New Methods for the Alignment of Instrumentation for Residual-Stress Measurements by means of Neutron Diffraction

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Abstract
Adequate alignment of instrumentation and specimens is imperative for the successful performance of residual-stress measurements by means of neutron diffraction. This paper presents a number of alignment methods that enable the user to align reproducibly a stress-measurement setup and a specimen positioned therein. Most of these methods employ the position and the direction of the incident neutron beam as their primary source of geometric reference. A mathematical description for each of the proposed alignment steps is given, which makes the alignment quantitative and enables quantitative assessment of the alignment quality after each alignment step. Examples from actual practice show that the alignment quality that can be achieved using these methods is better than 0.05 mm for translations and better than 0.05° for rotations.

Introduction
It is well known that, in the field of neutron diffraction residual-stress measurement, adequate alignment of instrumentation and specimens is imperative. There are many approaches to the alignment of spectrometers; there is, however, a need for alignment methods that have a more universal value. One limitation of most alignment methods is that it is hard to quantify the ultimate alignment quality, other than by experience. In this paper, we try to give an independent means of assessing how well a particular step in the alignment has been carried out so that the person who applies the method can find out what the quantitative alignment error means in terms of potential systematic errors in subsequent neutron diffraction stress measurements.

For this purpose, the alignment techniques we introduce are based on a firm geometrical analysis, which allows the application of sophisticated fitting techniques. The alignment steps are thus upgraded to small experiments including all steps from data acquisition to error analysis. It is the error-analysis step that is used to determine how well a particular step in the alignment has succeeded.

The kind of neutron stress measurement we refer to here is that where a neutron diffractometer is used to measure lattice spacings of a small part of a specimen (Allen, Hutchings, Windsor & Andreani, 1981; Prask & Choi, 1984). This small volume, of which the center of gravity is the measurement location, is called the gauge volume. The gauge volume can, in principle, be chosen anywhere in the specimen, with a specimen-positioning device that ideally consists of an x, y, z positioning table (‘depth profiling’). A full-circle goniometer can be used to reorient the specimen so that the lattice spacing of the gauge volume can be measured at different orientations in the diffraction geometry. For depth-profiling stress measurements, a standard diffractometer is usually equipped with beam-limiting apertures in the primary and diffracted beams. Ideally, these apertures can slide along the primary and diffracted neutron beams in order to accommodate different specimen geometries. Alignment of such an instrument includes requirements such as:

1. the beam apertures should ‘illuminate’ the center of rotation of the diffractometer, which is defined as the axis around which the neutron counter and the specimen table rotate;
2. when the primary-beam aperture moves, it should slide parallel to the primary neutron beam defined by the placement of a Soller collimator;
3. the secondary-beam aperture should slide along the detector take-off angle, which is defined by the angular position where the counter ‘sees’ the direct beam;
4. the relation between the specimen axis system and the diffractometer axis system should be known, so that the position and the orientation of the gauge volume in the specimen are known;
(5) a rotation of the specimen around any applicable axis should not alter the position of the center of gravity of the gauge volume in the specimen axis system.

In order to address these aspects of the problem of instrumental alignment, we have developed a number of geometrical alignment methods. The majority of these methods employs incident and diffracted neutron beams as the primary source of geometrical reference. They are treated next.

**Alignment methods**

In this section, we discuss the geometrical methods that have been successfully applied to align a diffractometer for residual-stress measurements. All but the first method (finding a rotation center by means of a dial gauge) make use of a monochromatic neutron beam extracted from a steady-state reactor. In these methods, the neutron beam is either partially obstructed or made to diffract from a scattering object. The obstruction as well as the diffraction take place in a controlled manner, which allows us to use the geometrical functions as model functions in a fitting process. One of the free parameters in such a fitting process should be the position or angle reference that one is looking for in a particular alignment step.

With regard to beam time, neither of the presented alignment experiments takes more than 20–30 min* to be completed (includes both the taking of data and data analysis). This is typically the same amount of time needed for other alignment methods, like setting up and using a theodolite. The additional accuracy of the methods presented here makes them very much worth implementing.

**Finding the center of rotation of a diffractometer using a dial gauge**

The ultimate goal in aligning the diffractometer is to place a specimen on an x, y, z translation stage in such a way that its location and orientation with respect to the geometry of the primary and diffracted neutron beams are known. These two beams define a gauge volume in space that has its center of gravity somewhere on the diffractometer axis. From this, it is clear that the first step in the alignment process is to make a physical reference to the center of rotation of the diffractometer. Therefore, a precisely machined cylindrical pin is placed on the x, y table that will eventually hold the specimen. The traditional way of finding the center of rotation is to rotate the specimen table while looking at the pin through a theodolite.

Manipulation of the x and y movements of the specimen table will eventually iterate the pin into the central position. Our method, however, employs a mechanical dial gauge instead of a theodolite (mainly because the translational accuracy is an order of magnitude better). We locate the center of a rotating cylindrical pin with respect to the axis of rotation while only rotating this cylinder over a sector of arc of 90°. The mathematics necessary for this are presented below.

