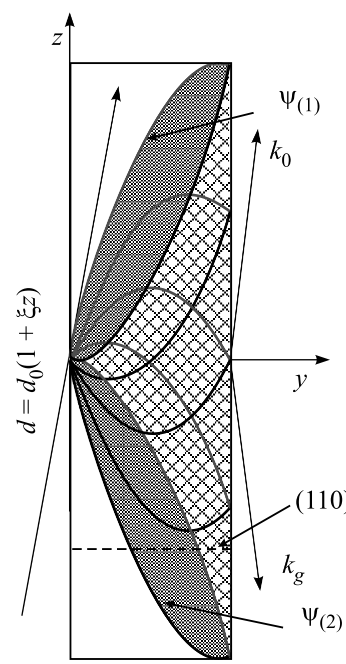

Fig.3. Example of the neutron trajectories in the deformed quartz crystal for the $\theta_B = 86°$ and $\xi = 6\cdot10^{-8}$/cm

trajectories are shown in a scale, corresponding to the length of crystal $L = 3.5$ cm (along Y axis) and height $h = 14$ cm (along Z axis). Each couple of the symmetrical with respect to Y axis trajectories in Fig.3 corresponds to the definite direction of the incident beam. The different couples correspond to slightly different incident beam directions within angle interval which is much less than the Bragg width. One can see that even for such a small crystal deformation the distance between the different Bloch wave trajectories can reach a few centimeters near the exit face of crystal. When this distance become equal to the height of crystal h, none of the neutrons can reach the exit crystal surface, because their trajectories as well as neutrons themselves go out from the crystal through its side faces.

The example of the measured intensity dependence on the deformation parameter ξ for the diffraction beam is shown in Fig.4. One can see that the width of this line W_ξ is less than 10^{-6}/cm.

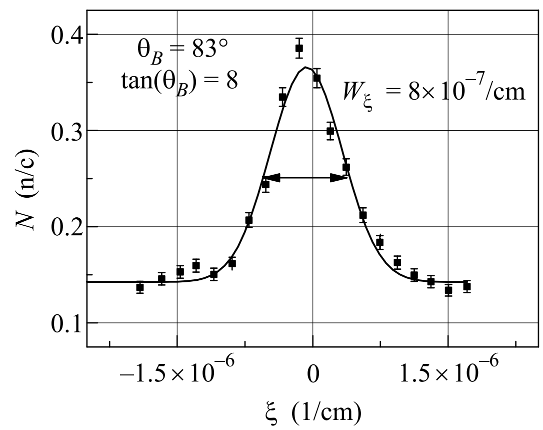

Fig.4. Example of experimental dependence of the diffraction beam intensity on the parameter ξ for the Bragg angle equal to 83°

The dependence of the W_ξ on $\tan\theta_B$ is shown in Fig.5.

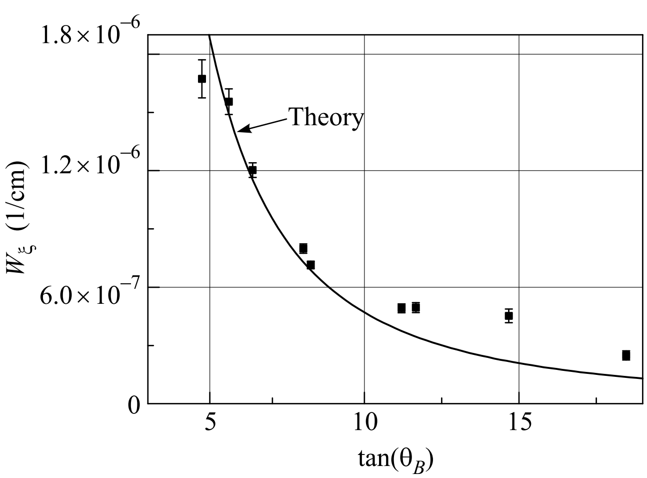

Fig.5. The dependence of W_ξ on the tangent of Bragg angle

One can calculate the width W_ξ using the equation of neutron trajectory (5)

$$W_\xi = \frac{h}{L^2c^2}\frac{8m_0 d}{\pi}. \tag{7}$$

The solid curve in Fig.5 is the theoretical dependence (7). There is a good agreement between calculations and experimental results up to $\tan\theta_B \equiv c = 10$.

