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INVESTIGATION OF ROCKING CURVE OF REFLECTION ON SINGLE CRYSTALS OF ADP UNDER INFLUENCE OF TEMPERATURE GRADIENT

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Abstract – Rocking curves of reflectivity for ADP crystal have been measured under influence of temperature gradient in Laue-case geometry. We observed that increase in value of the temperature gradient lead to increase of reflectivity and also increase of width of rocking curve slightly. Experimental results are compared with theoretical results based on the asymptotic solution of dynamical diffraction of X-ray wave in crystals with weak deformation. An agreement between both results is obtained.

Keywords: ADP crystal, X-ray reflection, temperature gradient, rocking curves

1. Introduction

The investigation of x-ray diffraction on deformed crystals under external influence began in 1930 [1, 2] then this technical expanded rapidly. The deformation in single crystals was carried out in various ways such as the thermal fields, ultrasonic resonance, mechanical bending. In [3] silicon crystal rocking curves are measured under condition of the Borrmann effect resonant by transverse ultrasonic vibrations. In the present work the effect of temperature gradient on the rocking curve of reflection for ADP crystal was studied experimentally and theoretically.

2. **Experimental results**

Experimental studies were performed according to the schemes with two crystals. X-ray tube BSV-Mo 27 was used as a source radiation. Experiment carried out for (002) reflecting atomic plane of ADP crystal with thickness of 1.9 mm in the presence of a temperature gradient perpendicular to the reflecting atomic plane. The intensity of reflected X-rays was recorded by a scintillation counter.

Figure 1 shows the rocking curves of reflectivity from (002) ADP crystal for different values of the temperature gradient applied to the crystal. As is seen, with increase of temperature gradient, reflectivity increases while the width of rocking curve increases slightly. As an example, at no temperature gradient reflectivity is 27% and FWHM is 4.6×10^{-5} rad but with increase in the temperature gradient to 18 deg/cm, reflectivity and FWHM changes to 47% and 5.6×10^{-5} rad, respectively.

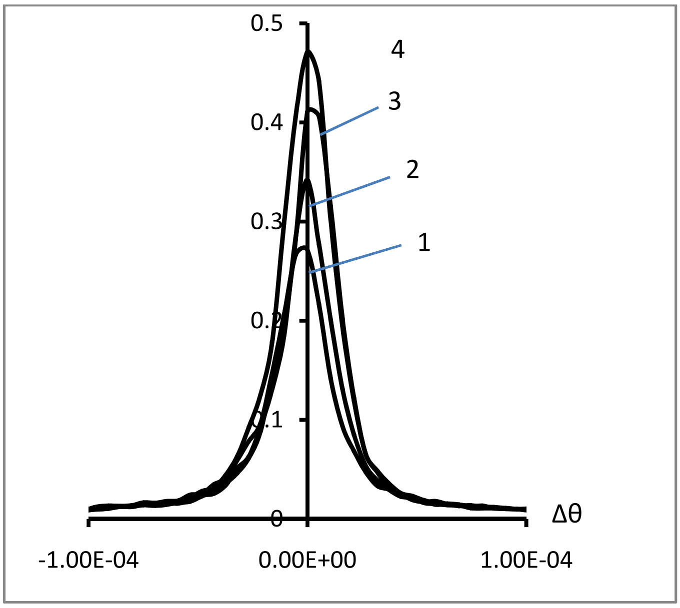

Fig.1. The rocking curves of reflectivity from (002) ADP crystal for different values of the temperature gradient (1- dT/d*x* = 0, 2- dT/dx =6 deg/cm, *3* - dT/dx =12, 4- dT/dx =18 deg/cm), experimental.

3. Theory

In our case (symmetrical reflection, Laue geometry) temperature gradient led to bend perpendicular reflecting atomic planes of lattice, the radius of curvature of these planes is the following:

$$R = \pm|\nabla(aT)|^{-1}, \tag{1}$$

where a is the linear coefficient of thermal expansion, and the sign of the curvature of the planes defined by the sign ∇ (aT).