**Theory.** Consider a vertical cylinder, a horizontal section of which is shown in Fig. 1. The center of the cylinder is $M(m_1, m_2)$ in a coordinate system $Oxy$ of which the origin is $O(0, 0)$. $O$ is also the center of rotation. In the direction of the positive y axis, a dial gauge is touching the cylinder at point $A(0, a)$. The reading of the dial gauge is $r_a$. A rotation of the cylinder by 45° around $O$, with respect to the dial gauge, is equivalent to bringing the dial gauge to point $B$, where the reading is $r_b$. A third point can be found by rotating the cylinder another 45° in the same direction, which brings the dial gauge to point $C$, where the radius is $r_c$. The dial gauge is now measuring in the direction of the positive x axis. $A$, $B$ and $C$ are three points on the circle centered at $M$ with coordinates

$$
A (0, a)
B \left(\frac{(a + r_a - r_b)}{2^{1/2}}, \frac{(a + r_b - r_c)}{2^{1/2}}\right)
C \left(a + r_c - r_a, 0\right).
$$

We now make the following substitutions:

$$
B - A = \Delta_{ba},
C - A = \Delta_{ca}.
$$

From the general equation for a circle

$$
(x - m_1)^2 + (y - m_2)^2 = r^2,
$$

we get

$$
M(m_1, m_2): \text{pin center}
O(0,0): \text{rotation center}
$$

Fig. 1. Dial gauge set up for finding the center of rotation of a cylindrical alignment pin.

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* This time estimate is given on the basis of our computer programs being used on data taken at beam port BT6 at the NBSR reactor at NIST, Gaithersburg.
the following three equations containing three unknowns can be constructed:

\[ m_1^2 + (a - m_2)^2 = r^2 \]
\[ \left[ \frac{1}{2}2^{1/2}(a + \Delta_{ba}) - m_1 \right]^2 + \left[ \frac{1}{2}2^{1/2}(a + \Delta_{ba}) - m_2 \right]^2 = r^2 \]
\[ (a + \Delta_{ca} - m_1)^2 + m_2^2 = r^2 \]

(4)

The unknowns \((m_1, m_2, a)\) are not readily solved for from (4) so we apply a numerical method in order to find a solution. The method we use is the method of Newton, which is described in some detail by Press, Flannery, Teukolsky & Vetterling (1986). The Newtonian iterative process solves a set of nonlinear equations of the form

\[ f(x_1, x_2, x_3, \ldots) = 0, \quad i = 1, 2, \ldots, N. \]

(5)

Equations (4) can be written in this form as:

\[ m_1^2 + (a - m_2)^2 - r^2 = 0 \]
\[ \left[ \frac{1}{2}2^{1/2}(a + \Delta_{ba}) - m_1 \right]^2 + \left[ \frac{1}{2}2^{1/2}(a + \Delta_{ba}) - m_2 \right]^2 - r^2 = 0 \]
\[ (a + \Delta_{ca} - m_1)^2 + m_2^2 - r^2 = 0. \]

(6)

One necessary step in this solution process is the availability of good initial values (guesses) for the unknowns. These can be found by solving (4) while systematically ignoring terms involving two or more \(\Delta\)'s. The system of equations then reduces to

\[ m_1 = \left[ -2a\Delta_{ba} - (2^{1/2} - 2)a\Delta_{ca} \right] \times \left[ (-2(2^{1/2}) + 2)a - 2(2^{1/2})\Delta_{ba} \right] + \left[ (2^{1/2} - 2)\Delta_{ca} \right]^{-1} \]
\[ m_2 = (2a\Delta_{ba} - 2^{1/2}a\Delta_{ca}) \times \left[ (2(2^{1/2}) - 2)a + 2^{1/2}\Delta_{ba} \right] + \left[ (2^{1/2} - 2)\Delta_{ca} \right]^{-1} \]
\[ m_1^2 + m_2^2 = r^2 + 2am_2 - a^2. \]

(7)

If in the first two equations \(a\) is replaced by \(r\), we will not have the correct solution but an excellent first guess for the start of the iteration process according to Newton. Using this method, one can find the center of rotation of one horizontal intersection of a cylinder and just one plane. We have obtained accuracies better than 0.02 mm using the present procedure.

The single knife edge

An important step in the alignment procedure for the neutron diffractometer in stress-measurement mode is the determination of the direction of the primary beam in the coordinate system of the specimen table (Brand, 1991, 1992). When radially moving primary and diffracted beam apertures are employed, their sliding directions should be along the directions of the corresponding beams.

The actual beam direction will be obtained by the double-knife-edge test, which is treated in the next section. The purpose of this single-knife-edge scan is to determine the correct position of the bracket that holds both the single- and double-knife-edge assemblies.

The principle of the single-knife-edge scan is very simple. The diverging primary neutron beam is covered by a neutron-absorbing wedge (the single knife). The coverage is removed in a stepwise manner while between the steps the intensity of the part of the beam that passes the wedge is measured. This process continues until the beam is completely open. Qualitatively, the measured intensity as a function of the wedge position yields a monotonically rising curve with a constant minimum at the beginning and a constant maximum at the end. From this curve, we will obtain the wedge position at which half of the beam is covered, which is the position at which the double-knife-edge scan will be carried out.

