Generalization of the Parallel Position in Diffraction using Elastically Curved Crystals

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Abstract

A theoretical and experimental study of double-crystal rocking curves with elastically deformed silicon wafers yields the result that rotating one of the crystals through 180° can change the peak intensity by a large factor, limited only by the sharpness of the intrinsic mosaic spread. The conventional double-crystal rocking curve with equivalent scattering vectors in what is called the parallel position has its counterpart for two crystals with different scattering vectors if each crystal is bent to its proper radius of curvature. Like the parallel-position case, the collimation does not enter into the width of the rocking curve. The rocking curve can be sharper than the usual parallel-position convolution of the two mosaic spreads. The often observed lack of agreement between rocking curves in what seem to be identical geometries is explained as a rotation of the mean of the mosaic spread across a crystal, which is equivalent to a bent crystal.

Introduction

It is a well known and well utilized fact that a pair of equivalent crystals, one used as a monochromator and the other as an analyzer of the beam, will reflect or transmit the twice-scattered beam over a range of angles that depends on the mosaic distribution of the crystals but not on the collimation of the beam when the two crystals have their scattering vectors equal and opposite to one another. This is called the parallel position (Bacon, 1975). Given two crystals with different scattering vectors, the arrangement for double scattering will have the two vectors in non-parallel directions. The range of angles of the twice-scattered beam then depends on the collimation of the beam unless, as is pointed out here, both crystals are suitably curved. The usual parallel position is a special case where the two curvatures are both infinite in radius.

It is a common experience of neutron crystallographers that the intensity of scattering for a symmetric crystal does not necessarily follow the known symmetry. In the simplest case, take a slab geometry and look at a reflection first from one side and then from the other. There is almost always some change in the rocking curves, which cannot be explained on the basis of the mosaic distribution of the crystal as a whole. It can be explained by the bent crystal effect. A linear variation in the mean of the mosaic distribution across a crystal is equivalent to a uniform bend.

We present the geometrical analysis of the rocking curves for two thin elastically deformed crystals. We give the expressions for the radii of curvature that produce the equivalent of the parallel position for crystals with different scattering vectors. The analysis supports our experimental observations on silicon wafers, e.g. we are able to show experimentally a change in the peak intensity of neutron scattering from an Si wafer by a factor of six in a case where the analysis predicts a factor of seven for rotation by 180° on the spectrometer table. The lack of exact agreement is due to the difficulty of properly bending the monochromating crystal.

We have not found any discussion in the literature of our generalization of the parallel position or any experiments that illustrate this point. But with such a simple point and such a vast literature in the realm of diffraction, it is not unlikely that our search has been inadequate. On the other hand, the point does not seem to be common knowledge, despite the current sophistication of neutron optics. (See, for example, Werner & Klein, 1984.)

Theory

As in any scattering problem, it is necessary to use diagrams to describe the geometric details. The problem is three dimensional in practice but all the effects that concern us here can be shown by projection onto the principal scattering plane, which is the plane of the page in Fig. 1. We show the crystals as thick lines to denote what in our practice are thin wafers of silicon (0.4 mm thick and 75 mm diameter) with the plane of the wafer perpendicular to the scattering plane. The analysis assumes a single scattering at each thin crystal, but could be generalized to include multiple scattering. The wafers are cut so that the normal to the surface is nominally a principal crystal axis, e.g. the [001] direction. The monochromating wafer is bent to a radius of curvature $R_m$ but this is such a large number that the bend does not show up on the diagram. This curvature is positive if it is toward the analyzing crystal, which itself is bent to a radius $R_a$. 

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The curvature of the analyzing crystal is positive if the bend is away from the monochromating crystal. (Note that this definition means that its curvature can reverse sign as the analyzing crystal is rotated on the spectrometer table.)

