An Experimental Test of a Double-Crystal Monochromator for Thermal Neutrons Based on Two Bent Silicon Crystals

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Abstract
Reflecting properties of a double-crystal (DC) monochromator consisting of two elastically bent perfect silicon crystals in the parallel non-dispersive (1, -1) setting were experimentally treated. Using an unconventional fully asymmetric geometry, the effective mosaicity may be significantly enhanced up to the value of about $10^{-2}$ rad. Test experiments were performed on the 111 and 400 reflections for wavelengths of 0.2 nm and 0.157 nm, respectively. The experimental results obtained are found to be in good agreement with the theoretical predictions published in a previous paper [Mikula, Kulda, Vrana & Chalupa (1984). J. Appl. Cryst. 17, 189-195].

1. Introduction
In the theoretically oriented paper I (Mikula, Kulda, Vrana & Chalupa, 1984) (here the references are given to other related papers), the possibility of employing the double-crystal (1, -1) arrangement of two elastically bent Si crystals for highly efficient monochromatization of thermal neutrons was proposed. The proposal consists of the use of a fully (or almost fully) asymmetrical geometry where the incident polychromatic beam enters the first crystal through the end face and passes through it parallel (or almost parallel) to the longest edge (see Fig. 1 of paper I). The associated effect of reflected beam widening is compensated for by the second crystal in the parallel (1, -1) setting in opposite geometry. Reflecting properties of this DC monochromator following from the theoretical estimations are expected to be much better than the ones of any DC monochromator based on two mosaic single crystals and they may even be compared with the best one-crystal mosaic monochromators.

The idea of such a DC monochromator (Mikula & Kulda, 1983) arose in the course of the measurements of the transmission function $T_\lambda(\lambda, R)$ of an elastically bent Si crystal bar (Mikula, Kulda, Červená, Chalupa, Hašková & Vávra, 1983) when very deep minima in the dependence of $T_\lambda(\lambda, R)$ on the neutron wavelength $\lambda$ were observed. The minima were brought about by Bragg reflections on sets of planes whose integrated reflecting power was strongly increased by bending.

In the case of an elastically bent perfect crystal the effective 'mosaicity' $\delta \theta$ is equal to the total change in Bragg angle for the incident beam on its path through the crystal. It is clear that $\delta \theta$ is proportional to the reciprocal value of the bending radius $R$. Hence, the maximum obtainable $\delta \theta$ is determined by the limiting value $R_{\min}$ for a given thickness of the crystal. For the symmetrical diffraction geometry the achievable $\delta \theta$ is usually of the order of some minutes and cannot compete with the value of the mosaicity of conventional monochromators. In our case this restriction is overcome by the employment of a strongly asymmetric geometry so that the effective path of the incident beam in the crystal and consequently $\delta \theta$ could be considerably enlarged.

Another way of increasing $\delta \theta$ is by using a stack of thin crystal lamellae, which allows a much smaller bending radius (Rekveldt, 1983). But, in such a case, the problem of the suitable selection of well-oriented lamellae may arise. Most of all, the relative orientation of one lamella to another is important for avoiding dips in the rocking curve that bring about a decrease of the integrated reflectivity, and difficulties in the control of resolution (Frey, 1974). Furthermore, when working with very small radii ($R \approx 1$ m) one should take into account the dependence of the peak reflectivity $r$ on $R$ as was indicated by Kulda (1984) and in paper I.

The purpose of this paper is to present the first experimental results concerning the reflectivity and focusing of the above-mentioned DC monochromator based on two bent Si crystals in the parallel (1, -1) setting.

2. Theoretical background
From paper I, the integrated reflectivity of the DC monochromator consisting of two crystal plates having the same length ($L_1 = L_2$) and radius of curvature ($R_1 = R_2$) is given by the simple formula

$$\rho = \delta \theta [r(R)]^2 A(\mu, L),$$

(1)
where $\delta \theta$ is the total change in the Bragg angle for an incident beam on its path through the crystal, $r(R)$ is the peak reflectivity (Kulda, 1984) and $A(\mu, L)$ is the attenuation factor depending on the linear attenuation coefficient $\mu$ and the length $L$ of the crystals (Freund, 1983).

For homogeneous bending, in the case of the fully asymmetric geometry (1) can be rearranged to the form (see paper I)

$$
\rho^\theta = (L/R)[1 - \exp(-Q R)]^2 \exp(-\mu L),
$$

(2)

where $Q = F^2 \lambda^2 / (V^2 \sin 2\theta_B)$, $F_h$ and $V$ are the structure factor and the volume of the unit cell, respectively. The calculation of an extremum of the function $\rho^\theta$ for a fixed $\delta \theta = L/R$ yields the optimum length $L_{\text{opt}}(\lambda)$ and radius of curvature $R_{\text{opt}}(\lambda)$ as functions of the neutron wavelength $\lambda$ and hence also a maximum integrated reflectivity $\rho^\theta_{\text{max}}(\lambda)$ that can be expected from an experiment.

