JETP Letters, Vol. 81, No. 3, 2005, pp. 99–101. Translated from Pis'ma v Zhurnal Éksperimental'noĭ i Teoreticheskoĭ Fiziki, Vol. 81, No. 3, 2005, pp. 129–132.

Observation of the Elastic Quasi-Mosaicity Effect in Bent Silicon Single Crystals

Yu. M. Ivanov*, A. A. Petrunin, and V. V. Skorobogatov

Petersburg Nuclear Physics Institute, Russian Academy of Sciences, Gatchina, 188300 Russia

** e-mail: yumi@pnpi.spb.ru*

Received December 6, 2004

A considerable elastic quasi-mosaicity effect has been observed upon the diffraction of x-rays on a bent silicon single-crystal plate. It has been shown that the effect depends on the choice of reflecting crystallographic planes and the orientation of the plate cut. The effect can be applied to improve the characteristics of silicon single-crystal monochromators of electromagnetic radiation and silicon single-crystal deflectors of charged-particle beams. *© 2005 Pleiades Publishing, Inc.*

PACS numbers: 07.85.–m, 61.10.–i, 61.85.+p

In crystal-diffraction gamma spectroscopy, the known elastic quasi-mosaicity effect for quartz arises when quartz plates, which are used for the diffraction of radiation in focusing spectrometers, are bent to a cylinder. The effect results in the broadening of the diffraction profiles of gamma lines and changes the linear dependence of the integrated reflection coefficient on photon energy to a quadratic dependence. This effect is attributed to the anisotropic properties of quartz, which lead to the bending of radiation-diffracting atomic plates coinciding with the normal cross sections of the unbent plate. The bending angle depends on the cut of the plate with respect to the crystallographic axes and can reach a value of several tens of angular seconds for certain crystallographic planes, which is several orders of magnitude larger than the natural mosaicity of quartz. The above explanation of the effect was given by Sumbaev [1–3] and used by him and his collaborators to increase the efficiency and resolution of focusing crystal-diffraction spectrometers.

At present, single-crystal silicon has become a widely used material for manufacturing diffraction plates. However, its elastic quasi-mosaicity is poorly studied. This circumstance stimulated the present study. Another motivation is the search for new methods for bending atomic planes of single-crystal silicon for the channeling of protons of high and ultrahigh energies by short crystals [4, 5].

A noticeable elastic quasi-mosaicity effect in silicon for the (022) crystallographic plane was predicted in [6], where some bending schemes in application to crystal-diffraction spectrometers were analyzed using the calculation procedure for the deformed state of a bent anisotropic crystal plate [7]. In accordance with the cut angle recommended in [6], a silicon plate with the (022) crystallographic plane perpendicular to the large faces was manufactured and analyzed on an x-ray diffractometer. No elastic quasi-mosaicity effect was found in this investigation.

To resolve the apparent contradiction, we performed new calculations of the elastic quasi-mosaicity effect using the procedure proposed in [7]. These calculations showed that the elastic quasi-mosaicity effect must be manifested for a silicon plate with the (111) plane perpendicular to the large faces, whereas the calculated elastic quasi-mosaicity effect vanishes for a plate with the (022) plane.

Figure 1 shows a plate of the orientation under consideration that is bent to a cylinder of radius ρ, along with plate-bending-induced change in the shape of the (111) crystallographic planes. In the calculation model, this change is associated with the coefficient k_9 entering into the expression for the x projection of the displacement Δr of an arbitrary plate point (x_0, y_0, z_0) in the plate coordinate system. This projection is represented in the form

$$\Delta r_x = -k_5 z_0^2 + k_{10} x_0^2 + 2k_{11} x_0 y_0 + k_9 y_0^2.$$

After bending, cross sections perpendicular to the large faces of the plate approximately take the shape of parabolic cylinders with the projection on the xy plane that is specified by the relation

$$x = k_9 y^2.$$

The coefficient k_9 for an arbitrary (hkl) crystallographic plane is determined by the elastic constants of the crystal, the cut angle of the plate in the (hkl) plane, the bending radius, and the bending method, which determines the boundary conditions of the problem. Figure 2 shows the coefficient k_9 as a function of the cut angle φ for the (111) plane and plate bending by the method of applied moments. As is seen, the coefficient

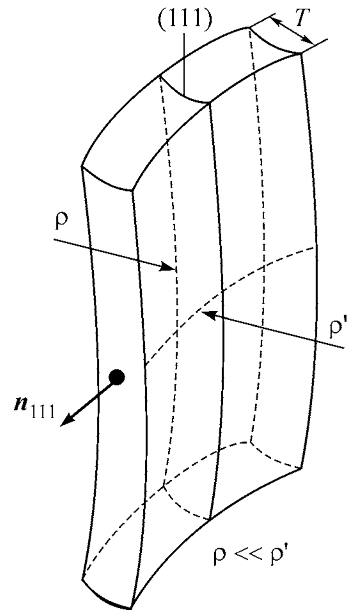

Fig. 1. Bending of the (111) crystallographic planes upon the bending of a silicon single-crystal plate to a cylinder of radius ρ. The radius ρ' characterizes the curvature in a plane perpendicular to the main bend plane.