Theory. The construction of the single knife edge is shown in Fig. 2. In this figure, the beam geometry is also shown. The single knife edge is built of an aluminium knife holder in which the knife, a cadmium-plated brass wedge, is held. The assembly is placed on the specimen table of the diffractometer and rigidly connected to it. The relative position of the knife edge perpendicular to the primary-beam direction is called \(x\). The position of the center line of the primary neutron beam is denoted \(x_0\). The form of the beam cross section at the site of the single knife edge is characterized by the beam divergence, \(\alpha\), the aperture width, \(w\), and the aperture distance from the knife edge, \(d\). The parameter we are looking for is \(x_0\), the knife position at which half of the primary beam is covered.

The single-knife-edge scan consists of the measurement of the intensity as a function of the position \(x\) of the knife edge. In order to be able to give an

![Fig. 2. Top view of the single-knife-edge assembly showing the beam geometry.](image-url)
indication of the accuracy of the determination of the beam position $x_0$, a theoretical model should exist that can be fitted to the single-knife-edge scan data. A standard fitting procedure, based on the Levenberg–Marquardt algorithm, will yield estimates of the free parameters of the theoretical model and their errors.

The scan starts with the single knife fully covering the primary neutron beam. The neutron detector, situated at the direct-beam position, will now only detect background radiation $I_b$. The detected intensity $I$ as the knife assembly is moved towards the positive $x$ direction (i.e. uncovering the beam) can be deduced from the intensity profile shown in Fig. 3. The total measured intensity at some $x$ is equal to

$$I(x) = \int_{x_0 - 1/2w - 1/2\alpha d}^{x} dI + I_b.$$  \hspace{1cm} (8)

The value of this function is equal to the hatched area of Fig. 3. It can be represented in a mathematical form when divided into five $x$ regions. The parameter $I_0$ that appears in the following equations is a proportionality constant.

(I) $x < x_0 - \frac{1}{2}w - \frac{1}{2}\alpha d$ 
$$I = I_b; \hspace{1cm} (9a)$$

(II) $x_0 - \frac{1}{2}w - \frac{1}{2}\alpha d \leq x < x_0 - \frac{1}{2}w + \frac{1}{2}\alpha d$ 
$$I = [(x - x_0 + \frac{1}{2}w + \frac{1}{2}\alpha d)^2/2\alpha d]I_0 + I_b; \hspace{1cm} (9b)$$

(III) $x_0 - \frac{1}{2}w + \frac{1}{2}\alpha d \leq x < x_0 + \frac{1}{2}w - \frac{1}{2}\alpha d$ 
$$I = (x - x_0 + \frac{1}{2}w)I_0 + I_b; \hspace{1cm} (9c)$$

(IV) $x_0 + \frac{1}{2}w - \frac{1}{2}\alpha d \leq x < x_0 + \frac{1}{2}w + \frac{1}{2}\alpha d$ 
$$I = I_0 - [(x_0 - x + \frac{1}{2}w + \frac{1}{2}\alpha d)^2/2\alpha d]I_0 + I_b; \hspace{1cm} (9d)$$

(V) $x \geq x_0 + \frac{1}{2}w + \frac{1}{2}\alpha d$ 
$$I = I_0 + I_b. \hspace{1cm} (9e)$$

In order to obtain the value of $x_0$ from (9), these equations must serve as the model function in a

Levenberg–Marquardt fitting procedure (Press, Flannery, Teukolsky & Vetterling, 1986). A number of intensity measurements are input to this fitting procedure as a function of the knife position. As the intensity values have errors based on counting statistics, their square-root values are given as the internal errors. The free parameters in the fitting process are $x_0, I_0, I_b, w$ and the product $\alpha d$. In practice, the function has proved very helpful in establishing correct values for the parameters mentioned. An example of the use of this function is given in Fig. 4.

The double knife edge

During the alignment procedure for the neutron diffractometer, we seek a physical reference for the primary-beam direction (Brand, 1991, 1992). This reference is used for aligning the sliding directions of the primary- and secondary-beam apertures by means of a dial gauge. The single-knife experiment treated above yields a specimen-table position at which a cadmium (single) knife is half closing the primary beam. This position is called $x_0$ (single knife edge half across the beam). At the stage that $x_0$ is known, another type of experiment must lead to the determination of the relative direction of the center line of the beam, which will be called $\psi_0$. The experiment that delivers this parameter is called the double-knife-edge scan.

