Neutron Interferometry: Antiphasing Effects Caused by Geometrical Aberrations

By U. Kischko*

Institut Laue-Langevin, Grenoble, France, and Institut für Physik, University of Dortmund, Federal Republic of Germany

And U. Bonse

Institut für Physik, University of Dortmund, Federal Republic of Germany

(Received 17 October 1984; accepted 8 May 1985)

Abstract

Intensity profiles of exit beams of a triple-Laue-case neutron interferometer have been measured photographically and compared with profiles calculated from the dynamical theory of perfect-crystal neutron diffraction. In order to avoid smear by an extended source a narrow incident beam only 0.2 mm wide was used. The spreading in the Borrmann triangles of the component crystals S, M, A of the interferometer was taken into account by a spherical wave calculation. The particular aim was to trace the influence of geometrical aberrations of the wafer thicknesses and deviations from so-called ideal geometries on the profile shapes and the phase homogeneity of the interferometer. It could be shown that previously observed 'plait'- or 'chessboard'-like patterns occurring in exit beams of neutron interferometers can be fully explained by the action of spherical wave interference disturbed by imperfections of the geometry. The agreement found between theory and experiment is very good. From the results, experimentally confirmed geometrical tolerances for the manufacture of neutron interferometers can be deduced.

1. Introduction

Part of a programme at the High Flux Reactor at the Institut Laue-Langevin (ILL) in Grenoble is to improve the performance (contrast and stability) of neutron interferometers. We go back to the causes of contrast deterioration by measuring profiles with narrow incident beams that do not suffer from horizontal smear from integration over the source. Previous profiles obtained in such a way show somewhat striking features: a 'chessboard' pattern (Bauspiess, Bonse & Rauch, 1976) and a 'plait' pattern in O and H beams. From the phase shift introduced by a wedge one expects a pattern of horizontal fringes in complete contrast to what is seen in Fig. 1 (Kischko, 1983). Initially the suspicion was that patterns of this type had to be attributed to some new hitherto unknown diffraction mechanism. The implication of the pattern of Fig. 1 with respect to interferometry is that within any horizontal line of the profile there are regions of apparently opposite phase. It is clear that when a detector measures the integrated intensity or when a wide incident beam is used instead of a narrow one, owing to the antiphasing effect described above, the contrast will fade. This is remarkable because common ideas of how contrast is lost in ångström-wave interferometers (X-ray, neutron) imply that 'somehow' geometrical errors and/or strain present in the crystal lattice are the cause of low fringe contrast.

Fig. 1. Intensity profiles behind four/five steps of a neutron interferometer with varying thickness of wafers. The pictures were taken using the beam geometry shown in Fig. 4 and with an Al wedge of linearly increasing thickness from bottom to top in the twofold reflected beam. Beam width determined by a slit 0.2 mm wide, Agfa D7 film, λ = 1.857 Å, exposure time: 75 h 30 min. The two photos were taken simultaneously.

*Present address: IBM Deutschland GmbH, MS T/W-Systeme, Sindelfingen, Federal Republic of Germany.
In this paper we clearly demonstrate the main reason for losing contrast to be deviations by \( >0.005 \text{ mm} \) of the wafer thicknesses \( t_s, t_M, t_A \) from ideal geometries of either \( t_M = t_s = t_A \) (Fig. 2) or \( t_M = 2t_s = 2t_A \) (Fig. 3), which yield a focal point at the exit surface. Similarly, Indenbom, Slobodetskii & Truni (1974) investigated theoretically the focusing of an X-ray beam by two successive Laue reflections from two crystal plates of the same thickness. We have investigated thoroughly both theoretically and by experiments the profile shapes in the \( O \) and \( H \) beams of the triple-Laue-case (LLL) neutron interferometer. To this end a so-called step interferometer was manufactured featuring varying wafer thicknesses at different heights as shown in Fig. 4 in order to make possible the simultaneous measurement of profiles with different geometries. A photograph of the step interferometer is shown in Fig. 5.