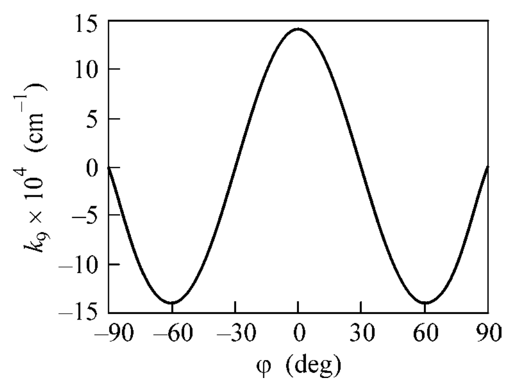

Fig. 2. Coefficient k_9 vs. the angle φ that characterizes the possible rotation of the plate cut about the normal to the (111) plane.

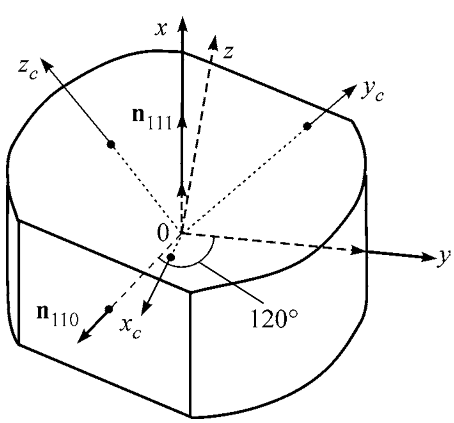

Fig. 3. Orientation of the plate coordinate axes *x,* y, and *z* that corresponds to the cut angle φ = 0° with respect to the silicon crystallographic axes x_c, y_c, and z_c for a sample grown along the [111] axis.

k_9 vanishes at the cut angles –90°, –30°, 30°, and 90° and takes an extreme value of 0.00141 cm^{-1} at the angles –60°, 0°, and 60°. The calculation was performed for a plate-bending radius of 1 m. Recalculation for another plate-bending radius is performed by dividing the coefficient k_9 by this radius measured in meters.

Figure 3 shows the orientation of the plate coordinate axes *x*, *y*, and *z* that corresponds to the cut angle φ = 0° with respect to the silicon crystallographic axes x_c, y_c, and z_c for a sample grown along the [111] axis. The axes of the *xyz* system are parallel to the plate edges, and the *xz* and *yz* coordinate planes are parallel to the large faces of the plate and the (111) crystallographic planes. The angle φ characterizes the possible rotation of the plate about the normal to the (111) plane and is measured from the *y* axis.

The calculated elastic quasi-mosaicity is determined by the bending of the (111) crystallographic planes, which is calculated for small strains as the difference between the derivatives of the function that describes the bending shape as calculated at the boundaries of the crystal. This bending is expressed by the formula

$$\Delta\theta = 2k_9T,$$

where Δθ is the plane bending and *T* is the plate thickness. It is seen that the elastic quasi-mosaicity follows the dependence of the coefficient k_9 on the cut angle φ.

On the basis of new calculations, a plate corresponding to the maximum coefficient k_9 was cut from single-crystal silicon. The plate has sizes 60 × 20 × 0.43 mm, and its orientation with the crystallographic axes is shown in Fig. 3 [the (111) plane is parallel to the 60 × 0.43-mm face]. The elastic quasi-mosaicity effect was experimentally observed on a two-crystal x-ray diffractometer [8] by measuring rocking curves before and after the bending of the plate to a cylinder.

Figure 4 shows the layout of the measurements. A tested silicon sample in the passage position was used as the first crystal, and a standard silicon crystal in the reflection position was used as the second crystal. The (111) crystallographic planes are diffracting planes in both crystals. An x-ray tube with a molybdenum anode was used as a radiation source. The beam incident on the sample under investigation was formed using a double-slit collimator, whose output slit had a width of 0.1 mm and a height of 5.0 mm. The angular divergence of the beam is equal to 1′, which is much smaller than the splitting of the fine-structure components. The Bragg diffraction angle for the MoK_{α_1} line in the first reflection order was equal to 6.5°, the natural width of the MoK_{α_1} line was equal to 9.2″, and the accuracy of determining the angular position of crystals was no worse than 0.5″.

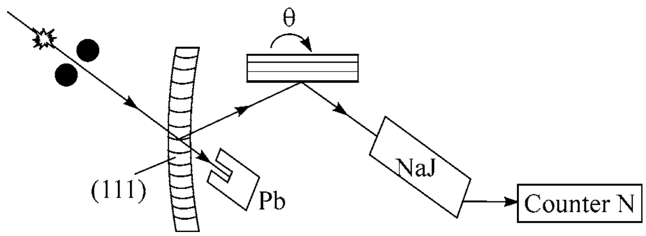

Fig. 4. Layout of rocking-curve measurement on a double-crystal diffractometer.