Besides using all the optimum parameters for $\delta \theta$, fixed in advance as described in detail in paper I, another method consisting in an arbitrary choice of the bending radius $R$ for fixed $L$ and $\lambda$, which yields the possibility of easy control of $\delta \theta$ and $\rho^\theta$, may be employed.

Figs. 1(a) and (b) display the dependences of $\delta \theta$ and $\rho^\theta$ on the reciprocal value of the bending radius for fixed $\lambda$ and several values of $L$. Fig. 1(a) corresponds to $\lambda = 0.2$ nm, 111 reflection and Fig. 1(b) corresponds to $\lambda = 0.157$ nm, 400 reflection.

### 3. Focusing

In an experiment for obtaining the maximum efficiency of the DC monochromator it is necessary for the second crystal to reflect all the neutrons coming from the first one over the whole angular divergence $\Delta \omega$. It was pointed out in paper I that, owing to the horizontal divergence $\Delta \omega$, the beam of neutrons reflected at a point $(x_n, y_n)$ of the first crystal passes through the second crystal not through a single point $(x_n, y_n)$ but spread over an area $\Delta x = l \Delta \omega / \sin \theta$ and $\Delta y = l \Delta \omega / \cos \theta$ along the $x$ and $y$ axes, respectively, where $l$ is the beam path length between the crystals. Here we use the coordinate system with respect to the crystal axes as indicated in Fig. 2. If we neglect the dependence of the local angular deviation $\delta \theta(x, y)$ brought about by bending (see paper I) on the co-

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**Fig. 1.** The dependence of the effective 'mosaicity' $\delta \theta$ (dashed lines) and the integrated reflectivity $\rho^\theta$ (full lines) on the reciprocal value of the bending radius for different lengths of the monochromator crystals. (a) 111 reflection, $\lambda = 0.2$ nm and (b) 400 reflection, $\lambda = 0.157$ nm.

**Fig. 2.** Schematic diagram of the defocusing and focusing geometries. (a) Incident and doubly diffracted beams pass the crystals along their longest edges. (b) The beams are not parallel to the longest edges of the crystals.
ordinate \( y \), all neutrons coming from a point \((x_n, y_n)\) can again be reflected by the second crystal only at points having an \( x \) coordinate \( x'_{n1} \) for arbitrary coordinate \( y'_{n1} \) from the interval \((y_{n1} - \Delta y/2; y_{n1} + \Delta y/2)\). Hence, for obtaining maximum efficiency, the thickness of the second crystal \( D_n \) should be greater than the thickness \( D_1 \) of the first one approximately by the value \( \Delta y \). The beam after being diffracted twice in the vicinity of the point \((x_{n1}, y_{n1})\) converges to the point \((x_{n1} + l/cos 2\theta; y_{n1})\) and its width \( \Delta Y_1 \) at a distance \( b \) from \((x_{n1}, y_{n1})\) is given by the expression

\[
\Delta Y_1 = |l/cos 2\theta - b|\Delta\omega. \quad (3)
\]

As this consideration is valid for all points \((x_n, y_n)\), the points of convergence are spread over a range having the length and width equal to the length and thickness of the first crystal or to the width of the entrance slit. A small uncertainty coming from the distribution of the points of convergence along the beam path may be neglected.

A further contribution \( \Delta Y_2 \) to the total width of the outgoing monochromatic beam stems from the bending through \( \delta\theta \) (see Fig. 2a). At the distance \( b \) from the centre of the second crystal, \( \Delta Y_2 \) is given by

\[
\Delta Y_2 = b\delta\theta = bL/R. \quad (4)
\]

If the second crystal is cut in such a way that the axis \( x' \) of the doubly diffracted beam is not parallel to the longest edge, focusing may take place (see Fig. 2b). Let us denote this deviation from the full asymmetry \( \Delta\psi \). The distance \( b_F \) of the focal point from the centre of the second crystal can be simply estimated as (Frey, 1975)

\[
b_F = R \sin[\Delta\psi]. \quad (5)
\]

Here it should be mentioned that, depending on the sense of the bending, \( \Delta\psi \) may be positive or negative. In this case the contribution \( \Delta Y_2 \) can be derived in the form

\[
\Delta Y_2 = |b_F - b|\delta\theta = |R \sin[\Delta\psi]| - b|\delta\theta. \quad (6)
\]

The inspection of (6) and (3) reveals that for

\[
l/cos 2\theta = R \sin[\Delta\psi] \quad (7)
\]

the width of the output beam at the distance \( b_F \) is practically given by the contribution \( \Delta Y_2 \) determined just by the thickness of the first crystal or by the width of the entrance slit.

