

Dynamical Diffraction of X-Ray in Single Crystal ADP with a Fan-Shaped Deformation

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Abstract: The effect of the fan-shaped deformation in the integral intensity of the reflected X-rays from single crystal of Ammonium Dihydrogen Phosphate (ADP) was investigated in case the Laue geometry. It was found with the increase of the temperature gradient, the integrated intensity of the reflected X-ray beam increase more than 100% for both of different linear absorption coefficients. A theoretical analysis of the dependence on the temperature gradient is applied to explain the results.

Key words: X-ray diffraction, ADP crystal, intensity of the reflected X-rays, fan-shaped deformation, analysis, single

INTRODUCTION

After the pioneering work of Fox and Carr (1931), Nishikawa *et al.* (1931) 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.

The phenomenon of full transfer of X-ray intensity from the direction of transmission into the direction of reflection has been observed in thin crystals under the influence of the temperature gradient (Mkrtychyan *et al.*, 1982).

Mirzoyan *et al.* (2010) first studied the phenomenon of reducing the linear absorption coefficient of quartz for a plane X-ray wave under the influence of a temperature gradient perpendicular to the reflecting atomic planes. Due to 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 approximately 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 (Mirzoyan *et al.*, 2010, 2014). It is 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 study presents the results of the effect of the fan-shaped deformations in the integrated intensity of the reflected X-rays from the single crystal ADP in Laue geometry under the influence of the temperature gradient parallel to the reflecting atomic planes.

MATERIALS AND METHODS

The crystal was deformed under influence of the temperature gradient perpendicular to the front surface of the crystal (opposite direction of axis Z). The crystal takes bent shape. In this case, the angle between reflecting atomic planes and axis Z is not zero and its value increases with the increase of temperature gradient.

The main parameter that determines the behavior of the wave field in the crystal is the scalar product $h \cdot u(r)$ where h is reciprocal lattice vector for the family of atomic planes (hkl) and $u(r)$ is the vector function of relative displacement of atoms due to the deformation (Authier, 2001). Under the conditions of constant temperature gradient (Penning and Polder, 1961), displacement vector components in the scattering plane ($y = 0$) have the following form:

$$U_x = \frac{XZ}{R}, U_z = \frac{(Z^2 - X^2)}{2R} \quad (1)$$

where, $R = \pm[\nabla(\lambda T)]^{-1}$ is the radius of curvature of the lattice planes perpendicular to ∇T and γ is the coefficient of thermal expansion of the crystal. So, we have:

$$h \cdot u(r) = \frac{hxz}{R} + \frac{h(1-\gamma)}{2R} (z^2 - x^2) \quad (2)$$

where, γ is factor of asymmetric and its value is less than or equal to unit in case of the Laue geometry. The value γ dependent on temperature gradient such that the increase of the temperature gradient results in the decrease of γ . According to Eq. 3, if $\gamma = 1$ the second term becomes zero and the wave field propagated in the crystal

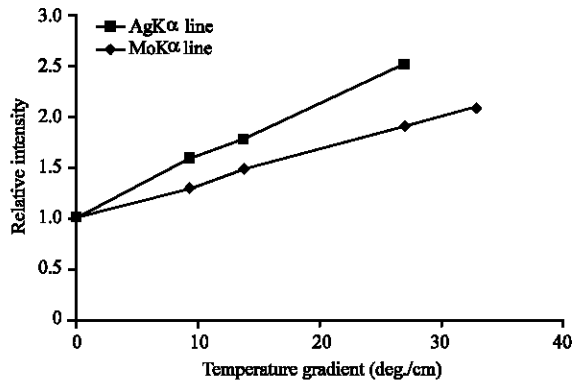


Fig. 1: Dependence of the integrated intensity of reflected beam on the temperature gradient, solid curve: AgKα line, dash curve: MoKα line, experimental

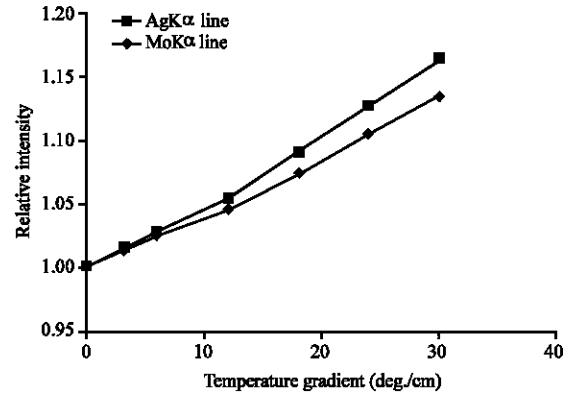


Fig. 2: Dependence of the integrated intensity of reflected beam on the temperature gradient $\bar{\gamma} = 0.8$, solid curve: AgKα line, dash curve: MoKα line, theoretical

