Diffraction Image of a narrow X-rays beam in Crystals with Weak Deformation

V.R. Kocharyan

Institute of Applied Problems of Physics of NAS RA
Yerevan, Armenia
e-mail: vahan2@yandex.ru

Experimentally investigated

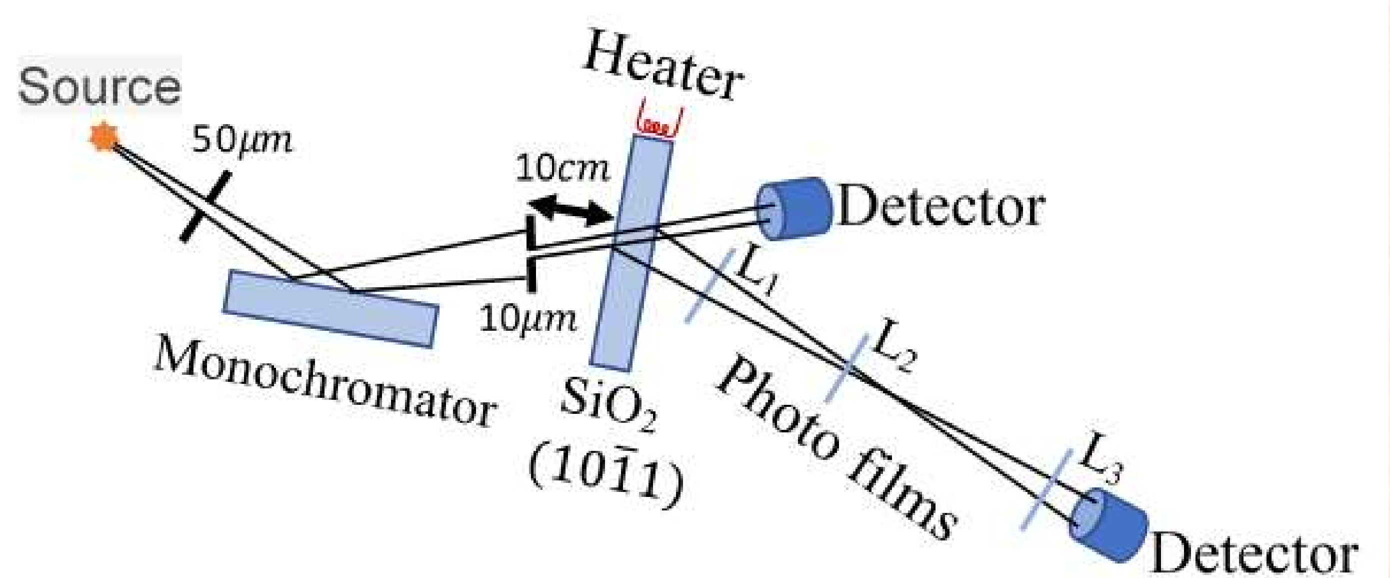
- ***Rocking curves (RC) of a quartz crystal,***
- ***pumping of X-rays from the transmission direction to the direction of reflection,***
- ***focusing of reflected beam.***

Theoretically considered

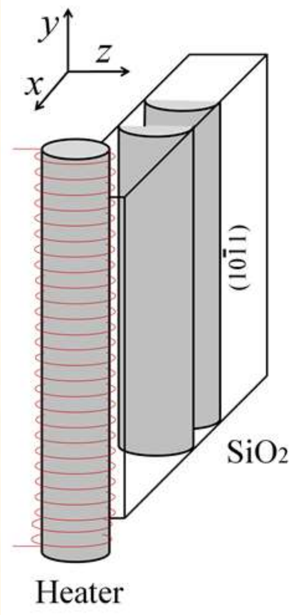
the problem of dynamic diffraction of X-rays from a point source on the spatial lattice of a crystal with a weak deformation field.

