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Hard X–ray Laue monochromator

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Abstract. Experimental studies of X-ray diffraction from reflecting atomic planes $(10\bar{1}1)$ of X-cut quartz single crystal in Laue geometry influenced by the temperature gradient were carried out. It is shown that by using the temperature gradient it is possible to reflect a hard X-ray beam with photon energy near the 100 keV with high efficiency. It has been experimentally proved that the intensity of the reflected beam can be increased by more than order depending on the value of the temperature gradient.

1. Introduction

The obtaining of intensive sources and base elements of short wavelength hard X-ray "optics" with controllable working parameters (energy, intensity, and focus length) gives an opportunity to improve technology in medicine and broaden the scope of application of X-ray diffractometry. In this regard, the issues of diffraction under external influence have special and actual place. For example, in order to optimize the required dose of exposure of patients 30 keV to 250 keV energy needs to be emitted from the white spectrum of the X-ray with the necessary bandwith, luminosity and radiation density. For the purpose of obtaining such beams the questions of diffraction under external influence occupy their special and actual place.

The authors of works [1, 2] were the first to detect the complete transfer of X-rays from the direction of passing to that of reflection in single crystals of quartz in Laue geometry when exposed to temperature gradient or ultrasonic vibrations. In [3] it was theoretically and experimentally proved that, using a temperature gradient and acoustic field, one can control the position of the focus of reflected radiation in space and time and can also convert a spherical wave into a plane one. These works do not experimentally investigate the transfer and control of the spectrum of reflected hard X-rays (over 25 keV).

2. Experiment

In order to obtain an intensive hard X–rays (over 25 keV) with controllable parameters, we have considered the X-ray diffraction on quartz monochromator in Laue geometry influenced by the temperature gradient. A rectangular plate of single crystal quartz (30x30 mm^2) with a thickness of 9 mm was used as the sample under investigation. The spectrums of reflected and passing X-ray beams from the reflecting atomic plane $(10\bar{1}1)$ of quartz single crystal were experimentally studied with various values of the temperature gradient. The experimental scheme is shown on figure 1. The experiments were carried out with the energy dispersive silicon spectrometer [4]. The temperature gradient in the crystal was created with the help of a heater 3 on figure 1. The heated part of the plate was parallel to the reflecting atomic planes $(10\overline{1}1)$, i.e. the temperatureo gradient was perpendicular to the reflecting atomic planes. The temperature gradient vector and the diffraction vector were antiparallel. A white spectrum of X-ray was used in the test which was generated by the tungsten X-ray tube RAP-150MN [5, 6] under up to 120 kV voltage and 95 μA current. The beam was collimated with two slits width of 1 mm before falling on the sample. The spectrum of the reflected beam was observed at the distance of 500 mm and at the angle near of 4.5°.

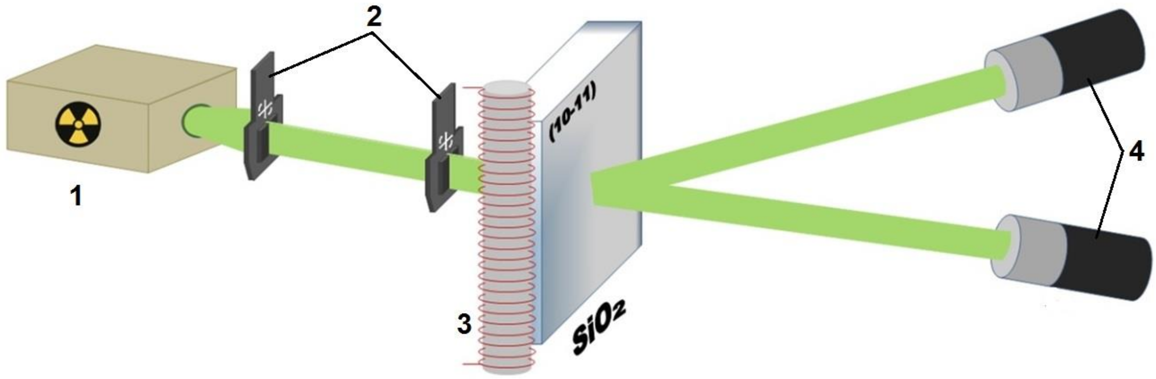

Figure 1. Experimental scheme: 1 – RAP-150MN; 2 – slit collimator; 3 – heater; 4 – detector.