The principle of this scan is as simple as the principle of the single-knife-edge scan. Now, however, two

![Fig. 3. Intensity profile across the incident beam at the location of the single knife edge.](image)

![Fig. 4. Experimental results of a single-knife-edge experiment. The solid line is the result of a successful fit of (9) to the data. For these data, a value of 28.33 (2) was obtained for the free parameter $x_0$ from (9).](image)
knives instead of one are used and the scan parameter is not a translation perpendicular to the beam direction but a rotation around the center of the diffractometer. The stepwise rotation begins at the situation where one knife covers the beam completely and continues until the other knife covers the beam. Between these two extremes, there exists a maximum corresponding to the situation where the two knife edges are in line with the beam. The purpose of the single-knife-edge scan has only been to find out at which knife position the double-knife-edge scan should be performed.

As the accuracy in direction of the beam must be estimated, a mathematical treatment of the function that describes the double-knife-edge scan is given. Using this function in a parameter-adjustment procedure will yield the uncertainties in the determined parameters.

Theory. The construction of the double knife edge is shown in Fig. 5. The beam geometry is also shown. The double knife edge is obtained by putting an extra knife into the empty place in Fig. 2. The advantage of this construction is that it makes it unnecessary to dismount the knife holder from the specimen table, thus mechanically conserving the result of the single-knife-edge scan. The different parts of the assembly are manufactured such that the connection line between the two knives is parallel to the back plane of the knife holder within 0.005°.

Both knife edges should be positioned symmetrically with respect to the center of rotation of the diffractometer. This is not very critical as there will be a free parameter Δl in the model that takes care of an unexpected misplacement. In practice, however, the misplacement should not exceed a few mm. In order to arrange the knife assembly this way, the coordinate table (i.e. the y movement, which is along the beam direction) is used to transport the assembly I₂ from the primary-beam aperture with respect to the single-knife-edge-scan situation, I being the distance between the knives.

The scan variable of the double-knife-edge scan is ψ, so the purpose of the scan is to determine the ψ value at which the line connecting the two knives is parallel to the primary-beam center line. This ψ value will be called ψ₀.

Usually, there exists a slight misplacement of the double-knife-edge assembly with respect to the result of the single-knife-edge scan: x₀. This is due to an incorrect ψ during the single-knife-edge scan (after all, ψ₀ was not known during the single-knife-edge scan). As a result, the fitting procedure on the double-knife-edge scan may yield a different value for the aperture opening w from that of the fitting procedure on the single-knife-edge scan. When these values for w are too far apart (e.g. more than 10% of w), it is advisable to repeat the single-knife-edge scan at the value of ψ that is the result of the then-declared 'preliminary' double-knife-edge scan. In that case, the double-knife-edge scan must be repeated at the newly determined x₀.

The beam geometry is defined by the same parameters as in the single-knife-edge scan: x, d and w. Between the scans, these should remain unchanged. In practice, this means that the position and opening of the primary-beam aperture must be maintained the same during both scans.

In the following, it is assumed that the scan starts at the situation where the knife closest to the aperture defining the primary beam is covering the beam completely so that only the background radiation Iₙ is detected by the neutron counter. The direction of ψ is chosen to be counterclockwise.

In Fig. 6, the intensity profile of the beam at the counter side of the double edge is given. The ordinate of Fig. 6 is ψ - ψ₀, so the integration parameter for the integration of dI will be ψ. In Fig. 6, the detected
The intensity \( I(\psi - \psi_0) \) is seen to be proportional to the hatched surface under the curve. It should be noted that the surface under the right-hand part of the curve has a negative contribution. The proportionality constant is set equal to \( I_0 \).

There exist two distinct geometrical modes for the double-knife-edge scan. The underlying reason is that the beam possesses a finite divergence \( \alpha \). This means that every obstacle that enters the primary beam gives rise to a trapezoidal intensity profile behind it. Unfortunately, the primary-beam aperture is not the only thing that can be regarded as an obstacle (two obstacles, to be exact); in addition, the first knife encountered by the beam serves as a moving obstacle that influences the profile to be covered by the second knife as the scan proceeds. Because the knives are rigidly connected by means of the knife holder, the profile encountered by the second knife is influenced by the first one in a predictable way. For the derivation of the intensity function for the double-knife-edge scan, we have to account for this phenomenon. The most important effect of the moving intensity pattern is that, depending on the value of the geometrical variables, two different situations (A and B) exist:

\[
\frac{1}{2} \psi < \left[ \frac{1}{2} w - \frac{1}{2} \alpha (d + \frac{1}{2} l - \Delta l) \right]/(\frac{1}{2} l - \Delta l).
\]

This corresponds to the situation that the divergence spread out by the first knife seen from the beam aperture (see Fig. 5) is covered by the second knife before it enters the lower divergence spread out by the aperture. The intensity function is again divided into seven regions:

\[(I)
\psi - \psi_0 < \left[ -\frac{1}{2} w - (d - \frac{1}{2} l - \Delta l) \frac{1}{2} \alpha \right]/(\frac{1}{2} l + \Delta l)
I = I_b;
\]

