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Дифракция импульсного пучка тепловых нейтронов на упруго-деформированной пластине монокристалла кварца

В работе представлены данные упругого рассеяния нейтронов, полученные методом времени пролета на изогнутой пластине монокристалла кварца. Полученные интегральные интенсивности брэгговского отражения от определенной плоскости кристаллической решетки, как функция упругого изгиба кристаллической пластины, показывают линейную зависимость в соответствии с теоретическим представлением.

Работа выполнена в Лаборатории нейтронной физики ОИЯИ.

Препринт Объединенного института ядерных исследований
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Eichhorn F. et al. **E14 - 10215**

Diffraction of a Pulsed Thermal Neutron Beam on an Elastically Bent Quartz Crystal Plate

The results of elastic neutron scattering with the time-of-flight method on a bent quartz single crystal plate are presented. Integrated Bragg intensities measured for a fixed lattice plane as a function of elastic bending of the crystal plate show a linear dependence in correspondence with the theoretical expectations.

The investigation has been performed at the Neutron Physics Laboratory, JINR.

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1. INTRODUCTION

For a number of neutron scattering investigations a problem arises - the opposite behaviour of the resolution function and luminosity of a monochromator or analyser unit. Therefore, in order to avoid the loss of intensity the resolution should not be better than necessary for a given problem.

It is possible to obtain a very high energy, wavelength or lattice constant resolution using the perfect crystals as a monochromator and analyser, due to the fact that a perfect crystal has a very narrow interference function, which means a precise relationship between the wavelength (energy) of incident or scattered neutrons and incidence or scattering angle. Therefore, the intensity of the scattered radiation or the luminosity of a perfect crystal is only relatively small. If one chooses a crystal with an increasing degree of lattice defects (up to the so-called mosaic crystal), then simultaneously the intensity increases, but the resolution decreases. The aim of our work was to test a crystal unit with an adjustable resolution and thus a luminosity which might be optimized for a given experimental problem. For this purpose we bent a nearly perfect quartz crystal plate elastically and homogeneously and measured the diffracted intensity.

It is known that the reflecting power of nearly perfect crystals for X-rays and neutrons increases, if they are distorted elastically[1]. So, a bent quartz crystal demonstrates an increase of the X-ray intensity nearly up to that of a mosaic crystal[1]. Bent crystals were also used for the intense monochromatization of thermal neutrons based on the geometrical effect of focusing[2,3] or on the decrease of extinction[4,5]. The diffraction of thermal neutrons on elastically bent silicon crystals was investigated both theoretically and experimentally[6,7].

2. MATERIAL AND ITS BENDING

The quartz crystal was grown hydrothermally by VEB Carl Zeiss Jena, GDR. From it a plate of about 150x180x3.1 mm^3 had been cut perpendicularly to the crystallographic z-axis (z-cut). It contains lattice defects in a small degree caused only by inhomogeneous growth. The surface was polished by the conventional method used in optics production. The plate was placed into a mechanical unit for bending[8] (Fig.1). The two symmetrically arranged pairs of long steel cylinders (2.3 in Fig. 1) were pressed against each other with the aid of a screw and a nut (6 in Fig. 1). The frames 4 and 5 distributed the force to the cylinders. Then the quartz crystal plate (1 in Fig. 1) was freely curved cylindrically. The axis of bending is parallel to

