Absorption correction of peak positions for neutron strain measurements

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Abstract. In angle-dispersive neutron strain scanning the information about residual strain comes from the whole gauge volume that is defined by slits in the incoming and diffracted beams. Since the intensity of the neutron beam decreases with the amount of material it has travelled, neutrons diffracted from different locations within the gauge volume contribute with different intensities to the recorded diffraction peak. This can lead to peak shifts, and thus apparent strains. The magnitude of this peak shift depends mostly on the beam attenuation and the size of the gauge volume, but also on the sample geometry and position of the gauge volume within the sample. The peak shift plays a significant role when the size of the gauge volume becomes large because of peak broadening by the sample. An analytic expression for the peak shift was derived for a simple geometry to evaluate a numerical simulation. The numerical simulation was developed to quantify necessary corrections in detail. The attenuation-induced peak shift was demonstrated by measurements on a strain-free powder sample and the results were compared with the numerical predictions.

1. Introduction
Neutron diffraction is a well-established technique for the non-destructive characterization of residual stress states in the interior of crystalline material [1, 2]. The physical principal is the same as for X-rays from a laboratory source, with the important difference that the penetration depth of neutrons is about a thousand times larger than for such X-rays. This enables neutron strain measurements at any location within several cm thick samples for many materials. Typical spatial resolutions are between 1 and 3 mm, depending on parameters such stress gradients, grain size, and sample thickness. There are angle-dispersive and energy-dispersive neutron strain scanners, the former work with monochromatic neutrons and record one single peak at a time, the latter work with a polychromatic beam and a time-of-flight (TOF) setup recording several diffraction peaks at once. In the following, only angle-dispersive neutron diffractometers will be discussed.

In angle-dispersive neutron strain scanning a sample is shifted through a neutron beam while the position of a Bragg reflection is recorded with an area detector [3]. The information about residual strain comes from the whole gauge volume that is defined by slits in the incoming and diffracted beams. (The advantage of a radial collimator in the diffracted beam will be discussed at the end.) The divergence of the beam also affects the size and shape of the gauge volume. Since the intensity of the neutron beam decreases with the amount of material it has travelled due to absorption and scattering, neutrons diffracted from different locations within the gauge volume contribute with different intensities to the measured diffraction peak. This leads to peak shifts, and thus apparent strains, which have to be corrected in extreme cases to obtain true strains. The magnitude of the peak shift also depends on the sample geometry and, thus, can change as a function of sample position relative to the
gauge volume. This means that a correction function is required for a whole strain scan along a line through a sample. However, this attenuation-induced peak shift is not included in standard data evaluation procedures for residual stress analysis, which is because it only plays a role when the size of the gauge volume becomes large. This is the case for sample-induced broadening of the diffracted beam. However, large peak broadening effects are not very often observed in engineering structural materials.

To be able to apply a correction for attenuation-induced peak shifts to measured strain data in such cases, a numerical simulation of the diffraction geometry including attenuation was developed. The numerical simulation was evaluated in two different ways: first, analytical expressions were derived for the peak shift for simple geometries, namely cylinder and plate samples. Second, a strain-free powder sample with a cylinder shape was measured and the results were directly compared with the predictions of the numerical simulation. The results show that the numerical simulation describes the attenuation-induced peak shift correctly and, thus, can be used for a correction of measured strain data.

2. **Analytical expression**

The effect of absorption on the peak position can be calculated analytically for simple geometries like e.g. the cylinder sample sketched in figure 1. It can also be easily formulated for plate samples. Incoming monochromatic neutrons travel along \(x\). It is assumed that the width \(w_1\) of the incoming beam is infinitesimally small and it has no divergence. The attenuation coefficient of the material is \(\mu\), corresponding to the total macroscopic cross section. Thus, the intensity of the incoming beam at a position \(x\) within the sample is

\[
I(x) = I_0 \exp(-\mu(x-x_0))
\]  

where the sample surface is at \(x_0\), and \(I_0\) is the intensity of the incoming beam. The width \(w_2\) of the slit in the diffracted beam shall also be infinitesimally small. It is assumed that there are spreads in the lattice parameter of the sample material as well as in the wavelength of the incoming beam that lead to a Gaussian profile of the diffraction peak. The peak recorded on a linear detector in the diffracted beam is then described by

\[
I(2\theta) = I_1 \exp\left(-\frac{(2\theta - 2\theta_0)^2}{2\sigma_a^2}\right)
\]

where \(2\theta\) is the diffraction angle and \(I_1\) is the maximum of the diffraction peak. The full width at half maximum (FWHM) of this diffraction peak is \(\beta = 2\sqrt{2 \ln 2} \sigma_a \approx 2.355\sigma_a\). With the distance \(d_2\) of the secondary slit from the sample centre, the diffraction occurs along a line within the sample, where the

![Figure 1. Geometry used for calculation of the analytical expression of the peak shift for cylinder sample.](image)
length of this line \( l = d_2 \tan \beta \) (cf. figure 1) corresponds to the FWHM, assuming that \( \beta \) is small. A diffraction power can be defined along this line as

\[
P(x) = P_0 \exp \left( -\frac{(x-x_1)^2}{2\sigma_x^2} \right)
\]

(3)

where \( x_1 \) is the centre point and \( \sigma_x \) is the standard deviation with \( \sigma_x = d_2 \sigma_s \). This diffraction power has to be multiplied by the available intensity to give the diffracted intensity \( I(x) \cdot P(x) \). By multiplying equations 1 and 3 and recollecting terms the peak shift due to absorption can be calculated as

\[
\delta = -\frac{\mu \beta^2 d_2}{2.355} = -0.1803 \mu \beta^2 d_2
\]

(4)

(details will be published elsewhere). The peak shift as a function of peak width for different attenuation coefficients \( \mu \) as calculated with equation 4 were compared with peaks shifts obtained from the numerical simulation for the geometry shown in figure 1 and a peak width of 0.91° (figure 2). The analytical results agree well with the results of the numerical simulation.