4. Experimental

The test experiment was performed by means of a triple-axis spectrometer TKSN-400 (Petržilka, Michalec, Chalupa, Sedláková, Čech, Mikula & Vávra, 1972) with a Zn 002 mosaic monochromator having a mosaicity of about 17° and placed on the first axis. Silicon crystal plates were placed on the second and third axes. The beam path between the Si crystals was \( l = 50 \) cm. Only one Soller collimator, having a horizontal divergence of 20°, was used and placed in the reactor hole. The silicon single-crystal plates used in the experiment were cut from a large dislocation-free perfect-crystal ingot grown in the [111] direction. After mechanical and chemical treatment, both crystal plates had the same dimensions of \(200 \times 30 \times 5 \) mm (length \times height \times thickness). In our experiment we could use the (111) diffracting planes making an angle of about 18-6° with the largest surface nearly parallel to the (112) planes. In the fully asymmetric geometry, the Bragg angle \( \theta_B \) of 18-6° determined the neutron wavelength \( \lambda_{111} = 0.2 \) nm. Similarly, after the rotation of both crystals around the \( x \) axis by 180°, the 400 reflection with a Bragg angle of \( \theta_B = 36-3° \) gave \( \lambda_{400} = 0.157 \) nm. The incident beam coming from the Zn monochromator entered the first crystal through a slit of width \( D_s = 1 \) mm.

At the beginning, the transmission function \( T_L(\lambda, R) \) versus the neutron wavelength \( \lambda \) was measured for undeformed perfect and bent crystals when the incident beam monochromatized by the Zn monochromator passed through the crystal plate along its longest edge. \( T_L(\lambda, R) \) is the ratio \( I_L^2/I_0 \), where \( I_0 \) is the intensity of incident neutrons and \( I_L^2 \) is the intensity of neutrons transmitted through the crystal bent to the radius of curvature \( R \) (for undeformed crystals \( R = +\infty \)).

Figs. 3(a) and (b) show parts of the dependence \( T_L(\lambda, R) \) versus \( \lambda \) in the vicinity of the values of 0.2 nm and 0.157 nm, respectively, for an undeformed crystal (curve 1) and for an elastically bent crystal (radius of bending \( R = 20 \) m – curve 2). Curve 3 in Fig. 3(a) represents a theoretical dependence (Freund, 1983). The difference between curves 1 and 3 is brought about by the rather large amount (about 40%) of second-order neutrons in the monochromatized incident beam for \( \lambda = 0.2 \) nm (Šimá, Chalupa & Vrana, 1981).

It can be seen from Fig 3(b) that besides the minimum corresponding to the 400 reflection at \( \lambda = 0.157 \) nm one can find further minima brought about by other Bragg reflections. The presence of such parasitic reflections competing with the reflection 400 may cause a considerable loss in the integrated reflectivity of the DC monochromator. On the other hand, one can expect the influence of the parasitic reflections in the case of the 111 reflection to be much smaller (see Fig. 3a). Owing to the large number of second-order neutrons in the incident beam and to the difference in the lattice spacings \( d_{002} \) and \( d_{300} \) of the Zn and Si crystal, the transmission function in both cases does not decrease to zero at the centre.

The efficiency of the DC monochromator defined as \( \rho^2/\delta\theta \) may be expressed experimentally be means of the ratio \( I_L^2/I_D^2 \), where \( I_D^2 \) is the intensity of
the doubly diffracted neutrons for crystals bent to a radius \( R \). After a simple consideration we arrive at

\[
\rho^\theta_{\exp}/\theta(R) = r(R)A(\mu, L)I^R_{\Delta C}(I^+_{\infty} - I^R_{\infty}).
\]  

(8)

The inspection of (8) reveals that, on the basis of the easily measurable values of \( I^R_{\Delta C}, I^+_{\infty}, I^R_{\infty} \) and well defined factors \( r(R) \) and \( A(\mu, L) \), one can obtain the efficiency of the DC monochromator in a straightforward way.

Figs. 4(a) and (b) display the experimental results of the efficiency \( \rho^\theta/\delta\theta \) versus the angular departure \( \Delta \theta \) of the second crystal from the precise parallel setting for the 111 reflection, \( R = 20 \, \text{m} \) and the 400 reflection, \( R = 64 \, \text{m} \), respectively.