Experimental investigation

The studies were carried out according to a two-crystal scheme based on a laboratory diffractometer. Mo tube served as the radiation source. A quartz crystal with a $(10\bar{1}1)$ surface was used as a monochromator. To isolate the MoKα1 radiation line, a narrow slit was placed after the monochromator. After a narrow slit at a distance of 10 cm in the Laue geometry, a sample (quartz crystal) was placed in the reflected position.

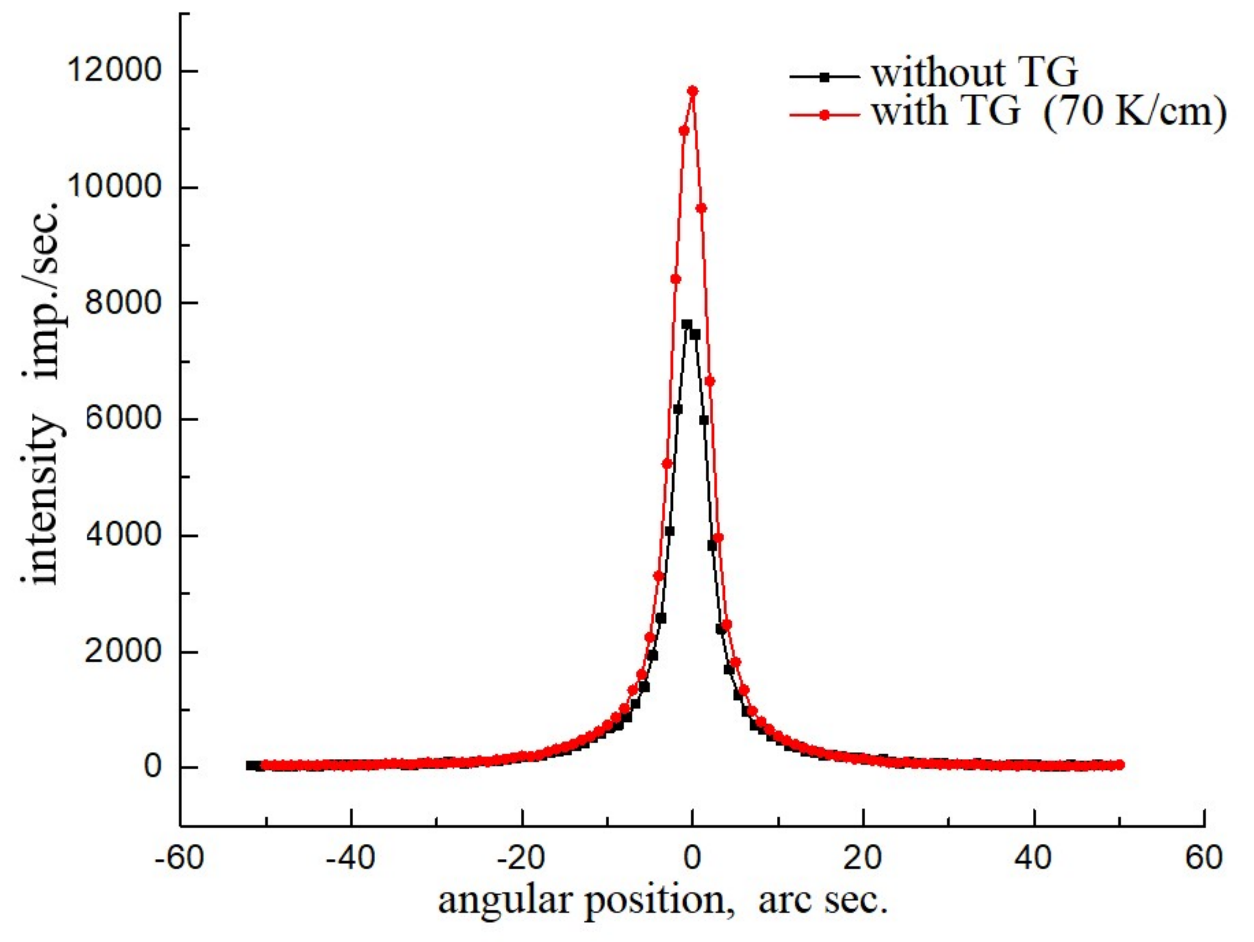


The experimental scheme



In the experiments, the temperature gradient was applied perpendicular to the reflecting atomic planes $(10\bar{1}1)$ of a quartz crystal. To measure the X-rays intensity a scintillation detector was used, and to observe the behavior of focusing at distances of L1, L2, and L3, the frontal section of the X-rays was recorded on photo film.

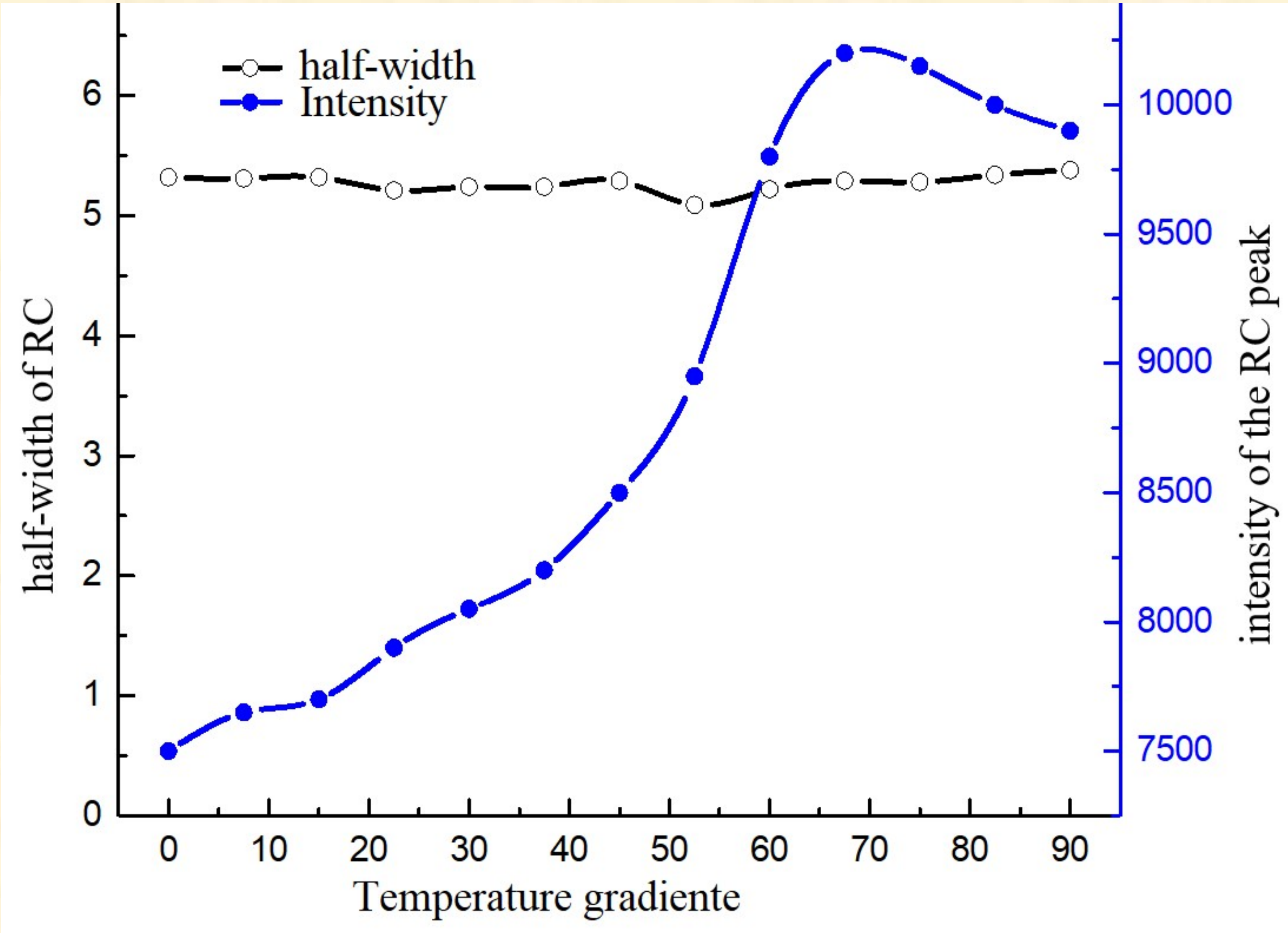
The rocking curves (RC) of a quartz crystal