The overall view of the geometry is shown in Fig. 1(b). The particular neutron path shown is for one, called the central ray, which hits the center of the monochromating crystal, is reflected from the central mosaic block (which is oriented in the center of the mosaic distribution averaged along the line perpendicular to the scattering plane through the center of that crystal) and then proceeds to the center of the analyzing (or sample) crystal along the \( \hat{z} \) axis. There is only one neutron wave vector \( k_0 \) (projected onto the principal scattering plane) that will satisfy this condition. The position on the source from which this neutron came is the center of the source plane, \( r_s = 0 \). When it hits the center of the analyzing crystal, Fig. 1(a), it is reflected from a mosaic block that is oriented in the center of the mosaic distribution averaged along the line perpendicular to the scattering plane through the center of that crystal. This is possible only if the analyzing crystal, Fig. 1(a), has been rotated so that the scattering vector \( \mathbf{G}_0 \) of that mosaic block is at the required angle with respect to the line joining the centers of the two crystals. The twice-scattered neutron then hits the center of the detector, which has been placed at angle \( F_0 \) away from the \( \hat{z} \) axis, where \( F_0 = 20^\circ \).

The most important point to remember is that the specification of two points, one on each crystal, and the energy of the neutron that goes between those points completely specifies all the geometric aspects of the problem for thin crystals.

There is only one orientation of a mosaic block (projected onto the scattering plane) at the point \( r_m \) in the monochromating crystal (measured in the scattering plane from the center of that crystal) that could have scattered a neutron in the momentum state \( \mathbf{k} \). There is only one place \( r_s \) on the source plane from which that neutron could have come. Further, there is only one possible orientation of a mosaic block at the position \( r_a \) on the analyzing crystal that could scatter that neutron.

Whether it scatters or not depends on whether the analyzing crystal has been rotated to provide such a mosaic block. If it has, then the twice-scattered neutron will arrive at a particular angle \( F = F_0 + \Delta F \) on the detector arc, which is determined by the two positions, \( r_m \) and \( r_a \), and the magnitude of \( \mathbf{k} \).

The probability of a neutron travelling such a path remains to be determined. This depends on the spatial orientation of the mosaic distribution of the monochromator as a function of \( r_m \) and of the analyzer as a function of \( r_a \). As the analyzer is rotated, the probability for double scattering changes. If the source is collimated to a width \( 2w_v \), then suitable neutrons will be available for a particular choice of \( r_m, r_a \), and \( k \) only if, for this choice, \( |r_s| \leq w_v \).

Let us assume that the mosaic distribution has the same width \( \eta_m \) at each point in the monochromating crystal and the same width \( \eta_a \) at each point in the analysing crystal. But the mean orientations of the mosaic distribution are functions of \( r_m \) and \( r_a \). The probability of scattering from the monochromating crystal is

\[
P_m(k, r_m, r_a) = P_m(k_0, 0, 0) \exp\left\{ -\frac{(r_m/\eta_m)^2}{2} \right\},
\]

where

\[
\varphi_m(r_m) - \varphi_m(k, r_m, r_a)
\]

is the deviation between \( \varphi_m(r_m) \), the mean direction of the mosaic at \( r_m \), and \( \varphi_m(k, r_m, r_a) \), the direction of the mosaic block in the monochromator required to scatter the neutron specified by \( k, r_m \), and \( r_a \). These angles are measured from the \( \hat{z} \) axis, the line joining

Fig. 1. Layout of the source(S)--monochromator(M)--analyzer(A)--detector(D) system. Analyzer and monochromator detail are shown in (a) and (c), respectively; the overall view is shown in (b). BP = Bragg plane.
the centers of the two crystals. Similarly for the analyzer crystal,

\[ P_a(k, r_m, r_a) = P_a(k_0, 0, 0) \exp \left\{ -\frac{(\varepsilon_a/\eta_a)^2}{2} \right\}, \]

where

\[ \varepsilon_a = \Phi_a(r_a) - \varphi_a(k, r_m, r_a). \]