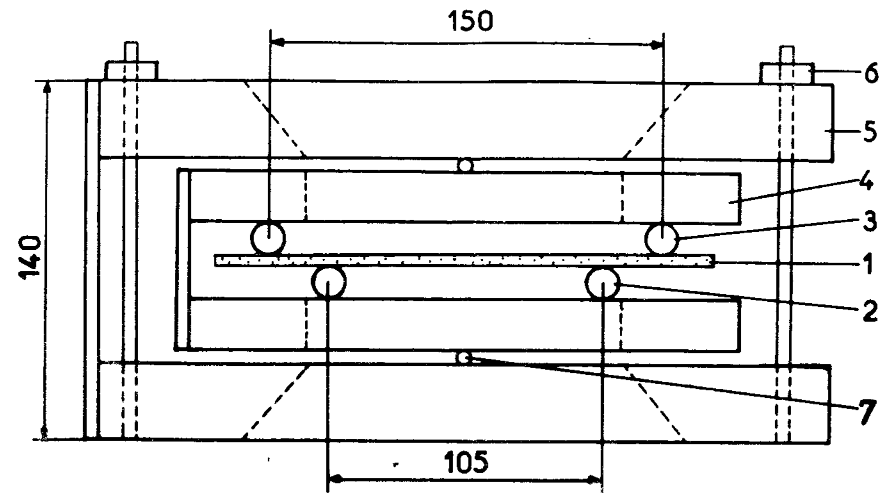

Fig. 1. Device for bending the quartz crystal plate. Denotation of the used symbols: 1 - quartz crystal plate, 2,3 - steel cylinders 15 mm in diameter, 4,5 - steel frames, 6 - a screw, 7 - a steel cylinder.

the crystallographic x-direction. The curvature was measured by a dial indicator following the deviation of the middle of crystal's surface from the plane of the unbent crystal plate.

3. THEORETICAL CONSIDERATIONS

Klar and Rustichelli[6] gave a detailed theoretical treatment of the dynamical neutron diffraction by ideally curved crystals. They demonstrated that the solution of fundamental equations of the dynamical theory for homogeneously bent crystals gives nearly the same result as a simpler calculation founded on the model which approximates the bent crystals to a suitable arrangement of perfect crystallites. We can use their results with the supposition that our bent quartz crystal plate is an arrangement of perfect crystals, which are tilted against one another at an angle smaller than the width of the interference function of a perfect crystal. This width is of the order of seconds of arc. Roughly speaking the integrated diffracted intensity depends both on the width and on the height of the interference function. Perfect and nearly perfect crystals have a maximum reflecting power of 1 in the Bragg case of nonabsorbing crystals. Only the width of this function increases if the crystal is bent. The full width at half maximum consists of the two parts: the first one is equal to the intrinsic width of perfect crystal's interference function and the second one increases nearly proportional to a factor $c \cdot A$, where c describes the effect of crystal bending on the dynamic interference. The parameter A depends on the properties of the neutrons and on the perfectness of the crystal. Exactly [6]

$$c = dy/dA .$$

The symbols used are the same as in Zachariansen's book [9]. It means

$$y = \frac{\pi \cdot V \cdot \sin 2\theta_B}{|F_{HN}| \cdot \lambda^2} (\theta_B - \theta),$$

V is the volume of the unit cell; θ_B is the Bragg angle; F_{HN} is the structure factor; λ is the wavelength; θ is the actual glancing angle; $A = \frac{|F_{HN}| \cdot \lambda \cdot t}{V \cdot \cos\theta_B}$; t is the thickness of the crystal plate.

Therefore the integrated diffracted intensity increases proportionally to the parameter c (the parameter A is constant for a given reflection on one and the same crystal). The parameter c linearly depends on the curvature (for instance, the deviation of the crystal surface in the middle of the bending device). A detailed numerical solution of the fundamental equations of the dynamical theory for distorted crystals [6] shows, that a nearly linear dependence of the integrated diffracted intensity on the papameter c exists, if the crystal is not too thin ($1 < A < 10$). This result corresponds to that obtained using a simpler model described above. If the curvature of the crystal increases, then no overlapping of the interference functions of neighbouring crystalline parts exists. This is valid for $c > 1$. It means that the integrated intensity reaches a saturation value for higher bending. Table 1 contains values of the parameter c for our experimental conditions. From it follows that one can expect an increase of the integrated intensity for reflections with low index and nearly no change in the integrated intensity for reflections with high index.