As you see, the half-width of the RC does not change, but the peak intensity RC increases in the presence of a temperature gradient.

Rocking curves of atomic planes $(10\bar{1}1)$ of a quartz crystal without and with a temperature gradient $\Delta T/\Delta x$ =70 K/cm

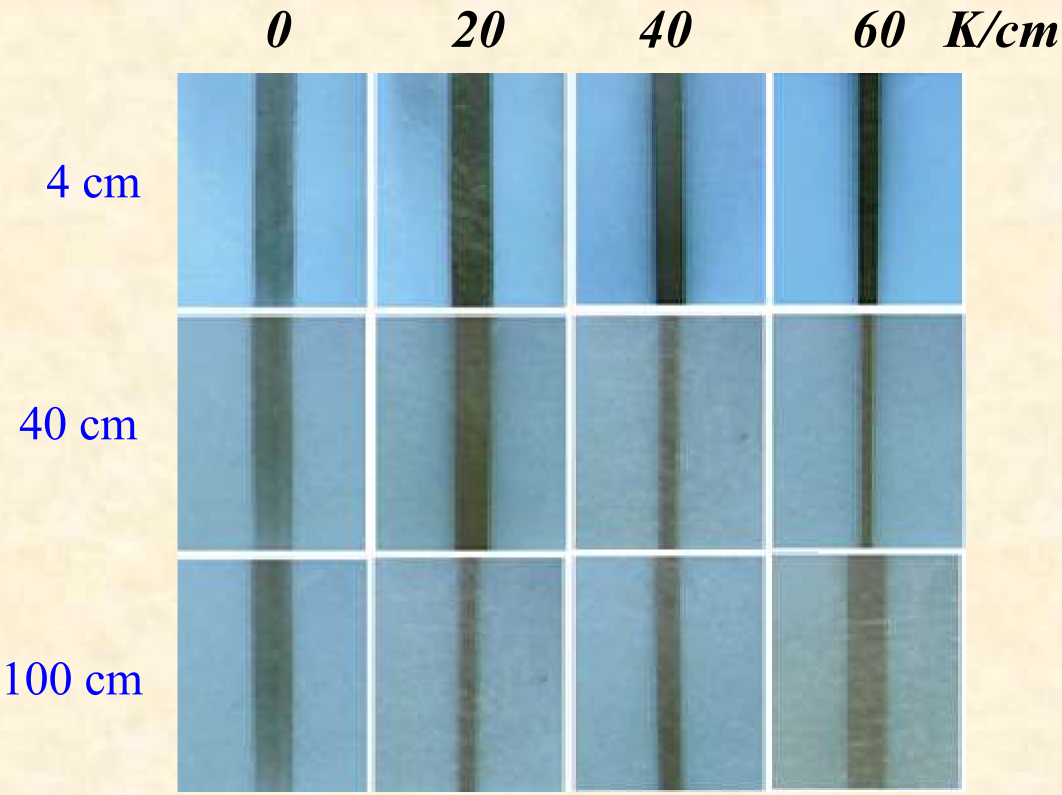
The pumping of X-rays from the transmission direction to the direction of reflection



Dependence of the half-width of the RC of $(10\bar{1}1)$ atomic planes of a quartz crystal and the peak intensity RC on the value of the external temperature gradient.