For the bent monochromator,

\[ \Phi_m(r_m) = \Phi_m(0) + r_m/R_m, \]

and for the bent analyzer,

\[ \Phi_a(r_a) = \Phi_a(0) + r_a/R_a. \]

The Laue conditions use the magnitude of the scattering vectors \( G_m \) and \( G_a \). The angle between the outgoing neutron from the monochromator and the direction of the scattering mosaic block is \( \theta_m(k, r_m, r_a) \) given by

\[ 2k \sin \{ \theta_m^\parallel(k, r_m, r_a) \} = |G_m| = G_m. \]

The angle between the incoming neutron to the analyzer and the direction of the scattering mosaic block is \( \theta_a^\parallel(k, r_m, r_a) \) given by

\[ 2k_0 \sin \{ \theta_a^\parallel(k_0, 0, 0) \} = |G_a| = G_a. \]

To decrease the bulk of the notation we let

\[ \theta_m = \theta_m^\parallel(k_0, 0, 0). \]

\( \theta_m \) is chosen by the experimenter (we use \( \theta_m = \pi/4 \)). It is the angle between the z axis and the mosaic block at the center of the mosaic distribution at the center of the monochromator; thus,

\[ \Phi_m(0) = \theta_m. \]

We define \( \alpha_m \) to be the angle between the Bragg plane of the center of the mosaic distribution and the plane of the monochromator. \( \cos \alpha_m \) is then \( G_m \cdot \hat{n}/G_m \), where \( \hat{n} \) is the vector normal to the wafer. This is the same at each point of the bent crystal. For the analyzer, the similarly defined angle is \( \alpha_a \), where \( \cos \alpha_a \) is then \( G_a \cdot \hat{n}/G_a \).

At the center of a double-crystal rocking curve the scattering vector \( G_a^\parallel \) at the center of the analyzer makes an angle \( \theta_a^\parallel(k_0, 0, 0) \) with the z axis where

\[ 2k_0 \sin \{ \theta_a^\parallel(k_0, 0, 0) \} = |G_a^\parallel| = G_a. \]

We use the notation

\[ \theta_a = \theta_a^\parallel(k_0, 0, 0). \]

When the analyzing crystal is rotated from this position by an angle \( \beta_a \), the orientation of the center of the mosaic spread for the center of the analyzing crystal \( \Phi_a(0) \) is given by

\[ \Phi_a(0) = \theta_a + \beta_a. \]

The positions \( r_m \) and \( r_a \) determine an angle \( \Psi_2 \) between the neutron path and the z axis, given by

\[ \tan \Psi_2 = \left\{ r_a \sin(\theta_a - (\alpha_a + \beta_a)) - r_m \sin(\theta_m - \alpha_m) \right\} \times \left\{ L_2^\parallel + r_m \cos(\theta_a - (\alpha_a + \beta_a)) \right\} \]

\[ - r_m \cos(\theta_m - \alpha_m)^{-1}. \]

The angles of the required mosaic blocks for scattering the neutron that will travel from \( r_m \) to \( r_a \) and have momentum of magnitude \( k \) are

\[ \varphi_m(k, r_m, r_a) = \theta_m^\parallel(k, r_m, r_a) - \Psi_2 \]

for the monochromator and

\[ \varphi_a(k, r_m, r_a) = \theta_a^\parallel(k, r_m, r_a) - \Psi_2 \]

for the analyzer.

**Generalization of the parallel position**

To handle the problem analytically we will assume that the mosaic spreads are very sharp. Below we will treat the effect of the mosaic spread by numerical integration and compare this to the results of a Monte-Carlo program designed for more complicated problems.