4. EXPERIMENT

To test the perfection of the crystal plate we measured the rocking curve on

Table 1

Values of the bending parameter c.

radius of curvature in m \ reflection	0003	0006	0009	00012	00015	00018
68.9	0.11	0.22	0.15	1.67	2.32	2.27
34.5	0.22	0.44	0.29	3.34	4.63	4.54
23.0	0.33	0.66	0.44	5.01	6.96	6.82
17.2	0.45	0.88	0.59	6.70	9.30	9.10

a neutron diffractometer at the steady Rossendorf research reactor. This curve for the ($1\bar{1}00$) reflection in the symmetrical Laue case is given in Fig. 2. The divergence of the neutron beam was limited by Soller collimators within the reactor channel and immediately in front of the BF_3 counter. In this experimental arrangement for completely perfect crystals the full width at half maximum was 6 minutes of arc, as determined by a silicon single crystal with a reflection width of 3 seconds of arc. Therefore, the crystal under investigation may be considered as a nearly perfect one. The intensity dependence on the glancing angle is given by the divergence and intensity distribution of the primary beam only and no influence of any crystal lattice distribution or lattice constant's variation is detectable. Certainly the width of a possible mosaic distribution is smaller than one minute.

The experiments with the bent crystal were performed at the pulsed reactor IBR-30 of JINR, Dubna. In Fig. 3 the experimental

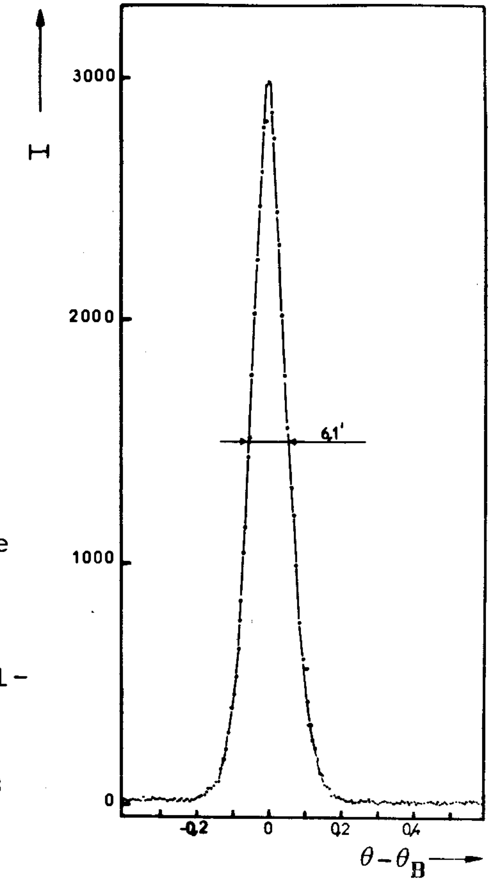

Fig. 2. The rocking curve of the used quartz crystal plate for the ($1\bar{1}00$) reflection in the symmetrical Laue case. I - intensity in pulses per minute, θ - deviation from the fixed Bragg angle θ_B in degrees.

setup is shown. The whole reactor-crystal flight path is about 33 m. The neutron beam strikes the quartz plate at a Bragg angle of 67.5°. Since the primary neutron beam is polychromatic the (0003) reflection and its higher orders are excited in the symmetrical Bragg case. The time-of-flight

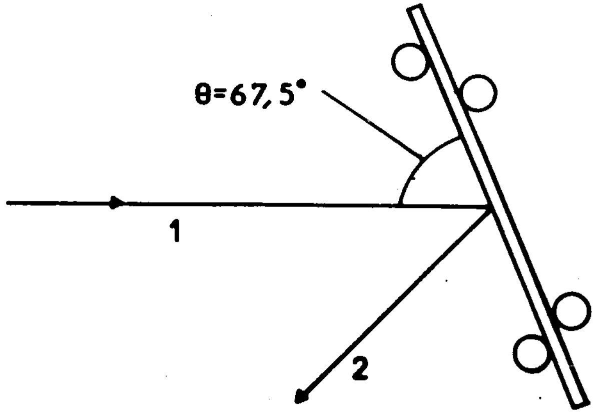

Fig. 3. The scheme of the experimental arrangement. 1 - incoming white neutron beam, 2 - from the crystal Bragg reflected beam.