Focusing of the reflected X-rays

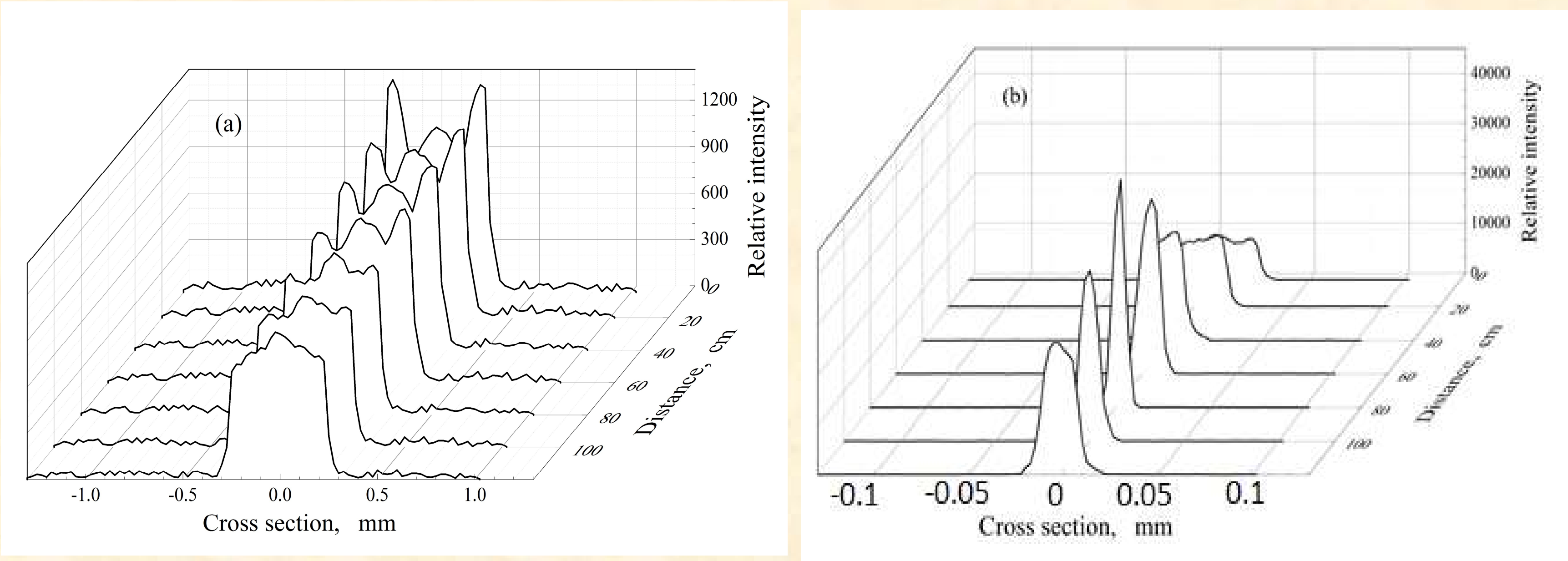
Experimentally considered the dependence of focus position of the reflected X-rays on the value of the temperature gradient. To find the location of the focus of X-rays at the distances of L1 (4 cm), L2 (40cm), L3 (100 cm) from the sample were taken frontal section of the beam with and without influence of a temperature gradient.



The frontal sections of the reflected X-rays from the reflecting atomic planes $(\mathbf{10\bar{1}1})$ of a single crystal quartz for different values of the temperature gradient.

Focusing of the reflected X-rays

As seen from the figures with the temperature gradient the reflected X-rays focus becomes ***closer to the crystal*** and there is a multiply increases of the intensity.



The frontal distribution of the intensity of the reflected X-rays from atomic planes $(10\bar{1}1)$ of a single quartz crystal of 1 mm thickness at different distances
a) without the influence of a temperature gradient
b) under the influence of a temperature gradient of 70ºK/cm.