We introduce the projections of \( r_m \) and \( r_a \) on the \( x \) axis, chosen perpendicular to the z axis and in the plane of the central ray;

\[ x_m = r_m \sin(\theta_m - \alpha_m) \]

and

\[ x_a = r_a \sin(\theta_a - \alpha_a). \]

It is convenient also to define here the analogous expressions for the effective radii of curvature of the monochromator and analyzer projected onto the \( x \) axis;

\[ X_m = R_m \sin(\theta_m - \alpha_m) \]

and

\[ X_a = R_a \sin(\theta_a - \alpha_a). \]

Then, for \( L_2 \gg r_m \) and \( r_a \), we can drop the cosine terms in (15) relative to \( L_2 \) and replace the \( \tan \Psi_2 \) by \( \Psi_2 \). As \( \beta_a \) is also a small angle, we can neglect it in (15) and write

\[ \Psi_2 = (x_a - x_m)/L_2. \]

From (16), (2), (5), (11), (18), (20) and (22), in sequence, we have

\[ \theta_a^\parallel(k, r_m, r_a) = \Psi_2 + \varphi_m(k, r_m, r_a) \]

\[ = \Psi_2 + \Phi_m(r_m) - \varepsilon_m \]

\[ = \Phi_m(0) + r_m/R_m + \Psi_2 - \varepsilon_m \]

\[ = \theta_m + x_m X_m + \left\{ x_a + x_m \right\}/L_2 - \varepsilon_m. \]
From (17), (4), (6), (14), (19), (21) and (22), in sequence, we have

\begin{align*}
\theta^B_{\beta}(k, r_m, r_a) &= \Psi_2 + \phi_a(k, r_m, r_a) \\
&= \Psi_2 + \phi_a(\epsilon_a) - \epsilon_a \\
&= \phi_a(0) + r_a/R_a + \Psi_2 - \epsilon_a \\
&= \phi_a + x_a/X_a + \{x_a - x_m\}/L_2 + \beta_a - \epsilon_a \\
&= 0 + x_a/X_a + \{x_a - x_m\}/L_2 + \beta_a - \epsilon_a \\
&= (24)
\end{align*}

The generalization of the parallel position is to satisfy the Laue conditions, (7) and (8), simultaneously for all values of \(x_a\) and \(x_m\) at \(\beta_a = 0\), when \(\eta_m = \eta_s = 0\), and for none when \(\beta_a \neq 0\). In general, as the angle \(\beta_a\) is changed, the Laue conditions will be satisfied for different sets of values of \(x_a\) and \(x_m\).

From (7), (8), (9) and (12) we can write

\[ \sin(\theta_m)/\sin(\theta_a) = \sin[\theta^B_{\beta}(k, r_m, r_a)]/\sin[\theta^B_{\beta}(k, r_m, r_a)]. \]

(25)

Substituting from (23) and (24) and expanding to second order in \(x_{ra}\) and \(x_{ra}\), we find a relation between \(\beta_a\) and \(x_{ra}, x_{ra}\), \(\epsilon_a\) and \(\epsilon_a\), of the form

\[ \beta_a = \epsilon_a - T\epsilon_a - A(x_{ra}, x_a) + B(\epsilon_a, x_{ra}, x_a), \]

where

\[ T = \tan \theta_a/\tan \theta_m \]

(26)

\[ A(x_{ra}, x_a) = -x_a/X_a + T x_m/X_m \]

\[ - (1 - T)(x_a - x_m)/L_2 \]

(28)

and

\[ B(\epsilon_a, x_{ra}, x_a) = (T^2 - 1)\tan \theta_a \]

\[ \times \{\epsilon_a + x_a/X_a + (x_a - x_m)/L_2\}^2 / 2. \]

(29)

The term \(A(x_{ra}, x_a)\), which is linear in \(x_{ra}\) and \(x_a\), is by far the most important. For the case of narrow mosaic, neglecting the terms in \(\epsilon_a\) and \(\epsilon_a\) and further neglecting the second-order term \(B(\epsilon_a, x_{ra}, x_a)\), one can make \(\beta_a = 0\) for all values of \(x_{ra}\) and \(x_a\) by the proper choices of \(X_m\) and \(X_s\):

\[ L_2/X_a = 1 - 1/T = (\tan \theta_a - \tan \theta_m)/\tan \theta_a \]