\[(II)
\left[ -\frac{1}{2} w - (d - \frac{1}{2} l - \Delta l) \frac{1}{2} \alpha \right]/(\frac{1}{2} l + \Delta l) < \psi - \psi_0 < \left[ -\frac{1}{2} w + (d - \frac{1}{2} l - \Delta l) \frac{1}{2} \alpha \right]/(\frac{1}{2} l + \Delta l)
I = \left\{ \left[ (\psi - \psi_0) \left( \frac{1}{2} l + \Delta l \right) + \frac{1}{2} w + (d - \frac{1}{2} l - \Delta l) \frac{1}{2} \alpha \right]^2 \times \left[ 2(d - \frac{1}{2} l - \Delta l) \alpha \right]^{-1} \right\} I_0 + I_b;
\]

\[(III)
\left[ -\frac{1}{2} w + (d - \frac{1}{2} l - \Delta l) \frac{1}{2} \alpha \right]/(\frac{1}{2} l) \leq \psi - \psi_0 < -\frac{1}{2} \alpha
I = \left\{ (\psi - \psi_0) \left( \frac{1}{2} l + \Delta l \right) + \frac{1}{2} w \right\} I_0 + I_b;
\]

\[(IV)
-\frac{1}{2} \alpha \leq \psi - \psi_0 < \frac{1}{2} \alpha
I = \left[ \frac{1}{2} w - (\psi - \psi_0) \left( \frac{1}{2} l + \Delta l \right) I_0 \right.
\left. - \left\{ \left[ (\psi - \psi_0) + \frac{1}{2} \alpha \right]^2/2 \alpha \right\} I_0 + I_b; \right.
\]

\[(V)
\frac{1}{2} \alpha \leq \psi - \psi_0 < \left[ \frac{1}{2} w - (d + \frac{1}{2} l - \Delta l) \frac{1}{2} \alpha \right]/(\frac{1}{2} l - \Delta l)
I = \left[ \frac{1}{2} w - (\psi - \psi_0) \left( \frac{1}{2} l - \Delta l \right) \right] I_0 + I_b;
\]
In order to use one of the sets of equations defined above [either (10) or (11)] to obtain \( \psi_0 \) from the data of a double-knife-edge scan, the equations serve as the model in a Levenberg-Marquardt fitting procedure (Press, Flannery, Teukolsky & Vetterling, 1986). The free parameters are \( \Delta l, w, I_o, I_b, \alpha \) and \( \psi_0 \). The decision between case I and case II is left to the fitting algorithm in order to avoid a non-logical outcome of the calculation. The model has proved to be very successful in calculating the parameters and their error estimates. An example of the use of the model is given in Fig. 7.

**Slit alignment using a powder specimen**

During a set of diffraction-peak registrations that together constitute a stress measurement, the specimen is usually rotated around a set of axes that should have their intersection point exactly at the center of gravity of the sampling volume. If this requirement is not fulfilled, the sampling volume will be at a different location in the specimen for each different orientation of the specimen.

In this section, a method is described that establishes the locations of the beam apertures with respect to the center of rotation of the goniometer. Specifically, we do this for an instrument configuration in which the detector is at the scattering angle to be used for the specimen of interest. We thus obtain information about the direct beam via diffraction of the direct beam by a powder specimen. This powder specimen will have a known location in the goniometer geometry, which must have been established by mechanical means (see the previous section). The basic principle is to step scan this powder specimen through the direct beam. From a mathematical model that describes the intensity obtained in the counter as a function of the position of the specimen, it is possible to obtain the position of the aperture with respect to the (known) location of the powder specimen. For this a specimen of cylindrical shape is preferred because it can be centered using the dial-gauge technique described earlier.

**Theory for horizontal alignment.** In Fig. 8, the top view of a horizontal beam of width \( 2w \) is given. In the same figure, a cylinder of radius \( r \) is drawn such that it is partly irradiated by the neutron beam. The center of the cylinder has a coordinate \( p \) that is known with respect to the center of rotation of the spectrometer. The position of the center of the neutron beam in the axis system in which \( p \) was defined is called \( x_0 \). The intensity resulting from the occupied part of the beam can be estimated by integrating over that surface, taking into account the path length that the beam has to travel for each location. This is where the attenuation coefficient \( \mu \) enters the problem. The intensity \( I_1 \) that results from the occupied part can be calculated from

\[
I_1(p) = I_0 \int_{x_1}^{x_2} \int_{y_1}^{y_2} \exp \left\{ -\mu [(r^2 - x^2)^{1/2} - y] + (r^2 - y^2)^{1/2} - x \right\} \, dx \, dy.
\]

(12)

\( I_0 \) in (12) is a proportionality constant. Depending on the size of \( r \) relative to \( w \), two different models exist for the step-scan function. Let us first consider the situation where \( r \leq w \). The step-scan function will
now consist of five parts, which have the following relationships with (12):

(I)  
\[ p \leq x_0 - w - r \]  
\[ l = l_b; \]  
\[ (13a) \]

(II)  
\[ x_0 - w - r < p \leq x_0 - w + r \]  
\[ l = l_1 + l_b \]  
\[ x_1 = x_0 - w - p, \quad x_2 = r; \]  
\[ (13b) \]

(III)  
\[ x_0 - w + r < p \leq x_0 + w - r \]  
\[ l = l_1 + l_b \]  
\[ x_1 = -r, \quad x_2 = r; \]  
\[ (13c) \]