In order to make sure of the effect of "transfer" the spectrums of passing and reflecting X-ray radiations were measured. For the chosen orientation of the crystal the diffraction first order matches 47 keV and second order 94 keV. Exactly for these energies in the solid spectrum of the passing beam the flops were observed, the depth of which is determined by the value of the temperature gradient and the energy resolution of the detector. The heating of the crystal side was made from 23 to 400°C, the opposite side was cooled with the help of convection. An increase in the intensity of reflecting beam in Laue geometry was observed in 45 times compared to the uniform temperature regime of the crystal quartz with 9 mm thickness. On figure 2 shown the filtered with 1.6 mm Cu radiation spectrum of "transfer effect" depending on the temperature gradient for the crystal quartz of 9 mm thickness. Energy of the first and the second order were determined from the spectrum and it values are equal to 46.86±0.05 and 93,33±0.05 keV, FWHM is 2.2±0.1 and 3.4±0.3 keV, correspondently.

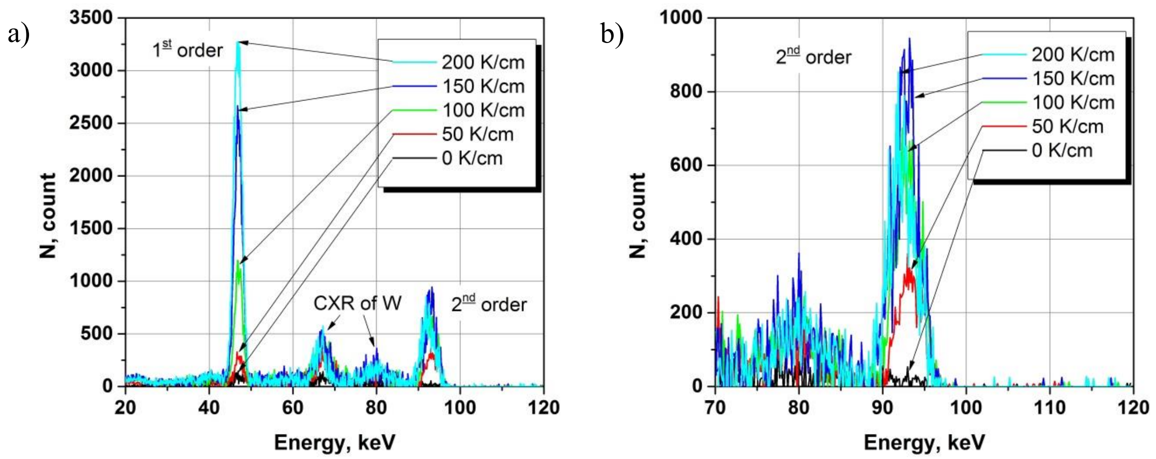

Figure 2. The spectrum of the reflected beam (a) and zoomed part (b) for the different value of the temperature gradient ΔT/Δx applied to the quartz single crystal with the thickness 9 mm.

The spectral measurements confirm the effect of transfer from passing beam of X-ray radiation to reflecting beam and its dependency from the temperature gradient that is created in the crystal. The multiple increases in the intensity is caused by the phenomenon of the full pumping of the X-ray from the passing direction to the reflecting direction with a big angular width which is much bigger than the angular width of the Darwin table and depends on the thickness of the observed mono-crystal. The saturation of the intensity parallel to the increase of the temperature gradients due to the fact that in big deformations the extinction length becomes much bigger than the effective thickness of the diffraction of each monochromatic X-ray waves.

3. Theory

Usually, an X-ray beam incident on the crystal has divergence and spectral width and in each direction spreads a totality of plane waves with different wavelengths.

In the calculations of diffraction the incident X-ray wave is decomposed into totality of plane monochromatic waves, each of which is scattered in accordance to the dynamic theory in the plane-wave approximation of the deformed crystal. Then the scattering wave integrated over the spectral and angular variable in the detector plane. In the calculations for each transmitted and reflected planar and monochromatic wave were obtained the solutions used in [7, 8].

In the XOZ-plane scattering, based on the experimental results [9, 10], in the presence of temperature gradient perpendicular to the reflecting atomic planes at a certain distance from the heating verge of the crystal the $U_x$displacement function can be written as:

$$U_x = \frac{t^2-(t-2z)^2}{8R}, \tag{1}$$

where t is the thickness of the crystal, R is the curvature radius of reflecting atomic planes.