Reflectivity of symmetric Laue geometry without influences of external force is defined by the following formula [5]:

$$I_R = \frac{e^{\frac{-\mu z}{\cos\theta_B}}}{2(1+p^2)} \times \left[\cosh\left(G_i \frac{z}{\cos\theta_B}\right) - \cos\left(\frac{2\pi kc|X_{hr}|}{\sin\theta_B}\sqrt{1+p^2}z\right)\right], \tag{2}$$

$$G_i = (2\pi k|X_{hi}|) \times \frac{1}{\sqrt{1+p^2}}, \tag{3}$$

where θ_B is the Bragg angle, μ is the linear absorption coefficient of the crystal, p is the deviation parameter from the Bragg angle, χ_{hi} and χ_{hr} are the imaginary and real parts of Fourier coefficient of the crystal polarizability, respectively.

In [4] it is given an asymptotic solution based on dynamical diffraction of X-ray wave in crystals with weak deformation. In [6] we were shown situation of our experiment satisfying condition of weak deformation. According to obtained results in [4], one should replace the term $2\pi k\chi_{hi}$ by $2\pi k\chi_{hi} - \frac{\alpha}{2\pi k|X_{hr}|}$ in the reflectivity formula. Here α is the parameter of crystal deformation and under influence of the temperature gradient is equal to

$$\alpha = \frac{h}{2R} = \pm\frac{ha}{2}\frac{dT}{dx}, \tag{4}$$

where h is the magnitude of diffraction vector of corresponding reflection. Expression (3) under influences of temperature gradient is converted to

$$G_i = (2\pi k|\chi_{hi}| \mp \frac{|\alpha|}{2\pi k|\chi_{hr}|}) \times \frac{1}{\sqrt{1+p^2}}. \tag{5}$$

The sign of α is determined by the sign of R in (1). The behavior of reflectivity dependence on the sign of α is determined with notice (2) and (5). It is obvious for $\alpha>0$ thast with increase in temperature gradient, reflectivity initially drops to a minimum and then begins to increase. This phenomenon was investigated in [6]. For case $\alpha<0$ reflectivity increases with the increase in temperature gradient. We suppose latter case for reflectivity from atomic plane (002) of ADP crystal.

4. Determination of χ_{hi} and χ_{hr}

For calculation of reflectivity it is necessary to know actual values of χ_{hi} and χ_{hr}. For this purpose, in case of absence of temperature gradient and exact Bragg angle (p=0) the reflectivity was measured then applying (2), the value of χ_{hi} is obtained

$$\chi_{hi} = 0.6 \times 10^{-8},$$

Also with measurement of Darwin width and using the relation below

$$\delta_{0s} = \frac{\sqrt{\chi_h \chi_{\bar{h}}}}{\sin 2\theta_B}, \tag{6}$$

the value of χ_{hr} is estimated:

$$\chi_{hr} = 0.2 \times 10^{-5}.$$

5. Rocking curve under influence of temperature gradient

For simplicity, we ignore term of cosine in (2). Theoretical formula of reflectivity was obtained by relations (2) and (5) for atomic plane (002) of ADP crystal with thickness 1.9 mm under influence of different temperature gradient. Figure 2 shows theoretical and experimental rocking curves of reflectivity for different values of temperature gradient.