(IV)  
\[ x_0 + w - r < p \leq x_0 + w + r \]  
\[ l = l_1 + l_b \]  
\[ x_1 = -r, \quad x_2 = x_0 + w - p; \]  
\[ (13d) \]

(V)  
\[ p > x_0 + w + r \]  
\[ l = l_b. \]  
\[ (13e) \]

Likewise, for \( r > w \):

(I)  
\[ p \leq x_0 - w - r \]  
\[ l = l_b; \]  
\[ (14a) \]

(II)  
\[ x_0 - w - r < p \leq x_0 + w - r \]  
\[ l = l_1 + l_b \]  
\[ x_1 = x_0 - w - p, \quad x_2 = r; \]  
\[ (14b) \]

(III)  
\[ x_0 + w - r < p \leq x_0 + w + r \]  
\[ l = l_1 + l_b \]  
\[ x_1 = -r, \quad x_2 = x_0 + w - p; \]  
\[ (14c) \]

(IV)  
\[ x_0 + w + r < p \leq x_0 + w + r \]  
\[ l = l_1 + l_b \]  
\[ x_1 = -r, \quad x_2 = x_0 + w - p; \]  
\[ (14d) \]

(V)  
\[ p > x_0 + w + r \]  
\[ l = l_b. \]  
\[ (14e) \]

The \( y \) boundaries for (12) are given by

\[ y_1(x) = -(r^2 - x^2)^{1/2} \]  
\[ y_2(x) = (r^2 - x^2)^{1/2}. \]  
\[ (15) \]

For the alignment of the primary-aperture assembly, we assume that no secondary-beam aperture is present in the secondary-beam path so that the entire powder specimen can be observed by the counter at all times. For the alignment of the secondary-beam aperture as depicted in Fig. 9, the same series of equations apply. There exists, however, one minor difference, which is related to the fact that the primary-beam-aperture opening may be smaller than the specimen diameter. Therefore, the expressions for the \( y \) boundaries become slightly different:

\[ y_1(x) = \max \left(-\frac{(r^2 - x^2)^{1/2}}{w_p}, \frac{(r^2 - x^2)^{1/2}}{w_p}\right) \]  
\[ y_2(x) = \min \left((r^2 - x^2)^{1/2}, \frac{(r^2 - x^2)^{1/2}}{w_p}\right). \]  
\[ (16) \]

In (16), \( w_p \) is the width of the primary slit.

**Theory for vertical alignment.** We now develop a similar set of equations for the vertical alignment of a primary-beam slit of width \( 2w \) and height \( 2h \). The set-up is now such that the \( \chi \) arc of the full circle has rotated the specimen in a vertical plane through the bisector of the incident and diffracted beams. The irradiated volume is still cylindrical; however, the top and bottom surfaces are inclined \( 45^\circ \) with respect to the cylinder axis. The intensity from this body located at a position \( p \) will be a volume integral of the through-specimen path length over this body. So, we need expressions for the through-specimen path length and the limits of integration in \( x, y \) and \( z \). We choose a Cartesian axis system as follows:

1. the origin of the Cartesian axis system is at the center of gravity of the irradiated body;
2. the vector expression for a neutron path in the incident beam passing through a point \( X(x, y, z) \) is

\[ \mathbf{x} = \begin{bmatrix} x \\ y \\ z \end{bmatrix} + \hat{x}_l \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}; \]  
\[ (17) \]

3. the vector expression for a neutron path in the diffracted beam passing through a point \( X(x, y, z) \) is

\[ \mathbf{x} = \begin{bmatrix} x \\ y \\ z \end{bmatrix} + \hat{x}_d \begin{bmatrix} -1 \\ 0 \\ 0 \end{bmatrix}. \]  
\[ (18) \]
In these equations, \( X(x, y, z) \) is an arbitrary point in the scattering volume. From this definition, it can easily be seen that the axis of the cylinder will be expressed by
\[
X = \left[ \begin{array}{c} x \\ y \\ z \\ 1 \end{array} \right]
\]
It can be derived that the boundaries for the diffracting body are
\[
x^2 + y^2 + 2z^2 = 2r^2 \quad \text{(cylinder)}
\]
\[
x = -w \quad \text{(bottom of cylinder)}
\]
\[
x = w \quad \text{(top of cylinder)}
\]
After finding the intersection points of both an incident neutron and a diffracted neutron with the cylinder, we can calculate the total through-specimen flight-path length for one neutron. Integration will yield the total intensity. So, for one diffracted neutron, we obtain a total through-specimen flight path of
\[
l(x, y, z) = \sqrt{x^2 + (y + \lambda d)^2 + z^2} + \sqrt{(x + \lambda d)^2 + y^2 + z^2}
\]
In (21), \( \lambda_i \) and \( \lambda_d \) are obtained from combinations of (17) and (18), respectively, with the equation of the cylinder [(20)]. Each combination usually yields two values for \( \lambda_i \) and \( \lambda_d \), which each correspond to one of two intersection points of a line with a cylindrical body. For our choice of axis system and linear equations [(17) and (18)], the largest of the two values for \( \lambda_i \) and \( \lambda_d \) is always the correct one.