DIFFRACTION OF X-RAYS FROM QUARTZ CRYSTAL UNDER THE EXTERNAL TEMPERATURE GRADIENT

The diffraction of X-rays in crystal is described by the Takagi equations

$$\frac{\partial \psi_0}{\partial s_0} = -i\pi kc\chi_{\bar{h}}\,\psi_h$$

$$\frac{\partial \psi_h}{\partial s_h} = -i\pi kc\chi_h\;\psi_0 + i\alpha\,\psi_h$$

The polarizability for deformed crystals is as follows:

$$\chi(\vec{r}) = \sum_m \chi_m\, e^{-2\pi i\vec{h}_m(\vec{r}-\vec{U}(\vec{r}))}$$

In symmetric Laue geometry displacement function at definite distance from a heating face of crystal can be represented as

$$\boldsymbol{hu} = q\;((z\;tan\theta_B)^2 - x^2),$$

were ψ_0, ψ_h are amplitudes of Bloch waves in crystal lattice , $(s_0 s_h)$ - coordinates in an oblique system with axes parallel to the direction satisfying the Bragg condition. The transition to coordinates in the Cartesian coordinate system with axes (x, z) is performed using the following formulas

$$s_0 = \frac{1}{2}\left(\frac{z}{\cos\theta} + \frac{x}{\sin\theta}\right) \qquad s_h = \frac{1}{2}\left(\frac{z}{\cos\theta} - \frac{x}{\sin\theta}\right)$$

where χ_m-are the Fourier amplitudes of the microscopic periodical polarizability $\chi(\vec{r})$ of the crystal .

DIFFRACTION OF X-RAYS FROM QUARTZ CRYSTAL UNDER THE EXTERNAL TEMPERATURE GRADIENT

Under the condition of weak deformation:

$$q \ll \sigma\overline{\sigma}.$$

where $\sigma\overline{\sigma} = \pi^2 k^2 c^2 \chi_h \chi_{\overline{h}}$

In this approximation, the Green-Riemann function is represented as

$$G(s_0, s_h) = e^{iqs_0s_h} J_0\left(2\sqrt{s_0 s_h(\sigma\overline{\sigma} - iq)}\ \right),$$

where J_0 is the zero-order Bessel function.

Thus, the integral formula for determining the amplitude of a Bloch wave can be represented as the sum of two wave modes, which in turn can be represented in the following integral form

$$\psi_h(x,z) = \frac{1}{\sqrt{2\pi}\sqrt[4]{\frac{(\sigma\overline{\sigma}-iq)}{\sin^2\theta_B}}} \int_{x+z\tan\theta_B}^{x-z\tan\theta_B} \frac{e^{iS_+(x',x,z)} e^{R_-(x',x,z)} + e^{iS_-(x',x,z)} e^{R_+(x',x,z)}}{\sqrt[4]{(z\tan\theta_B)^2 - (x-x')^2}} dx'$$

where

$$S_{\mp}(x',x,z) = \frac{qxx'}{2*\sin^2\theta_B} + \left(\frac{k\cos^2\theta_B}{2L_1} - \frac{q}{4\sin^2\theta_B}\right)x'^2 \mp \frac{\sqrt{\sigma\overline{\sigma}}}{\sin\theta_B}\sqrt{(z\tan\theta_B)^2 - (x-x')^2}$$

$$R_{\mp}(x',x,z) = \mp\frac{q}{2\sin\theta_B\sqrt{\sigma\overline{\sigma}}}\sqrt{(z\tan\theta_B)^2 - (x-x')^2}.$$