Let, in the Laue geometry, the monochromatic plane wave of X-rays is incident on the crystal. In this case, considering (1) for the two-wave approximation the Takagi's equations take the following view:

$$\begin{cases} \dfrac{\partial D_h}{\partial z} - i\dfrac{C\chi_h K}{2\cos(\theta)} e^{-i\vec{h}\vec{u}} D_0 - i\dfrac{(\chi_0 - b)K}{2\cos(\theta)} D_h = 0 \\ \dfrac{\partial D_0}{\partial z} - i\dfrac{\chi_0 K}{2\cos(\theta)} D_0 - i\dfrac{C\chi_{\bar{h}} K}{2\cos(\theta)} e^{i\vec{h}\vec{u}} D_h = 0 \end{cases}, \tag{2}$$

where D_0 and D_h are the amplitudes of the reflected and transmitted field, the parameter $b = -2\sin(\theta)\Delta\theta$ characterizes the deviation from the exact Bragg angle, χ_0 and χ_h are the Fourier components of the dielectric permittivity, K is the wave number, θ is the angle of incidence, $\vec{h}$ is the diffraction vector, $\vec{u}$ is the displacement vector, and C is the polarization multiplier.

The boundary conditions for amplitudes of each monochromatic plane waves of X-rays D_0 and D_h on the input surface of the crystal $z = 0$ take the following form: $D_0 = D_{ins}$ and $D_h = 0$. Introducing the designations:

$$\eta = \frac{bK}{4\cos\theta},\ \alpha = \frac{1}{2}\frac{\partial \vec{h}\vec{u}}{\partial z},\ C_h = \frac{C\chi_h K}{2\cos\theta},\ C_{\bar{h}} = \frac{C\chi_{\bar{h}} K}{2\cos\theta},$$
$$D_h = \tilde{D}_h e^{i(\frac{\chi_0 K}{2\cos(\theta)}z - \frac{bK}{2\cos(\theta)}z - \frac{\vec{h}\vec{u}}{2})},\ D_0 = \tilde{D}_0 e^{i(\frac{\chi_0 K}{2\cos(\theta)}z - \frac{bK}{2\cos(\theta)}z + \frac{\vec{h}\vec{u}}{2})}. \tag{3}$$

Based on the boundary conditions and the designations (3), from equation (2) for amplitudes of each monochromatic plane wave of X-rays D_0 and D_h we get finally:

$$D_h(z) = \frac{C_h D_{ins}}{2\sqrt{W(0)W(z)}} \left(\begin{aligned} &\exp\left(\frac{2A - C_i}{C_r} f(z) - \frac{K\chi_{0i}}{2\cos(\theta)} z\right) \exp\left(i[\varphi(z) + \psi_1(z) + f(z)]\right) \\ &- \exp\left(\frac{C_i - 2A}{C_r} f(z) - \frac{K\chi_{0i}}{2\cos(\theta)} z\right) \exp\left(-i[\varphi(z) + \psi_2(z) + f(z)]\right) \end{aligned} \right), \tag{4}$$

$$D_0=\frac{D_{ins}}{2\sqrt{W(0)W(z)}}\left(\left(i(W(z)-\eta-\frac{\partial\alpha}{\partial z})-\frac{1}{2W(z)}\frac{\partial W(z)}{\partial z}\right)\exp\left(\frac{2A-C_i}{C_r}f(z)-\frac{K\chi_{0i}}{2\cos(\theta)}z\right)\exp\left(i[\varphi(z)+\psi_1(z)+f(z)]\right)\right.$$
$$\left.+\left(i(W(z)+\eta+\frac{\partial\alpha}{\partial z})+\frac{1}{2W(z)}\frac{\partial W(z)}{\partial z}\right)\exp\left(\frac{C_i-2A}{C_r}f(z)-\frac{K\chi_{0i}}{2\cos(\theta)}z\right)\exp\left(-i[\varphi(z)+\psi_2(z)+f(z)]\right)\right), \quad (5)$$

where

$$f(z)=\frac{2Az+\eta-At+\sqrt{(2Az+\eta-At)^2+C_r}}{\eta-At+\sqrt{(\eta-At)^2+C_r}},$$

$$\varphi(z)=\frac{(2Az+\eta-At)\sqrt{(2Az+\eta-At)^2+C_r}-(\eta-At)\sqrt{(\eta-At)^2+C_r}}{4A},$$

$$\psi_{1,2}(z)=\pm\left(\frac{K\,\mathrm{Re}\,\chi_0}{2\cos\theta}+2\eta\right)z\pm A\left(zt-z^2\right)$$

$$C_r=\mathrm{Re}(C_hC_{\bar h}),\qquad C_i=\mathrm{Im}(C_hC_{\bar h}).$$

A is the deformation parameter, which is equal to $A=\frac{h}{2R}$ in the presence of temperature gradient.

For the purpose of qualitative comparison of reflecting and passing radiation with experimental results calculations are made with the help of this method when an X-ray beam with white spectrum falls on the crystal quartz. In the calculations the diffraction in Laue geometry is viewed for reflecting atomic planes $(10\bar{1}1)$ of single crystal of quartz with 9 mm thickness when the crystal is in Bregg condition for 94 keV photon energy.