The position scan function, which divides into three regions, is:
\[
\begin{align}
\text{(I)} & \quad p - x_0 < -r + h \\
I & = I_0 \\
\text{(II)} & \quad -r + h < p - x_0 < r + h \\
I & = I_0 + I_1 \\
\text{(III)} & \quad p - x_0 > r + h \\
I & = I_1
\end{align}
\]

Experimental confirmation. The results presented in Figs. 10, 11 and 12 clearly indicate that the centers of the primary and secondary beams can readily be located, both horizontally and vertically. The accuracy by which the parameter \( x_0 \) is determined for the different models meets the highest standard one could
wish. As the position at which the specimen axis coincides with the vertical axis of the spectrometer is obtained separately (i.e. by means of a mechanical dial gauge), the horizontal and vertical positions of the beam apertures can be readily corrected such that they point to the center of the spectrometer.

**Entering curves**

After the sequence of alignment procedures described above has been utilized, the neutron diffractometer, including its beam-aperture systems, can be expected to be well aligned. In order to start a measurement, the location of the specimen axis system in the beam geometry should be established (Brand, 1991, 1992). During this step, the ability of a specimen to diffract neutrons will again be used.

The aperture systems that are connected to the diffractometer define a rhombic prism in space: the gauge volume. The axis of the prism is expected to coincide with the diffractometer axis. When the specimen is moved towards the diffractometer center, the specimen material will start to diffract neutrons as the sample volume becomes part of the specimen. The diffracted intensity of a certain peak is a function of the specimen position relative to the diffractometer axis and of the parameters that define the shape and the size of the sample volume. Depending on the form, the orientation and the composition of the specimen, beam attenuation might play an important role.

In the next subsections, two models – called entering curves – are presented that give the integrated intensity as a function of the relative specimen position. There will be a treatment of two geometrical situations, i.e. the diffraction vector $\mathbf{q}$ parallel and perpendicular to the specimen surface, where the vector $\mathbf{q}$ can be defined as parallel to the bisector of the incident and diffracted beams. The specimen we have
chosen for the derivations is a bar-shaped specimen that contains no texture.

When the integrated intensity of a diffraction peak is measured as a function of the relative position of the specimen surface for the two orientations of the incident vector $q$, the location of the center of gravity of the sample volume can be found by means of a least-squares fitting procedure using both models. The fit results belonging to each of the two models should give the same value for the relative surface position at which the diffractometer axis is situated exactly in the specimen surface. Comparing these results is a way to confirm the quality of the alignment achieved.

Theory for entering curve at $\psi = 0^\circ$ (reflection). The primary- and secondary-beam apertures, both of width $w$, define a rhombic prism in space. The rhombus is defined by $w$ and $2\theta$ (see Fig. 13). In the well aligned situation, the point of intersection of the diagonals of the rhombus coincides with the center of rotation of the diffractometer. The function to be derived will be such that at $x_0$ the intersection of the diagonals of the rhombus lies in the specimen surface.

From the region defined thus, a diffracted intensity $I$ is expected that differs from the background value when some part of the region contains specimen material. The measured integrated intensity from a partly occupied region (to be characterized by $x$) can be calculated by integrating over the occupied part of the surface region. One aspect of the $\psi = 0^\circ$ case is that the intensity, obtained from a coordinate somewhere below the specimen surface, is attenuated owing to absorption along the total travelling path for a neutron to and from that particular coordinate. This depth-dependent attenuation is described by an absorption factor, which includes the absorption coefficient $\mu$.

In the left part of Fig. 13, the cross section of the stationary rhombic prism is shown, together with the moving specimen. The function that describes the integrated intensity as a function of the relative specimen position is divided into four $x$ regions. In the next equations, $I_0$ is a proportionality constant, $I_b$ is the background intensity and $p_0$ is half the rhombus diagonal that is oriented perpendicular to the specimen.

$$p_0 = (\sin \theta / \sin 2\theta)w. \quad (27)$$

From the parameters defined up to now, the model that gives the integrated intensity as a function of the relative position $x$ will be:

(I) $$x < x_0 - p_0$$

$$I = I_b; \quad (28a)$$

(II) $$x_0 - p_0 \leq x < x_0$$

$$I = I_0[(x - x_0 + p_0) / \mu] - I_b \sin(\theta / 2\mu^2)\left\{1 - \exp\left[\left[-2\mu / \sin \theta\right] (x - x_0 + p_0)\right]\right\} + I_b; \quad (28b)$$

(III) $$x_0 \leq x < x_0 + p_0$$

$$I = I_0(\sin \theta / 2\mu^2)\left\{-2\exp\left[\left[-2\mu / \sin \theta\right] (x - x_0 + p_0)\right] + 1\right\} + I_0[(x_0 + p_0 - x) / \mu] + I_b; \quad (28c)$$

(IV) $$x \geq x_0 + p_0$$

$$I = I_0(\sin \theta / 2\mu^2)\left\{-2\exp\left[\left[-2\mu / \sin \theta\right] (x - x_0 + p_0)\right] + \exp\left[\left[-2\mu / \sin \theta\right] (x - x_0 - p_0)\right] + I_b. \quad (28d)$$

Equations (28) give the expected integrated intensity as a function of $x$ and a number of parameters. From the measurement of $I$ at a series of $x$ values, the values of the unknown parameters can be obtained by a Levenberg-Marquardt process (Press, Flannery, Teukolsky & Vetterling, 1986). The free parameters that will enter this process via the function defined above are $x_0$, $w$, $I_0$, $I_b$ and $\mu$.

