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Dynamic Diffraction of X-Ray in Quartz Single Crystal with Fan-Shaped Deformation

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Abstract. The effect of the fan-shaped deformation in the integrated intensity of the reflected X-ray from quartz single crystal (SiO_2) was investigated in case of Laue geometry for different reflecting atomic planes. It was found that with the increase of the temperature gradient, in the case of parallel vectors of diffraction and temperature gradient, the integrated intensity of the reflected X-ray beam increase more than 100% for different atomic planes of the crystal. The dependence of intensity of the reflected beam on the temperature gradient has been theoretically analyzed.

1. Introduction

After the pioneering work of [1, 2], the study of deformed single crystals by X-ray radiation was rapidly expanded. The deformation in single crystals was carried out under the influence of different external forces of the temperature gradient, ultrasonic resonance, mechanical bending.

In Ref. [3], the phenomenon of transfer of X-ray intensity in the direction of the reflection under the influence of the temperature gradient has been observed in thin crystals ($\mu t \sim 1$, where μ is the linear absorption coefficient and t is the thickness of the single crystal).

In Ref. [4], the phenomenon of reducing the linear absorption coefficient of quartz by X-ray plane wave was studied under the influence of a temperature gradient perpendicular to the reflecting atomic planes. Due to the changes in the coefficient of linear absorption of the single crystal of quartz, the total intensity of the transmitted and reflected beams in the Laue geometry, increased by ≈30%.

The dependence of the integrated intensity of X-ray beams diffracted from single crystals *ADP* and *KDP* in the Laue geometry was investigated under the influence of temperature gradient perpendicular to the reflecting atomic planes [5, 6]. It was found that the integrated intensity of the X-ray beam reflected from a single crystal depends almost linearly on the magnitude of the temperature gradient.

This paper presents the results of the effect of the fan-shaped deformations on the integrated intensity of the reflected X-rays from quartz single crystal in Laue geometry under the influence of the temperature gradient parallel to the reflecting atomic planes. Based on the theoretical analysis, the observed phenomenon was explained.

2. The experimental procedure and results

Experiments were performed by diffractometer-*DRON-3M*, X-ray tubes *BSV-29* with anode of Mo and with the horizontal size of focal spot 0.4 mm and vertical size 8 mm. The tube voltage and current were 40kV and 20 mA, respectively. The thickness of the single crystal of quartz was 3 mm. The linear absorption coefficient of quartz for *MoKα* radiation equals 10.4 cm^{-1}. The experimental scheme is shown in Figure 1, which shows the size and location of the slots.

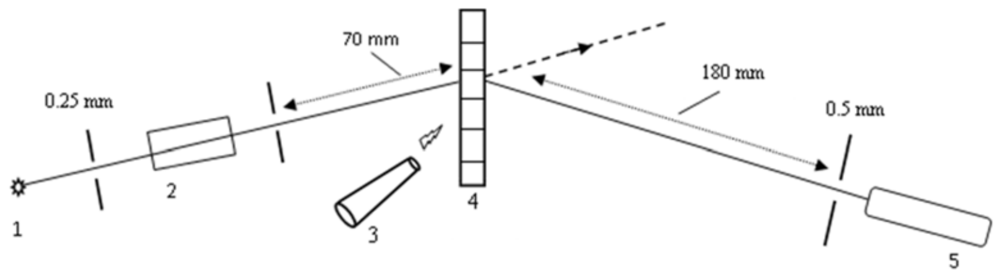

Fig.1. Diagram of the experiment.1- Source, 2-Soler slit, 3-Hot-air blower, 4- Sample, 5-Scintillation counter

The temperature distribution on the surface of the crystals must be uniform so that intensity distribution of the reflected beam uniformly exits from different places of the single crystals. As seen in Figure 1, the front surface temperature is higher than the exit surface of the single crystal since only the front surface is heated by hot-air blower.

Figure 2 shows the plots of the integrated intensity of the reflected beams from the atomic planes of $(10\bar{1}1)$, $(21\bar{3}1)$ and $(10\bar{1}0)$ versus the value of the temperature gradient applied parallel to the reflecting atomic planes in the Laue geometry. As seen, the integrated intensity of the reflected beam increases with the increase of the value of the temperature gradient for the plane $(10\bar{1}0)$ more than twice, and for the plane $(21\bar{3}1)$ about three times. However, the integrated intensity of all these cases was not saturated.

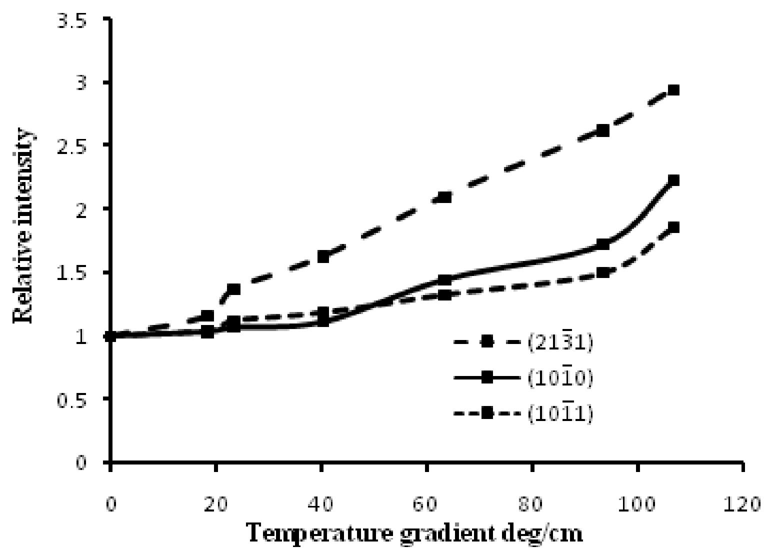

Fig.2. Dependence of the integrated intensity of reflected beam on the temperature gradient for different atomic planes