(30)

\[ L_2/X_a = T - 1 = (\tan \theta_a - \tan \theta_m)/\tan \theta_m. \]

(31)

Equations (30) and (31) are the generalization of the parallel position. If they are satisfied, the rocking curve is as sharp as the mosaic spread will allow. Note that \(X_m\) and \(X_s\) depend only on \(G_a\) or \(\theta_{\alpha}\) for fixed geometry where \(\theta_{\alpha}\) and \(L_2\) are determined. However, there may be several reflections that have the same \(G_a\) but different \(x_{ra}\) (21), and thus different \(R_a\).

The standard parallel position is the special case of \(T = 1\), for then the two crystals are reflecting from Bragg planes of equal spacing and \(\theta_{\alpha} = \theta_m\). For any pair of spacings of the Bragg planes of the two crystals there is a radius of curvature of each, which will give a sharp rocking curve. This is demonstrated experimentally below. But first it is necessary to discuss the role of the mosaic spread.

### Rocking-curve width

The monochromator and the analyzer crystals together form a collimator. Given an infinite plane source the monochromator will be uniformly bathed in neutrons of all wavelengths and directions. A fraction of these will be diffracted and bathe the analyzer uniformly. (Like a two-slit collimator looking at an infinite source, the intensity is uniform across each slit.) The probability of a neutron being doubly diffracted will depend on the rotation angle \(\beta_a\) of the analyzer;

\[ dP(\beta_a) = P_0 \{dr_m/2w_m\} \{dr_a/2w_a\} \]

\[ \times \exp\{-[(\beta_a + A(x_{ra}, x_a))/\eta_{\beta}\}^2 / (2\pi)^{1/2}/\eta_{\beta} \}

(32)

where the full width of the monochromator is \(2w_m\) and that of the analyzer is \(2w_a\). \(P_0\) is a normalization parameter. The other quantities are as in (1) and (3). The angle \(\beta_a\) enters because the four variables \(r_m, r_a, \epsilon_a\) and \(\epsilon_a\) are not independent, being related by (26) for each setting of \(\beta_a\). If the nonlinear terms, \(B(\epsilon_a, x_{ra}, x_a)\), are dropped and \(\epsilon_a\) eliminated, then integration over \(\epsilon_a\) gives

\[ P(\beta_a) = P_0 \int_{-w_m}^{w_m} \{dr_m/2w_m\} \int_{-w_a}^{w_a} \{dr_a/2w_a\} \]

\[ \times \exp\{-[(\beta_a + A(x_{ra}, x_a))/\eta_{\beta}\}^2 / (2\pi)^{1/2}/\eta_{\beta} \}

(33)

where

\[ \eta_{\beta} = (T^2 \eta_m^2 + \eta_s^2)^{1/2}. \]

(34)

At the values of \(R_m\) and \(R_s\) that produce the sharpest rocking curve, \(A(x_{ra}, x_a) = 0\). The rocking curve is then Gaussian with a width given by \(\eta_{\beta}\), which is the weighted convolution of the mosaic half-widths of the monochromator and analyzer crystals. Note that the weighting is not the same for the two crystals except in the special case of the regular parallel position, \(T = 1\) (Bacon, 1975). For \(T < 1\), \(\eta_{\beta}\) is narrower than for the regular parallel position. When \(X_m\) and \(X_s\) are not at their optimum values given by (30) and (31), \(A(x_{ra}, x_a) \neq 0\), in general. Equation (33) can then be integrated numerically to get the broadened rocking curve.