The results of the calculations are brought in the figure 3. As we can see, the calculations also confirm the existence of multiple increase of intensity which is caused by the phenomenon of full pumping of the X-ray from passing direction (figure 3b) to the reflecting direction (figure 3a) with big spectrum width. In the experimental results in the spectrum of the passing beam near the Bregg angle the flop does not reach 0 value which is due to the resolution of the spectrometer.

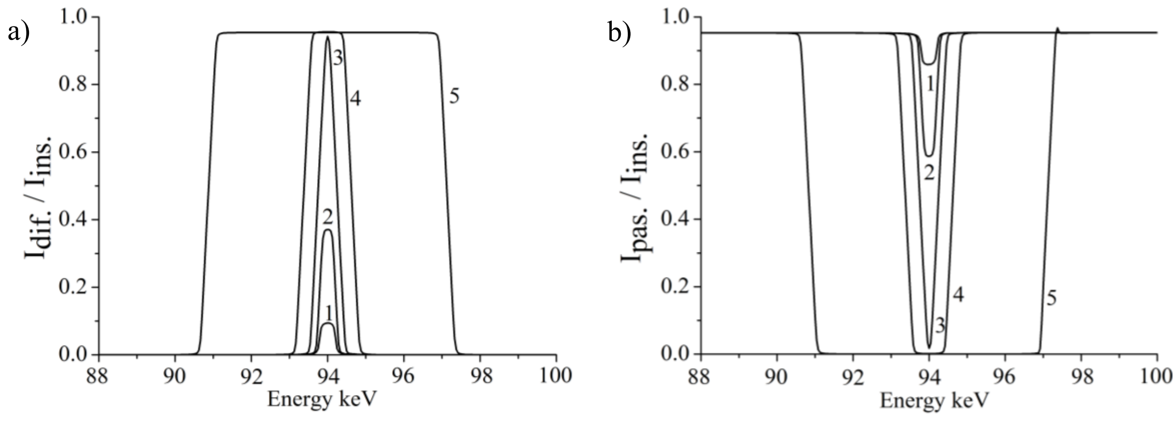

Figure 3. The spectrums of the reflected (a) and passed (b) beams for the different values of the parameter deformation of the reflecting atomic planes of the quartz single crystall with the thickness of 9 mm: 1) A = 0; 2) A = 250; 3) A = 800; 4) A = 2000; 5) A=10000.

On figure 4 shows the spectrum of reflecting beam from reflecting atomic planes of a single crystal of quartz to different thicknesses at a certain value of the parameter A. The calculations are made for the X-rays with an energy of 94 keV at a radius of curvature of the reflecting atomic planes ~ 15 m (parameter A = 10000). From figures it is clear that at a certain value of the parameter A, than greater the thickness of the single crystal, the wider the spectrum of the reflecting X-ray beam i.e., the wider the spectrum of full pumping beam. For example, a single crystal of quartz with a thickness of 1 cm, the atomic planes are curved with the curvature of 15 m fully reflect the X-rays with a spectral width of $\Delta E \approx 6 \div 7$ keV, a crystal with a thickness of 5 cm fully reflects $\Delta E \approx 25$ keV.

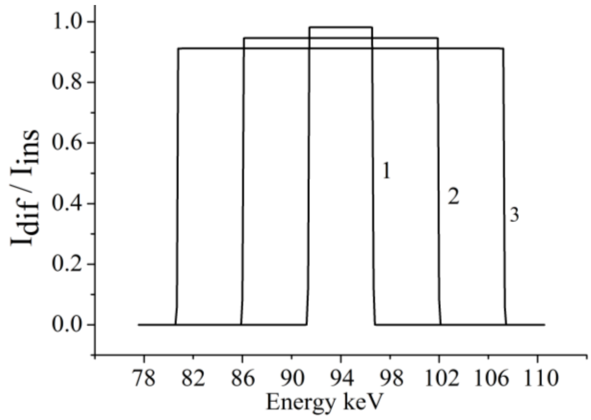

Figure 4. The spectral distribution of the reflected X-rays with energy of 94 keV from the single crystal of quartz for value of parameter A = 10000: 1) t = 1 cm, 2) t = 3 cm, 3) t = 5 cm.

Conclusion

Thus, we have obtained multiple times increase in the intensity of the reflecting hard X-rays, full pumping of X-ray from passing direction to the reflecting direction with big spectral width, its dependency from the thickness of the researched single crystal and value of the applied temperature gradient. It is shown that by using quartz crystals in Laue geometry with external temperature gradient it is possible to create a monochromators with higher of luminosity and linear filters in the region of hard X-ray radiation with controllable parameters.

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