3. Numerical simulation

A numerical simulation was used for the calculation of the peak shift for other positions of the sample relative to the gauge volume, where it is more difficult to obtain an analytic expression. The simulation was done in two dimensions, because in a first approximation only the geometry in the scattering plane is relevant. Cylinder and plate samples (reflection and transmission geometry) were taken into account so far (actually, a circle or rectangles in two dimensions). Neutrons in the primary beam with a mean wavelength of 1.64 Å were selected, the wavelength that was mainly used for the measurements at the strain scanner ARES-2 of the HZG neutron facility [4]. The monochromator with elastically bent perfect Si single crystals [5] was included in the simulation.

Behind the primary slit with width \( w_1 \) at a distance \( d_1 \) from the centre the beam enters the sample and the point of diffraction in the sample along the path of the beam is chosen by a random number. Diffraction is calculated by reflection of the neutron path at the diffracting lattice planes in a powder sample. The mean lattice parameter can be chosen such that the diffraction angle is close to 90°, which is normally used for strain measurements to obtain a near-rectangular gauge volume. A Gaussian distribution of lattice parameters was used with a given width, which can be adapted to the peak broadening observed in a measurement. This distribution of lattice parameters, together with the wavelength spread, gives a broadened peak. After the reflection at the lattice planes, it is tested if the
diffracted ray passes the secondary slit of width $w_2$ at distance $d_2$ from the centre. Those rays passing the slit are finally recorded on a virtual detector placed at a distance of 1 m from the sample.

The location of the sample can be changed with respect to the position of the gauge volume. In this way, scans of radial and tangential strains along a line through the sample can be simulated.

When the attenuation is set to zero, a gauge volume is obtained that is expected when attenuation plays only a minor role (figure 3a). However, when there is strong attenuation and the diffraction peaks are significantly broadened, the gauge volume is shifted towards the primary slit, leading to a peak shift (figure 3b). Moreover, there is also some weighting of the gauge volume towards the secondary slit. The location of the gauge volume shown in figure 3 is 7 mm from the centre of the cylinder as indicated in the insets. A large peak width of 1.5° and a large distance $w_2$ of 100 mm were used for this exemplary calculation to get a strong visible effect. The scattering angle was 101° as for the powder measurement.

First, the simulation was tested by calculating the peak shift for the simple geometry that was used for deriving the analytical expression and a peak width of 0.91°, which was observed in the powder measurement. The simulation results match exactly with the analytical expression (figure 2). The second test involved the stress-free powder sample introduced in the following section.

4. Stress-free powder sample

A powder sample was used to evaluate the predictions of the numerical simulation. No peak shifts are expected in a scan of the powder sample because no residual strain gradients are present in the sample. The measurements were done at the strain scanner ARES-2 at the HZG neutron facility [4]. The powder container had a diameter of 20 mm and thin Al walls. Ni powder was used because it has a relatively large attenuation coefficient. The attenuation coefficient $\mu = 0.55$ cm$^{-1}$ for the powder sample was determined by a transmission measurement. The (311) reflection was used at $2\theta = 101^\circ$ ($\lambda = 1.64$ Å). The radius of curvature of the monochromator crystal was optimized for $2\theta = 90^\circ$; thus, at $101^\circ$ the peak was slightly broadened to a width of 0.91°. Large attenuation and large peak width was desired in this case to obtain a large attenuation-induced peak shift. The slit width was 2 mm; the slit heights were 10 mm (slit 1) and 30 mm (slit 2). Both slit distances were 50 mm.

The peak shifts along sample diameters on scan lines for measuring radial and tangential strain directions calculated with the simulation were 0.12° and –0.07°, respectively (figure 4). This is the difference between the values at $+10$ mm and $-10$ mm. Since the peak positions can have a constant offset that depends on geometrical details, only the slopes of the curves shown in figure 4 were evaluated and compared with the measurements so far. In other words, the simulation results were shifted on the angular scale such that they fit to the measurements. With this restriction, calculated and measured peak shifts fit well within the statistics. Two things can be concluded from these measurements: i. there is a significant attenuation-induced peak shift with significant values for an
attenuation of 0.55 cm\(^{-1}\) and a peak width of 0.91°; ii. the developed numerical simulation is adequate for describing this attenuation-induced peak shift.

It should be noted that it is expected that significant values of the attenuation-induced peak shift are only observed when simple slits are used for strain scanning. With a radial collimator instead of the secondary slit, an increase of the gauge volume is avoided and, thus, an increase of the peak shift to significant values is expected to be suppressed. This was shown, e.g., by Pirling et al. [6]. A quantitative consideration of radial collimators will be subject of further work and published elsewhere.

5. Summary
The shift of a measured Bragg peak in a strain scanning experiment due to beam attenuation was analyzed. This shift can usually be neglected in residual stress analysis, but it becomes significant when there is strong peak broadening in the sample and simple slits are used for the measurement. A numerical simulation for the calculation of the peak shift was developed. A comparison with the results of an analytical expression for a simple geometry confirmed the correctness of the simulation. Moreover, the scanning results of a stress-free powder sample matched exactly the predictions of the numerical simulation. Thus, the numerical simulation can be used for correcting strain data that is influenced by attenuation-induced peak shifts.

References
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