The above integration assumes an infinite plane source. If one works backwards from the coordinates \(k, r_m, r_a\) to trace the origin of each neutron on the
Table 1. Comparison of theory and Monte Carlo (MC) results for several analyzer reflections

Theory results are labeled 'exact' when all terms in (26) are used and 'linear' when \( B(\gamma_m, \gamma_a, x_a) = 0 \) in (26).

<table>
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<th>Analyzer hkl</th>
<th>422</th>
<th>400</th>
<th>311</th>
<th>111</th>
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<td>( \theta_m(\degree) )</td>
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<td>35-26</td>
<td>28-60</td>
<td>14-48</td>
</tr>
<tr>
<td>( T )</td>
<td>1-0</td>
<td>0-707</td>
<td>0-545</td>
<td>0-258</td>
</tr>
<tr>
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<td>0</td>
<td>-25-24</td>
<td>+25-24</td>
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<tr>
<td>( R_a(cm) )</td>
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<td></td>
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<tr>
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<td>-608-3</td>
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<tr>
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<td>( \infty )</td>
<td>-1224-7</td>
<td>-608-3</td>
<td>-176-6</td>
</tr>
<tr>
<td>MC</td>
<td>( \infty )</td>
<td>-1238(4)</td>
<td>-586(3)</td>
<td>-177-8</td>
</tr>
<tr>
<td>( X_a(cm) )</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
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<td>-599-4</td>
<td>-174-1</td>
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<tr>
<td>( R_X(cm) )</td>
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<td>-720-8(2)</td>
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source, it becomes readily apparent that in many cases the width of the source that can be used is much larger than the width of the crystals. As our source is not wider than the width of the large crystals, the sample crystal is not uniformly bathed.

**Monte Carlo**

To take the source width into account as well as the mosaic spread of the crystals, we created a Monte Carlo program to match our experimental setup. In trying to understand the Monte Carlo program results, we developed the present theory, which makes the slow and cumbersome Monte Carlo program obsolete. However, the two techniques provide independent checks on each other.

In our modelling of the system, we match our experimental arrangement. For the monochromator we use a (001)-cut silicon wafer, 0-4 mm thick and 75 mm in diameter. We use a 90° take-off angle \( \theta_m = \pi/4 \). The reflection is the 422 with \( \gamma_a = -35-26° \). Other system parameters, see Fig. 1, are \( L_1 = 2-8, L_2 = 5, L_3 = 1 m, 2w_m = 5 \) and \( 2w_m = 7-5 cm \). The analyzer is also a (001)-cut silicon wafer. From double-crystal rocking curves in the parallel position with flat crystals we estimate that \( \eta_m = \eta_a = 0-025° \).

Some of the reflections that are found in rotating the crystal on the spectrometer table with the [011] axis along the table axis (normal to the plane of the page in Fig. 1) are shown in Table 1. The values of \( R_m \) and \( R_X(X_m \) and \( X_a) \) for the sharpest rocking curves from (30) and (31) are tabulated for the linearized theory (linear) and for the theory including the second- and higher-order terms (exact), which is done numerically. These results are compared to those found by varying \( R_m \) and \( R_a \) in the Monte Carlo (MC) program. The linear and exact theories agree to better than 0-1% in all cases, which justifies dropping the non-linear terms in (26). The Monte Carlo results agree with the linear theory to < 1% accuracy in most cases, the worst case being ~4% difference. Note that we have found it very difficult to bend silicon wafers uniformly to a 4% accuracy.

In all cases \( X_m \) and \( X_a \) are negative as expected since \( \tan \theta_m > \tan \theta_a \) in all cases. Thus the curvatures, projected onto the x axis, are all down relative to the z axis. Note that \( X_m \) and \( X_a \) are the same for the 311 and 311 reflections and also for the 111 and 111 reflections. However, in both cases \( R_a \) depends on the particular analyzer reflection used; that is, \( R_a \) depends on the angle \( x_a \) that the crystal must be rotated from the Bragg plane to put the scattering vector, \( G' \), in the right direction.