without feeling any tension. So, the change in γ is significant from the point of view of the diffraction formation of the wave field in the lattice. Now, using the results of Trouni *et al.* (2012), Mirzoyan *et al.* (2014) integrated intensity can be written as:

$$R_i = \frac{\pi |xhr|}{2\sin 2\theta_b} e^{-\frac{\mu t}{\cos \theta_b}} I_0 \left(\frac{t}{\cos \theta_b} \left(2\pi k |xhri| - \frac{|\alpha|}{2\pi k |xhr|} \right) \right) \quad (3)$$

where, $I_0(y)$ function is modified Bessel, χhr and χhi are real and imaginary parts of the Fourier coefficients of the crystal polarizability, μ is linear absorption coefficient of the crystal, t is thickness of the sample and:

$$\alpha = \frac{(1-\gamma)h}{2R} = \frac{(1-\gamma)h\lambda}{2} \frac{dT}{dx} \quad (4)$$

The sign of α is determined by the sign of R . From the behavior of the Bessel function, it is obvious that in case $\alpha < 0$ with the increase in $|\alpha|$, the integrated intensity first drops to a minimum $\alpha = 4\pi^2 k^2 |\chi hi| |\chi hr|$ at then rises exponentially (Mirzoyan *et al.*, 2010, 2014). In case $\alpha > 0$, the integrated intensity also rises with increasing $|\alpha|$ but unlike the first case, there is not a minimum. The latter case corresponds with the above experimental results. Figure 1 and 2 show the variations integrated intensity with the temperature gradient. Plots in Fig. 1 and 2 demonstrate that the changes of integrated intensity of reflected beam in low temperature gradient are linear. In addition, decreasing the values of asymmetric factor of crystal, leads to the increase of integrated intensity of the reflected beams.

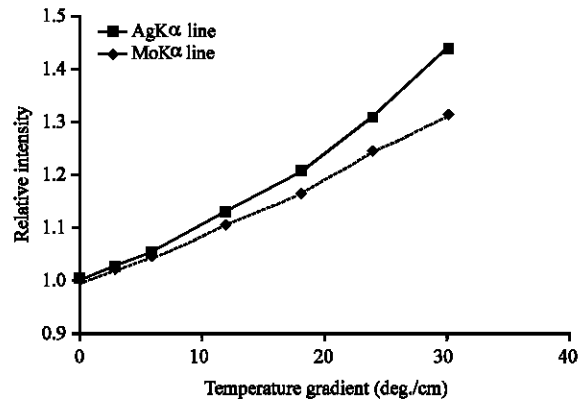


Fig. 3: Dependence of the integrated intensity of reflected beam on the temperature gradient, $\bar{\gamma} = 0.6$, solid curve: AgKα line, dash curve: MoKα line, theoretical

RESULTS AND DISCUSSION

The experimental procedure and results: Experiments were performed by diffractometer-DRON-3M, X-ray tubes BSV-29 used with anodes of Ag or Mo and with the horizontal size of focal spot 0.4 mm and vertical size 8 mm. Integrated intensity of the diffracted X-ray beam was measured by using scintillation counter with FEU-85. Thickness of single crystal of ADP was 1.88 mm. The hot-air blower was used to increase of temperature of the front surface of crystal. Using this device has the advantage of uniformly heating the front surface of the crystal. Figure 3 shows variations of the integrated intensity of the reflected beam from the atomic planes (002) of single crystal of ADP for AgKα and MoKα lines with the temperature gradient applied parallel to the

reflecting atomic plane in the Laue geometry. As can be seen for both lines, despite the fact that the linear absorption coefficient of $\text{MoK}\alpha$ twice $\text{AgK}\alpha$, for $\text{AgK}\alpha$ 2.75 cm^{-1} and $\text{MoK}\alpha$ 5.4 cm^{-1} , the integrated intensity of the reflected beams has a linear character. It is evident that in both cases $\mu t \leq 1$ (μ is the linear absorption coefficient and t the thickness of single crystal) provides thin crystal condition and therefore the dependence of the intensity of the reflected beam on the temperature gradient be have similarly. Considering the experimental results, it can be concluded that the presence of the temperature gradient and the deformation of reflecting atomic planes causes the integrated intensity of the reflected beam to increase.

CONCLUSION

It is shown that with the increase in temperature gradient applied parallel to the reflecting atomic planes of ADP single crystal, deformation of fan-shape atomic planes, the integrated intensity of reflected beam increases relatively linearly. The theoretical results obtained which are based on an approximate solution of dynamical diffraction of the X-ray wave in weakly-deformed crystals are in agreement with experimental results.

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