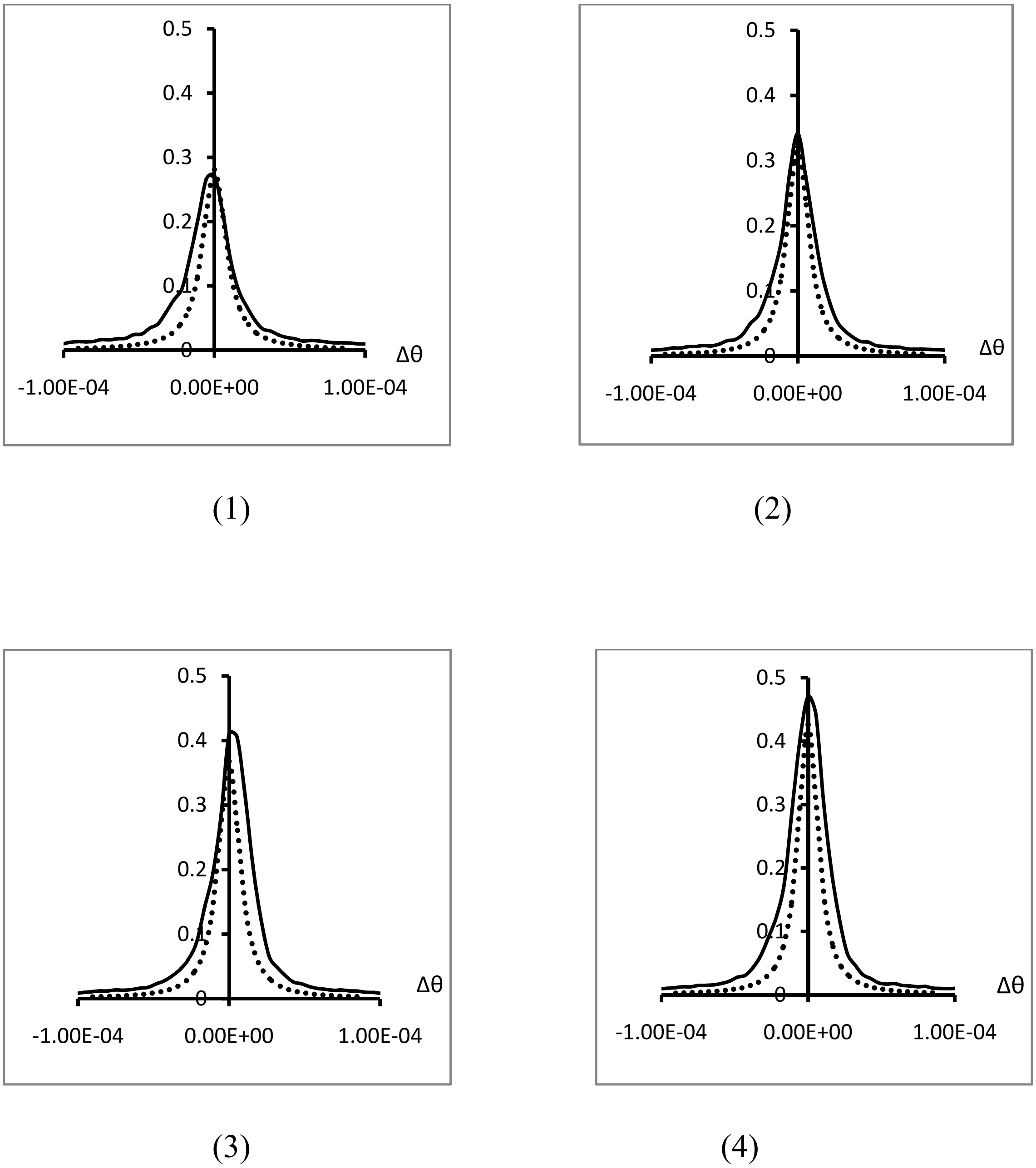

Fig.2. The rocking curves of reflectivity from (002) ADP crystal for different values of the temperature gradient; solid curve: experimental, dotted curve: theoretical, 1- dT/dx = 0 deg/cm , 2- dT/dx =6 deg/cm, 3- dT/dx =12 deg/cm, 4- dT/dx =18 deg/cm.

As can be seen, the values of theoretical reflectivity at exact Bragg angle ($\Delta\theta = 0$) are in good approximation with corresponding practical results. Table 1 shows Percentage of difference between experimental and theoretical values of reflectivity. On the other hand, width of theoretical rocking curves changes weakly with the increase of temperature gradient while in practical case width of rocking curves has slight increase.

Table.1. Experimental and theoretical values of reflectivity at exact Bragg angle.

$\Delta T/\Delta x$ (degree/cm)	Reflectivity (theoretical)	Reflectivity (experimental)	Percentage of difference
0	0.28	0.27	4%
6	0.32	0.34	6%
12	0.37	0.41	11%
18	0.43	0.47	9%

6. Conclusion

In this paper, by applying an asymptotic solution of dynamical diffraction of X-ray wave in crystals with weak deformation, a formula for reflectivity was obtained for ADP single crystal under influence of temperature gradient, which is in relatively good agreement with experimental results.

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