The widths of the rocking curves, \( \eta(\degree) \), are calculated from (34) and compared to Monte Carlo results in Table 1. The agreement is within 0-6% in all cases. Note that, for fixed take-off angle, \( \theta_m \), it is the analyzer Bragg angle, \( \theta_a \), that determines the weighting of the monochromator mosaic width, \( \eta_m \), in (34). In our case, with \( \theta_m = \pi/4 \), this results in very narrow rocking curves when \( \theta_a \) is small. In the 111 case, \( \theta_a = 14-48° \) and \( T = 0-258 \). This results in a rocking-curve width, \( \eta(\degree) = 0-0258° \), just 0-008° wider than the intrinsic width of the analyzer, \( \eta_a = 0-025° \).
If the monochromator and the analyzer are bent to the radii that produce a sharp rocking curve and then the analyzer is rotated through 180°, which reverses the sign of the curvature, the peak intensities differ greatly, but the integrated intensities are the same. The ratios of the peak heights on flipping the analyzer crystal by 180° are shown in Table 1. The most spectacular effect is for the 111 reflection, where the mosaic spread of the monochromator does not affect appreciably the line width. The optimum radius of curvature of the monochromator crystal is quite small, $R_m = 1.77$ m, but well within what can be achieved with elastic bending of silicon wafers. The predicted change in peak intensity for a 180° rotation of the analyzer crystal, bent to a radius of $R_a = 7.2$ m, is a factor of 18.4. This is illustrated in Fig. 2. The rocking curve for a flat analyzer, $R_a = \infty$, is also shown.

**Maps**

The natural coordinates for describing the double-crystal rocking experiment are the positions on the two crystals where each neutron hits when the mosaic spread is very narrow. For our system geometry, Figs. 3 and 4 show four maps each for the 422 and the 311 analyzer reflections using $r_m$ and $r_a$ as the coordinates for showing contours of constant $\Delta k = (k - k_0)/k_0$, contours of constant $\Psi_3$ (the angle the outgoing neutron from the analyzer makes with the central ray) and contours of constant $\Delta \Gamma$ (the angle by which the detector must be moved from the central ray to intercept the neutron). In the conventional parallel-position case, Fig. 3, the $\Psi_3$ contours are parallel to the $\Delta k$ contours. Thus, the outgoing angle and the energy are correlated. Note that for the detector a finite distance, $L_3$, from the analyzer, the detector angle, $\Delta \Gamma$, does not map with $\Delta k$. In the generalized parallel-position case, Fig. 4, the $\Psi_3$ and $\Delta k$ contours are not, in general, parallel.

In our geometry, the source width is limited to $-2.5 \leq r_s \leq 2.5$ cm. For the 422 analyzer, Fig. 3, we see that this limits the rocking-curve intensity to $\sim 77\%$ of the neutrons that would be available if the source were opened up up to $-4.7 \leq r_s \leq 4.7$ cm. For the 311 analyzer, Fig. 4, the narrow source limits the rocking curve intensity to $\sim 41\%$ of the neutrons available if $-7.7 \leq r_s \leq 8.0$ cm. Recall that, at $R_m$ and $R_a$ optimum, the rocking-curve width does not depend on collimation.

**Experiments**

The experiments that motivated these calculations were various studies of monochromating crystals made of stacks of silicon wafers elastically bent in order to create strain gradients to increase the reflec-

![Fig. 2. Theoretical rocking curves from (33) with $R_m = -1.77$ m, $\theta_m = 45^\circ$, $\theta_a = 144.8^\circ$, $\eta_m = \eta_a = 0.025^\circ$.](image1)

![Fig. 3. Contour maps for a 422 monochromator reflection and a 425 analyzer reflection. $R_m = R_a = \infty$. Units are cm for $r_s$ and $^\circ$ for $\Psi_3$ and $\Delta \Gamma$.](image2)