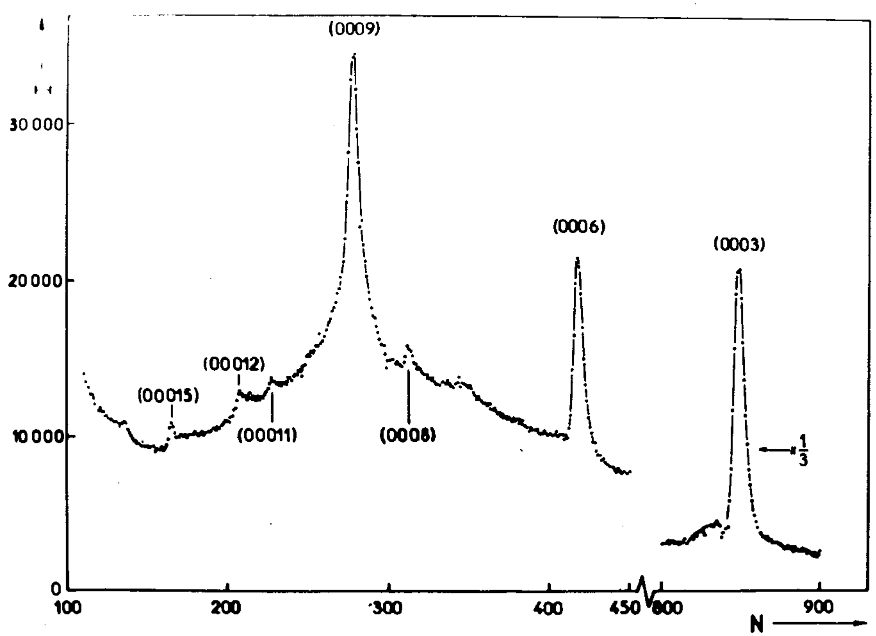

Fig. 4. A typical TOF spectrum for the bent crystal plate obtained after about 2 hours of measuring time. I - intensity in pulses per channel, N - channel number. The channel width was 32 μsec.

spectrum of diffracted neutrons was obtained with a 4K- memory time analyzer with the channel width of 8 and 32 μ sec. A typical time-of-flight spectrum is shown in Fig. 4. We have carried out the measurements with the bent crystal plate with a radius of curvature ranging from ∞ to 17 m. The axis of bending is perpendicular to the plane of incident and diffracted neutron beams.

Table 2 shows the wavelength λ, the value of the structure factor $|F_{HN}|$, the parameter A for the given thickness, and the FWHM of the interference function.

Table 2

Values of λ, $|F_{HN}|$, A, and FWHM for the experimental conditions taken

reflection	λ in Å	$|F_{HN}|$ in 10^{-14} m	A	FWHM in sec of arc
0003	3.32	0.96	230	1.75
0006	1.66	0.61	73	2.78
0009	1.11	4.32	346	0.88
00012	0.83	1.98	119	0.23
00015	0.66	2.34	113	0.17
00018	0.55	3.12	125	0.16

5. RESULTS

In the time-of-flight spectrum (Fig. 4) the (0003) reflection and its higher orders (0006), (0009), (00012), (00015), and (00018) can be noticed, moreover, the reflections (0008), (00011) appear. The α-quartz used possesses a rhombohedral structure with lattice constants $a = 4.91$ Å and $c = 5.39$ Å. According to the crystallographic conditions the reflections from the basal plane must have the Miller indices (000ℓ), $\ell = 3n$; so the reflections (0008) and (00011) must vanish (Fig. 4). The reflection (0009) coincides with a satellite of the pulsed reactor, therefore, we do not take it into consideration.

Table 1 shows the integrated diffracted intensity in relative units for the reflections observed in dependence on the curvature of the crystal plate. The measured intensities for different tests are standardized comparing the background intensities over the whole spectrum of neutrons. The width of the interference function is expected to increase with increasing curvature of the crystal as a greater wavelength interval can be reflected within a given divergence angle. For our experimental conditions this additional width is expected to be about 0.3 per cent of the reflection width in the time-of-flight spectrum for the minimum radius of bending. This value lies more than one order under the experimental error, so that the change of the width of the interference peaks could not be observed.