4. Discussion. As follows from the equations (1) and (2) the "Kato force" arises due to dependence of the deviation parameter α on the spatial coordinates Z and Y. Therefore if we put the undeformed perfect crystal in the certain force field affecting the neutron along reciprocal lattice vector $\mathbf{g}$, we will have the same results as for the deformed crystal.

The effect of external field on the diffracting neutron was considered in [6] and influence of gravity on a neutron diffraction in an elastically bent crystal was experimentally observed [3].

It is easy to see that the external force $\mathbf{F_{ext}}$ affecting the neutron along the vector $\mathbf{g}||\mathbf{Z}$, see Fig.1, is equivalent to action of the gradient of interplanar distance in the same direction. So we will have

$$\xi_f = F_{\rm ext}/2E_n, \tag{8}$$

where E_n is the neutron energy.

Therefore the equation for neutron trajectory in crystal in the external field will have the form

$$\frac{\partial^2 z}{\partial y^2} = \pm\frac{c^2 g}{2m_0}\frac{F_{ext}}{2E_n}. \tag{9}$$

Let's compare this Kato trajectory with the usual one for neutron under the same external field in the free space for the same neutron energy. The last is described by usual Newtonian equation which has a form

$$\frac{\partial^2 z}{\partial y^2} = \frac{F_{\rm ext}}{2E_n}. \tag{10}$$

As follows from (9) and (10) the "curvature" of the diffracting neutron trajectory in the crystal is magnified by the factor

$$K_e = \pm c^2 g/2m_0, \tag{11}$$

as compared with the usual one. This factor depends on Bragg angle as $\tan^2\theta_B$. We should emphasize that the width of the curve shown in Fig.4 in the units of external force affecting the neutron is about $6\cdot 10^{-9}$ eV/cm, that is only a few times more than the neutron gravitational interaction with the Earth field ($\sim 10^{-9}$ eV/cm).

The numerical calculation of the factor K_e for (110) and (200) quartz planes gives

$$K_e^{(110)} = \pm 1.8 \cdot 10^5\, c^2, \qquad (12)$$

$$K_e^{(200)} = \pm 1.4 \cdot 10^6\, c^2. \qquad (13)$$

So for the Bragg angle $\theta_B = 87^0$ ($c = 20$) this factor will be equal to

$$K_e^{(110)} = \pm 0.72 \cdot 10^8, \qquad (14)$$

$$K_e^{(200)} = \pm 0.56 \cdot 10^9. \qquad (15)$$

The effect of diffraction enhancement of the angular deflection of a neutron trajectory inside the crystal is well known, see for instance [4], and can reach the values of $10^5 - 10^6$, but we would like to pay attention that such effect can be considerably magnifyed by the additional gain factor proportional to $\tan^2\theta_B$ for the Bragg angles close to $\pi/2$.

5. Conclusions. The effect of strong influence of a small crystal deformation on the neutron diffraction beam intensity was observed for the case of Laue diffraction in transparent crystal. It was shown for the first time that the effect considerably increases for the Bragg angles close to $\pi/2$ as $\tan^2\theta_B$.

The additional gain factor determined by the value of Bragg angle can reach $\sim 10^3$. So the joint factor of diffraction enhancement for the neutron trajectory bending due to external field can reach $\sim 10^9$ (not $10^5 - 10^6$ as for Bragg angles $\sim 45°$).

The observed effect gives a new possibilities for precise investigation of a neutron interaction with the external fields. The estimations have shown that for specially designed two crystal setup the resolution to the external field (width of the line, see Fig.4) can reach $\sim 10^{-13}$ eV/cm and the sensitivity to measure the neutron energy variation can be better than 10^{-18} eV/cm. That could allow to improve the limit on the neutron electric charge by about 2–3 orders of magnitude as compared with [10] and to carry out the measurement of the ratio of the neutron inertial and gravitational masses at the level $\sim 10^{-5}$ or even better.

The authors would like to thank the personnel of the WWR-M reactor (Gatchina, Russia). This work was supported by RFBR (grants # 05-02-16241, # 06-02-81011).

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