![Fig. 4. Contour maps for a 422 monochromator reflection and a 311 analyzer reflection. $R_m = -6.08$ and $R_a = -13.62$ m. Units are cm for $r_s$ and $^\circ$ for $\Psi_3$ and $\Delta \Gamma$.](image3)
tivity (Arrott & Templeton, 1985). In testing the monochromating crystals we used double-crystal rocking curves where the test crystals were in the analyzer crystal position and an elastically bent stack was used as a monochromator. The monochromator curvature was in the wrong direction to produce the dramatic effects calculated above. But still we saw changes in intensity on rotation of the sample crystals by 180° that were too large to be ignored. It was only after working out the theory that we realized that much bigger effects would come from turning the bent-crystal monochromator over. Confirmation of this prediction was readily accomplished. But for quantitative comparison we undertook to do the experiment with single wafers rather than our stacks, mainly because, with our methods of elastically bending crystals in stacks, one is never quite sure of the radius of curvature of other than the end members of the stack. Also, because the stacks have mosaic widths larger than the single wafers by a factor of $\sim n^{1/2}$, where $n$ is the number of wafers in the stack, we expected more dramatic effects from the single wafers.

For the sake of a quantitative experiment we took two wafers and elastically deformed them into spherical caps. The method is to use Belleville (slightly conical) washers 70 mm outer diameter and 64 mm inner diameter made out of aluminium on both sides of the wafer. When compressed, this puts a torque on the outer edge of the wafer. The response should be a quadratic bend. This can be checked optically using the sun as a source. The images are never of optical quality. That polished silicon wafers are not of perfectly uniform thickness is probably the major cause of this. The radii of curvature were adjusted to 10 and 5 m. The 5 m crystal was used as the monochromator with its curvature away from the analyzer crystal. The 422 reflection from the monochromator at a 90° take-off angle produces a beam of 0.175 nm wavelength neutrons. Double-crystal rocking curves were obtained for the 10 m radius crystal for the reflections $\pm 422$, $\pm 400$, $\pm 3\bar{1}1$ and $\pm 1\bar{1}1$. The corresponding calculations were carried out using numerical integration of (33) with $\eta_m = \eta_a = 0.025^\circ$. Note that none of the four reflections have $R_m$ and $R_a$ at optimum for rocking-curve sharpness, as given in Table 1. The results of the experiments and the comparison with theory are shown in Fig. 5. For each reflection the theory was normalized to match the mean height of the broad peak. But there is no adjustment other than that. Fig. 5(a) is for the same reflection as the monochromator. This would be the parallel position if the crystals were not bent. The structure in the curves, most apparent in Figs. 5(b) and (c), indicates that the crystals are not well conforming to the desired spherical cap bend. It is clear that the theory is quite adequate to account for the observations even if the experiment does not quite do justice to the theory. If we had known that the comparison was going to be as good as it is, we probably would have taken more care to get uniform bending of the crystals.

We do not show data for the 022 in as much as this is the subject of another paper on the relation of the direction of the strain gradient to the scattering vector in dynamical theory (Arrott & Templeton, 1985).

It is clear that one can take advantage of this theory in particular experiments. The most obvious one is in using the double-crystal rocking curve for the analysis of small-angle scattering as originally developed by Werner (Werner, Wiener, Gurmen & Arrott, 1970; Gurmen, Werner & Arrott, 1975). In Werner's method the sample crystal is placed between the monochromator and the analyzer. The small-angle scatter-
ing is found by subtracting the rocking curves with and without the sample (suitably normalized for attenuation in the sample). The power of this method is that it is not necessary to use any collimation other than that provided by the monochromator and analyzer. The use of suitably bent crystals can narrow the rocking curve by a factor $\leq 2^{1/2}$. Also, for small $T$, the monochromator width can be increased to improve counting rate without a large effect on the analyzer rocking-curve width. (See also Kulda & Mikula, 1983.)

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References