The measurement results are shown in Fig. 5, where both rocking curves are presented. The FWHM of the rocking curve of the unbent plate is equal to 6″ and is close to the width of the folding of diffraction curves of two ideal crystals. After the bending to a radius ρ = 92 cm, the rocking-curve width increases by a factor of 4 and reaches 24″ = 120 μrad. The observed broadening of the rocking curve agrees with the calculated elastic quasi-mosaicity, which is equal to 26″ and indicates a considerable elastic quasi-mosaicity effect in a bent plate. An increase in the width was accompanied by a considerable increase in intensity at the maximum of the rocking curve, which is a subject of special investigation that will be reported elsewhere.

Note that the shape of the bent plate differed from the cylindrical shape and was close to the saddle shape with a radius of ρ' = 410 cm in a plane perpendicular to the main bend plane (see Fig. 1). Deviation from the cylindrical shape is a common property of plates upon the bending by the method of applied moments, and the radius ρ' and curvature sign depend on the crystal symmetry, chosen crystallographic plane, and plate cut angle. Deviation from the cylindrical shape leads to broadening of the rocking curve. However, this broadening in the above measurement was much smaller than the elastic quasi-mosaicity effect.

A plate for a control experiment was made from the same ingot. This plate was identical to that studied above but differed in the cut angle, which was taken to be φ = –30° and corresponds to a calculated value of $k_9 = 0$. In the unbent state, the rocking curve of the plate with φ = –30° nearly coincides with a similar curve for the plate with φ = 0°. However, the control plate after the bending to a radius of ρ = 75 cm has absolutely different properties: the rocking curve is only slightly broadened and intensity at the maximum decreases simultaneously. This result is entirely explained by the deviation of the shape of the bent control plate from the cylindrical shape in the complete absence of the elastic quasi-mosaicity effect.

The experiment revealed the considerable elastic quasi-mosaicity effect in silicon and showed that a small change in the orientation of the cut of single-crystal silicon plates may significantly vary their deformed state upon bending. We think that the use of this effect may improve the characteristics of silicon single-crystal monochromators of electromagnetic radiation and silicon single-crystal deflectors of charged-particle beams.

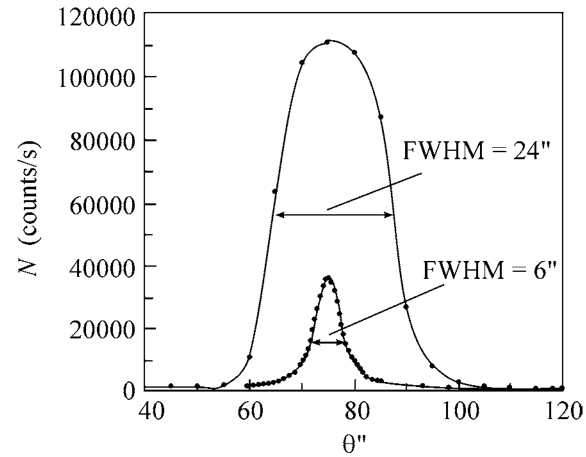

Fig. 5. Rocking curves for a plate notched at an angle of φ = 0° (6″) before and (24″) after bending.

We are grateful to S.A. Vavilov and M.A. Koznov for assistance in manufacturing the crystals and L.P. Lapina for help in preparing the manuscript. This work was supported by the Russian Foundation for Basic Research, project nos. 01-02-18005 and 01-02-17992.

REFERENCES

1. O. I. Sumbaev, Zh. Éksp. Teor. Fiz. **32**, 1276 (1957) [Sov. Phys. JETP **5**, 1042 (1957)].
2. O. I. Sumbaev, *Crystal-Diffraction Gamma Spectrometers* (Gosatomizdat, Moscow, 1963) [in Russian].
3. O. I. Sumbaev, Zh. Éksp. Teor. Fiz. **54**, 1352 (1968) [Sov. Phys. JETP **27**, 724 (1968)].
4. A. G. Afonin, V. T. Baranov, V. M. Biryukov, *et al.*, Phys. Rev. Lett. **87**, 094802 (2001).
5. A. G. Afonin, V. T. Baranov, V. M. Biryukov, *et al.*, Pis'ma Zh. Éksp. Teor. Fiz. **74**, 57 (2001) [JETP Lett. **74**, 55 (2001)].
6. V. M. Samsonov and E. G. Lapin, Preprint No. 587, LIYaF AN SSSR (Leningrad Inst. of Nuclear Physics, USSR Academy of Sciences, Leningrad, 1980).
7. V. M. Samsonov, Preprint No. 278, LIYaF AN SSSR (Leningrad Inst. of Nuclear Physics, USSR Academy of Sciences, Leningrad, 1976).
8. S. G. Skornyakov, A. I. Smirnov, and G. P. Solodov, Preprint No. 1133, LIYaF AN SSSR (Leningrad Inst. of Nuclear Physics, USSR Academy of Sciences, Leningrad, 1985).

Translated by R. Tyapaev