DIFFRACTION OF X-RAYS FROM QUARTZ CRYSTAL UNDER THE EXTERNAL TEMPERATURE GRADIENT

$$S_{\mp}(x',x,z)=\frac{qxx'}{2*\sin^2\theta_{\boldsymbol{B}}}+\left(\frac{k\cos^2\theta_{\boldsymbol{B}}}{2L_1}-\frac{q}{4\sin^2\theta_{\boldsymbol{B}}}\right)x'^2\mp\frac{\sqrt{\sigma\bar{\sigma}}}{\sin\ {}_{\boldsymbol{B}}}\sqrt{(z\tan\theta_{\boldsymbol{B}})^2-(x-x')^2}$$

Obviously, the behavior of the second derivatives of the two eikonals S_+ and S_- differ significantly from each other. If for S_+ the derivative retains its sign throughout the entire region of existence of the wave field, then for S_- the derivative sign changes when passing through a certain point, where the second derivative is equal to zero. This means that this mode forms a focus near this region. Now, from the joint solution of two equations of equality to zero of the first and second derivatives of the eikonals, we have for the focus coordinates

$$x=0,\ z=F_{in}=\frac{L_{ef}}{\Gamma} \quad \text{where} \quad L_{ef}=\frac{L_1 k\sin^2 2\theta_{\boldsymbol{B}}}{k\sin^2 2\theta_{\boldsymbol{B}}-2L_1 q},\quad \Gamma=\frac{\mathrm{k}\sin\theta_{\boldsymbol{B}}\sin 2\theta_{\boldsymbol{B}}}{2|\sigma|}.$$

It can be seen from that, with an increase the deformation parameter q the focal spot moves deeper into the crystal, so approaches to the exit surface of the crystal,

and at $\mathrm{q}=\frac{k\sin^2 2\theta_{\boldsymbol{B}}}{2L_1}$, F_{in} becomes infinite. In this case, the rays propagate in parallel.

A further increase in q leads to a reverse displacement of the focal spot towards the input surface of the crystal (we have an imaginary focus) .

DIFFRACTION OF X-RAYS FROM QUARTZ CRYSTAL UNDER THE EXTERNAL TEMPERATURE GRADIENT

The formation of a diffraction field behind a crystal is formulated using the Huygens-Fresnel principle, based on the fact that the distribution of the amplitude of the diffracted field on the output surface of the crystal is given, and the function of a point source is a spherical wave.
The resulting integral form of the diffracted field amplitude differs from the analogous amplitude in the crystal only in that L_1 is replaced by $L_1 + L_2$ where L_1 is the source-crystal and L_2 is the crystal-detector distances along the Bragg directions.
As a result, for the coordinates of the focal spot outside the crystal, we will have

$$\xi = 0, \qquad F_{out} = \Gamma t - L_{ef}$$

Where t-is the crystal thickness,

$$\Gamma = \frac{\mathrm{k}\sin\ _{\boldsymbol{B}} \sin 2\theta_{\boldsymbol{B}}}{2|\sigma|}, \quad L_{ef} = \frac{L_1 k \sin^2 2\theta_{\boldsymbol{B}}}{k \sin^2 2\theta_{\boldsymbol{B}} - 2L_1 q} \quad \mathrm{q} = \frac{k \sin^2 2\theta_{\boldsymbol{B}}}{2L_1}$$

The behavior of the reflected wave field in vacuum is similar to the behavior of the field in a lattice. With an increase in the deformation parameter q, the focal length first approaches to the exit surface of the crystal, at a certain value of q it becomes infinite (imaginary focus), and with a further increase in q, it begins to move towards the exit surface of the crystal.

CONCLUSIONS

- ***We experimentally show that an increase of the value of the temperature gradient leads to a multiple increase in intensity without a change in the half-width of the rocking curves.***

- ***We experimentally and theoretically show that with the increase of the value of the temperature gradient or deformation parameter the focus becomes closer to the crystal, and the focal spot is narrowed in the diffraction plane.***

Thank you for your attention!

Institute of Applied Problems of Physics of NAS RA, Yerevan, Armenia
Vahan2@yandex.ru