Theory for entering curve at $\psi = 90^\circ$ (transmission). For the situation where $\psi = 90^\circ$, i.e. when the diffraction vector $q$ is parallel to the specimen surface, the derivation of the integrated intensity as a function of the relative specimen position is less complicated than the $\psi = 0^\circ$ case. In the $\psi = 90^\circ$ case, the total path length for neutrons in the specimen material (the sum of the path to and the path from a specific coordinate) is not dependent on the position in the specimen. This is because of the bar-shaped form of the specimen. Therefore, all absorption information will be hidden in the parameter $I_0$.

The geometry for this case is given in the right-hand part of Fig. 13, where it can clearly be seen that the
beam leaves the specimen on the side opposite to that by which it entered the specimen. The parameter that symbolizes the situation where the intersection point of the two rhombus diagonals meets the specimen surface is called $x_{g0}$. The length of the diagonal that is now perpendicular to the specimen surface is called $p_{90}$; its value is

$$p_{90} = \frac{1}{2} \arctan \left( \frac{\cos \beta}{\sin \beta \sin \gamma} \right).$$

The model that gives the integrated intensity as a function of relative specimen position is divided into four $x$ regions:

(I) \hspace{1cm} x < x_{g0} - p_{90} \hspace{1cm} I = I_b; \\
(II) \hspace{1cm} x_{g0} - p_{90} \leq x < x_{g0} \hspace{1cm} I = I_0(x - x_{g0} + p_{90})^2 + I_b; \\
(III) \hspace{1cm} x_{g0} \leq x < x_{g0} + p_{90} \hspace{1cm} I = I_0 \left[ 2p_{90}^2 - (x_{g0} + p_{90} - x)^2 \right] + I_b; \\
(IV) \hspace{1cm} x \geq x_{g0} + p_{90} \hspace{1cm} I = 2I_0p_{90}^2 + I_b.$$

Equations (30) give the expected integrated intensity as a function of $x$ and a number of parameters. From the measurement of $I$ at a series of $x$ values, the values of the unknown parameters can be obtained by a Levenberg-Marquardt fitting process (Press, Flannery, Teukolsky & Vetterling, 1986). The free parameters that will enter this process via the model defined above are $x_{g0}$, $w$, $I_0$ and $I_b$.

**Examples of entering curves.** In Fig. 14, an example of a successful fit of equations (28) to experimental data is given. The data were taken from a bar-shaped container filled with iron powder. The gradually dropping intensity at higher depth values clearly shows the effect of attenuation ($\mu$ is about 0.06 mm$^{-1}$ for iron powder). As is obvious from the figure, one cannot find the position where the gauge volume is half-way in the specimen [$x_0$ in equations (28)] simply by taking the position corresponding to half the maximum intensity. The attenuation effect becomes even more pronounced as $w$ increases.

Fig. 15 shows an example of a transmission entering curve (transmission: $q$ parallel to the sample surface). The sample we employed has a rectangular cross section so the path length for an individual neutron is not affected by the position from which it diffracts. Therefore, depth-dependent attenuation does not play a role in the shape of the curve. In this particular case, $x_{g0}$ corresponds to the position where the intensity is one half of the maximum value. However, determining $x_{g0}$ that way would make it impossible to perform an adequate error analysis, which is only possible if equations (30) are fitted to the data.
Entering curves can be measured in two ways. The first method is to obtain real values for the integrated intensity as a function of specimen-surface position, which implies scanning a complete diffraction peak for each specimen position. The second method is first to determine the maximum of a typical diffraction peak, then bring the instrument to that position and scan the specimen position. Because the peak position suffers a slight shift as a function of specimen position, one might find the second method less attractive. However, tests performed by us have shown that there is no significant difference between the two methods as far as the determination of $x_0$ and $x_{90}$ is concerned. There is a small but significant difference for parameters like $w$ and $\mu$, but we still prefer the second method because it is much faster and it is the positions that are the parameters of most interest.

Concluding remarks

With the alignment methods outlined in this paper, an instrument for residual stress measurements by means of neutron diffraction can be reproducibly aligned. The total gauge-volume positioning error, which can be derived from the uncertainties in the individual alignment steps, can be kept as low as 0.03 to 0.05 mm in the $x$, $y$ and $z$ directions. For gauge volumes as small as $1 \times 1 \times 1$ mm, this is sufficiently accurate.

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