The output beam was photographed by means of an X-ray film in contact with a Gd foil. Owing to the construction of the experimental device, the photographs of the output doubly diffracted beam could be made at distances \( b_0 = L/2 = 10 \, \text{cm} \) (just behind the second crystal), \( b_1 = 36 \, \text{cm} \) and \( b_2 = 117 \, \text{cm} \) in the \( x \) axis direction.

Fig. 5 shows photographs of the outgoing beam corresponding to the 111 and 400 reflections, respectively, for several radii of curvature. In the case of the 111 reflection, the outgoing beam was precisely parallel to the \( x \) axis of the crystal. In the latter case in order to avoid the effect of the parasitic reflections, the angle between the outgoing beam and the \( x \) axis was \( \Delta \psi = -1.1^\circ \).

Fig. 3. The transmission function \( T(\lambda, R) \) versus the wavelength in the vicinity of (a) \( \lambda = 0.2 \, \text{nm} \) and (b) \( \lambda = 0.16 \, \text{nm} \). Dependences 1 and 2 correspond to the nondeformed crystal and to the one elastically bent to the radius \( R = 20 \, \text{m} \), respectively. Curve 3 corresponds to the theoretical dependence of the nondeformed perfect crystal.

Fig. 4. The efficiency \( \rho^\theta/\delta\theta \) of the DC monochromator versus the rocking angle \( \Delta \theta \) of the second crystal in the vicinity of the precise parallel setting (curve 2). (a) 111 reflection, \( \lambda = 0.2 \, \text{nm} \); (b) 400 reflection, \( \lambda = 0.157 \, \text{nm} \). Curve 1 gives the maximum theoretical efficiency.
5. Discussion

It can be seen from (8) and Figs. 4(a) and (b) that the efficiency of the DC monochromator on an absolute scale is significantly influenced by the attenuation factor $A(\mu, L)$, depending on the length of the crystals. It should be noticed that, for a commonly used effective mosaic spread of about 20', the optimum length $L_{\text{opt}}$ of the monochromator crystals is significantly lower in comparison with $L = 20$ cm of those available (see paper I). An agreement between the experiment and the theory may be considered according to the ratio $\rho_{\text{exp}}/\rho_{\text{th}}$, which is 0.94 and 0.78 for the 111 and 400 reflections, respectively. In both cases the value of this ratio was found to be constant within 5% for different bending radii. The rather low value of the ratio $\rho_{\text{exp}}/\rho_{\text{th}}$ for the 400 reflection originates from the competitive role of the nearest parasitic reflections (see § 3) and from the fact that, for $\Delta \omega = 17'$, the value $\Delta y = \Delta Y_f(b=0) = 7.4 \text{ mm}$ considerably exceeds the thickness of the second crystal used in the experiment, while $\Delta y$ corresponding to the 111 reflection is equal to 3.2 mm. In the course of the experiment the loss of the intensity of the doubly diffracted beam brought about by a rather large value of $\Delta y$ could be partly compensated for by the use of slightly smaller $R_n$ in comparison to $R_0$. In practice, owing to the divergence of the incident beam, it is always necessary to find an optimum radius $R_n$ (with respect to $R_0$), which corresponds to a maximum intensity of the doubly reflected beam. Then for $R_n < R_0$, the experimental value of $\Delta y$ is somewhat smaller in comparison with the theoretical one. This problem was dealt with in more detail in the paper of Kulda & Mikula (1983). Owing to the geometry and a relatively small distance between the crystals used in this experiment, the optimum $R_n$ differs from $R_0$ by less than 10%. Consequently, the results of the theoretical treatment performed in our previous paper and in this one may be applied with sufficient accuracy.

Figs. 6(a) and (b) display the theoretical dependences of the DC monochromator efficiency on the bending radius $R$ for the 111 reflection, $\lambda = 0.2 \text{ nm}$ and the 400 reflection, $\lambda = 0.157 \text{ nm}$, respectively. The curves from 1 to 4 correspond to different lengths of the crystals and the dashed one corresponds to the dependence of the peak reflectivity $r$ on $R$. The curves from 1 to 4 represent the maximum efficiency that can be obtained in an experiment. For a sufficiently large

![Fig. 5. Photographs of the doubly diffracted output beam taken at different positions along the beam for several bending radii of the crystals: $b_0 = L/2 = 10 \text{ cm}$, $b_1 = 36 \text{ cm}$ and $b_2 = 117 \text{ cm}$.](image)