Considering the experimental results, it can be concluded that the increase in intensity of reflected beam is caused by the increase in the reflectivity of atomic planes and their bending [7] under the influence of the temperature gradient.

3. Theory

We consider the case of a symmetrical transmission in the Laue geometry, with the oriented crystal near the Bragg condition and reflecting atomic planes perpendicular to the front surface of the crystal.

When the crystal is influenced by the temperature gradient perpendicular to the front surface of the crystal (opposite direction of axis *Z*), the crystal is deformed and the reflecting planes of perpendicular to this surface take the form shown in Fig. 3. In this case, the reflecting planes make a small angle φ with the axis *Z*. In the absence of the temperature gradient of $\varphi = 0$.

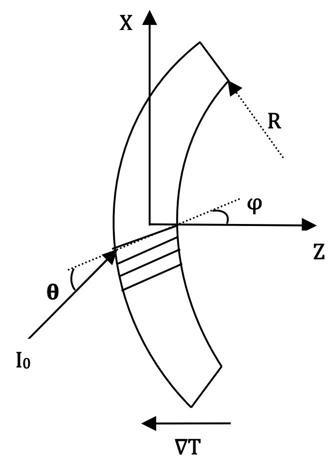

Fig.3. Diagram deformed crystal under temperature gradient perpendicular to front surface

The main parameter that determines the behavior of the wave field in the crystal is the scalar product $\boldsymbol{h}.\,\boldsymbol{u}(\boldsymbol{r})$, where $\boldsymbol{h}$ is reciprocal lattice vector for the family of atomic planes *(hkl)*, and $\boldsymbol{u}$ is displacement vector of scattering centers from their equilibrium positions due to the deformation [8]. Under the conditions of constant temperature gradient, displacement vector components in the scattering plane $(y = 0)$ have the following form [9]

$$U_x = \frac{xz}{R} \qquad , \qquad U_z = \frac{(z^2 - x^2)}{2R}\,, \tag{2}$$

Where $R = \pm[\nabla(aT)]^{-1}$ is the radius of curvature of the atomic planes perpendicular to ∇T and a is the coefficient of thermal expansion of the crystal. Therefore, we have

$$\boldsymbol{hu}(\boldsymbol{r}) = \frac{hxz}{R} + \frac{h(1-\gamma)}{2R}(z^2 - x^2), \tag{3}$$

where $\gamma = \frac{\gamma_h}{\gamma_0}$ is factor asymmetrical as γ_0 and γ_h are direction cosines for the incident and reflected directions, respectively.

According to Eq. (3), if $\varphi = 0 (\gamma = 1)$ the second term becomes zero, and the wave field is propagated in the crystal without feeling any tension. However, even small shifts from symmetrical geometry are significant from the point of view of the formation of the diffraction of the wave field in the lattice. Now, using the results of Refs. [6,10], integrated intensity of reflected beam with weak deformation can be written as

$$R_i = \frac{\pi|\chi_{hr}|}{2sin2\theta_b} e^{-\frac{\mu t}{cos\theta_b}} I_0 \left(\left(\frac{2\pi k|\chi_{hi}|}{cos\theta_b} - \frac{\alpha}{2\pi k|\chi_{hr}|} \right) t \right), \qquad (4)$$

where $I_0(y)$ function is of modified Bessel, χ_{hr} and χ_{hi} are real and imaginary parts of the Fourier coefficients of the crystal polarizability, μ is linear absorption coefficient of the crystal, t is a thickness of the sample, and

$$\alpha = \frac{\partial^2(\boldsymbol{h}.\boldsymbol{u})}{2\partial z^2} = \frac{(1-\gamma)ha}{2} \frac{dT}{dx}, \qquad (5)$$

The behavior of the integrated intensity is as a function dependent on the deformation parameter α, the integrated intensity decreases with α increasing, it reaches a minimum at

$$\alpha = \frac{4\pi^2 k^2 |\chi_{hi}||\chi_{hr}|}{cos\theta_b}, \qquad (6)$$

With further increase in α, the integrated intensity exponentially increases in the range of applicability approximation formula (4). Note that due to the smallness of the parameter α, the minimum integrated intensity is very close to the value $\alpha = 0$. The rest of the formula (4) fairly well describes the experimental dependence of R_i on α.

4. Conclusion

Thus, it was shown that with by applying the temperature gradient parallel to the reflecting atomic planes of quartz single crystal, atomic planes deformed to fan-shape and with the increase in the temperature gradient, the integrated intensity of the reflected beam increased. The experimental results obtained, were qualitatively described using an approximate solution of dynamical diffraction of the X-ray wave in weakly deformed crystals.

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