6. DISCUSSION

Table 3 demonstrates clearly the increased integrated diffracted intensity with increasing elastic deformation of the quartz crys-

Table 3

Relative integrated diffraction intensities

radius of curvature in m \ reflection	0003	0006	0008	00012	00015	00018
∞	20920	30060	5037	7865	7323	4693
68.9	37920	70000	7555	9120	8370	5495
34.5	41660	75450	8302	9127	8401	4619
23.0	47400	76380	10080	8137	6979	3778
17.2	57000	84540	9840	8425	9727	3537

tal plate. In Fig. 5 the dependence of the intensity of the (0006) reflection on the curvature of the crystal plate is shown. In correspondence with the theoretical expectations a linear dependence exists between intensity and bending. Table 4 gives the slope of straight lines in Fig. 5. They are defined by the dependence of the integrated diffracted intensity on the curvature. The intensity of reflections with lower Miller indices (0003, 0006) increases remarkably if the crystal is bent. This dependence tends to zero (within the experimental error) for higher reflection orders (00012, 00015, 00018) as expected.

From the above considerations we can conclude that the increase of intensity is caused by the fact that with the bent crystal one can better use the divergence of the primary beam in the reflections of low order.

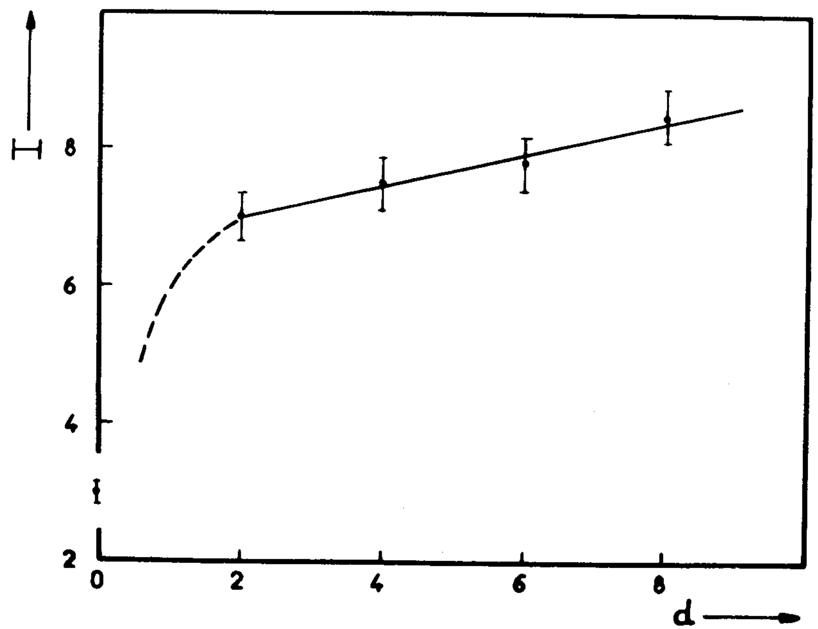

Fig. 5. Integrated intensity of the (0006) reflection as a function of the curvature of the crystal plate. I - intensity in arbitrary units, d - deviation of the middle of the crystal's surface from the unbent position in units of 10^{-2} mm.

Table 4

Slope of the straight line, defined by the dependence of the integrated diffraction intensity on the curvature/10^6 pulses mm^{-1}.

reflection	0003	0006	0008	00012	00015	00018
	32.2	23.2	4.7	0.1	1.3	-2.5

Between the intensity of the unbent crystal and the extrapolated value of the linear dependence of the intensity on the crystal bending a jump exists, especially for the reflections of low order. We know that the quartz crystal plate has not a completely perfect crystal lattice, i.e., contains some defects, so we can think about the influence of a secondary extinction effect on the intensity variation. Our actual crystal should consist of large "mosaic" blocks, which have a dynamic reflection power R_i^{dyn} and which are tilted only by a very small angle (less than 1′) against one another. Then no influence of this extinction exists if the crystal is bent. Using this assumption, then the quotient of the linearly (to curvature radius ∞) extrapolated intensity of the bent crystal $R_i^{bent}(r \to \infty)$ and the intensity of the unbent crystal R_i^{unbent} is /10/

$$\frac{R_i^{bent}(r \to \infty)}{R_i^{unbent}} = \sqrt{1 + 2gR_i^{dyn}} \; .$$

The parameter g is inversely proportional to the half-width of the assumed "mosaic distribution". It is possible to fit the measured jumps with $g \approx 2 \times 10^4$, which corresponds to a half-width of nearly 3.5 seconds of arc. The fact that the width of a possible mosaic distribution is much smaller than one minute of arc is consistent with our measurements.

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