![Fig. 6. The efficiency $\rho^\theta/\delta \theta$ (full lines) and the peak reflectivity $r$ (dashed line) as functions of the bending radius $R$. Curves 1, 2, 3, 4 correspond to different lengths of the crystals of 5, 10, 15 and 20 cm, respectively. (a) 111 reflection, $\lambda = 0.2 \text{ nm}$. (b) 400 reflection, $\lambda = 0.157 \text{ nm}$.](image)
The calculated values of the uncertainty contributions $\Delta Y_1$, $\Delta Y_2$, $\Delta Y_3$ at the distances $b_1 = 36$ cm and $b_2 = 117$ cm

<table>
<thead>
<tr>
<th>Reflection</th>
<th>$R_1$ (m)</th>
<th>$\Delta Y_1(b_1)$ (mm)</th>
<th>$\Delta Y_2(b_1)$ (mm)</th>
<th>$\Delta Y_3(b_1)$ (mm)</th>
<th>$\Delta Y_1(b_2)$ (mm)</th>
<th>$\Delta Y_2(b_2)$ (mm)</th>
<th>$\Delta Y_3$ (mm)</th>
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<td>111</td>
<td>20</td>
<td>14</td>
<td>26</td>
<td>38</td>
<td>12</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>111</td>
<td>80</td>
<td>14</td>
<td>26</td>
<td>9</td>
<td>2</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>400</td>
<td>17</td>
<td>50</td>
<td>17</td>
<td>0</td>
<td>10</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>400</td>
<td>64</td>
<td>50</td>
<td>17</td>
<td>2</td>
<td>0</td>
<td>1</td>
<td></td>
</tr>
</tbody>
</table>

$R$, where $r^2 = 1$ may be put with sufficient accuracy, the efficiency $\rho^0 / \delta \theta$ is constant and determined only by the attenuation. On the other hand, for $R \rightarrow 0$, where $r^2 \rightarrow 0$, the DC monochromator becomes inefficient. It can be seen from the expression for $r^2(R)$ in (2) that this behaviour for the small values of $R$ is brought about by the presence of the exponential factor $\exp(-QR)$. Consequently, the expression $r^2(R)$ depends through $Q$ on the neutron wavelength and also on the structure factor.

Table 1 presents the calculated values of the contributions $\Delta Y_1$, $\Delta Y_2$, $\Delta Y_3$ at the distances $b_1$, $b_2$ for the 111 and 400 reflections. Inspection of Fig. 5 reveals that the widths of the images of the outgoing beams are in good agreement with the expectations from the calculation. The effect of focusing is demonstrated in the case of the 400 reflection for $R = 17$ m and the distance $b_1$. In this case, the value of $b_1$ differs slightly from that of $b_F$ equal to 32 cm. A faint shadow corresponds to the contribution $\Delta Y_1$, which was partly eliminated by the employment of the optimized radius $R_H$, which was about 1 m smaller with respect to $R_T$.

An advantage of our DC system may be found in the very low background inherent in all DC monochromators. This property may be characterized by the background-to-peak ratio. Here the background is the intensity taken at a distance of $n \times$ FWHM from the peak of the double-crystal rocking curve. For the 111 reflection and $R = 20$ m this ratio at $4 \times$ FWHM was $3 \times 10^{-5}$.

An important parameter characterizing any monochromator is the ratio between the integrated reflectivities corresponding to the first- and higher-order reflections. This ratio was experimentally measured for the 400 reflection at $\lambda = 0.157$ nm and the 800 reflection at $\lambda = 0.078$ nm. The obtained experimental value $\rho_{400}^0 / \rho_{800}^0 = 17$ is in a good agreement with the calculated one, which was 14.

Conclusion

The first experimental results concerning the reflectivity of the new type of the DC neutron monochromator based on two elastically bent perfect silicon crystals are presented. It can be stated that the experimental results are in full agreement with the predictions given by the theoretical estimations. The minimum width of the outgoing beam is determined by the predictions of the first crystal. The drawback of this DC monochromator is a rather small variation of the wavelength $\lambda$ of the monochromatized neutrons in the vicinity of $\lambda_0$ for which the crystal plates were cut (see paper I). It originates in the necessity of using the fully (or nearly fully) asymmetric geometry, enabling a relatively long flight path of the incident beam through the crystal. As the maximum usable crystal thickness is determined by a limit value of the bending radius, an employment of such a simple arrangement of the DC monochromator seems to be especially suitable for experiments with small samples and for instruments on neutron guide tubes where the width of the primary incident beam and its horizontal divergence are relatively small.

Further theoretical and experimental investigations in this direction are being carried out.

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References