The actual dimensions of wafers and distances between the wafers achieved after the manufacturing process were directly determined using a locally measuring Abbé comparator. Profiles were calculated on the basis of the spherical wave theory (Bauspiess, Bonse & Graeff, 1976; Petrascheck, 1979). Special consideration was given to the properties of the

---

Fig. 2. Ray-tracing profiles of the triple-Laue-case (LLL) neutron interferometer with narrow incident beam. \( S \) beam splitter, \( M \) mirror, \( A \) analyser crystal. \( t_s = t_m = t_A \). The profile of the \( O \) exit beam as calculated from cylindrical wave theory is shown at the top of the figure (the \( H \) exit beam is not shown). Note the fairly large smear of intensity over the inner third of the beam cross section. The numbers below the profiles denote the \( q_n \) coordinate as defined by equation (11). \( t_s, t_m \) and \( t_A \) are the thicknesses of crystals \( S \), \( M \) and \( A \), respectively.

Fig. 3. As Fig. 2, but with intensity focusing in the exit beam because \( 2t_s = t_m = 2t_A \).

Fig. 4. Schematic view of the neutron step interferometer. In steps 2, 4 and 5, \( t_s = t_m = t_A \), whereas in steps 1 and 3, \( 2t_s = t_m = 2t_A \).

Fig. 5. Photo of the neutron step interferometer.
source, which in the experiments includes the ILL High Flux Reactor combined with a neutron guide and the monochromator crystal in front of the interferometer (Bauspiess, 1979). It is found that chessboard and plait patterns can be completely understood as resulting from deviations from ideal geometry in the interferometer.

2. Theory

A wave-optical treatment of the zero absorption LLL interferometer based on the spherical wave theory as suggested by Kato (1961) has been worked out by Bauspiess, Bonse & Graeff (1976) and, including arbitrary absorption, by Petrascheck & Folk (1976). The diffracted wave behind the interferometer is obtained by Fourier expansion of the incident spherical wave, multiplying each plane-wave component by the corresponding plane-wave transmission coefficient of the interferometer and superimposing the modified components behind the interferometer. In the absorption-free case, both wavefields that are created inside the crystal by dynamical diffraction have to be taken into account: type 1 with antinodes on the atomic sites and type 2 with nodes on the atomic sites and hence anomalous low absorption. At any entrance surface the Laue-case boundary conditions require again both wavefield types to be excited. So it is necessary to superimpose rays that have changed their propagation mode while travelling through the interferometer (Figs. 2 and 3). The whole Borrmann-fan wave is excited by a spherical wave and inter- and intrabranch interference occurs and is manifested in the spatial intensity distribution (Authier, Milne & Sauvage, 1968). As a result the spatial intensity distribution depends on the thickness of each wafer and the overall relative defocusing $\Delta z/T$ (Fig. 6) with the defocus

$$\Delta z \equiv (z_A^1 + z_B^1 - z_A^2 - z_B^2)/2$$

and the combined thickness

$$T \equiv t_S + t_M + t_A.$$ (2)

In parabolic treatment the curvature of the incoming wave front is not neglected, so that the source-to-film distances in $O$ and $H$ beams, $w_o$ and $w_h$, are parameters in the calculation. For comparison with experiment we give a brief summary of the results. We define $K = (K_x, K_y, K_w)$ with respect to the coordinate system $u, v, w$ of Fig. 6 with $u$ normal to the plane of drawing. Let the incident spherical wave be given by its Fourier expansion

$$\exp(2\pi ikr)/r = (1/r^3)e^{(2\pi iK't)/(K^2 - k^2)}.$$ (3)

Then the intensity distribution due to that wave behind the complete interferometer is calculated. With $\Delta_0$ the extinction distance and $k = 1/\lambda$, where $\lambda$ is the wavelength in vacuum, the following abbreviations are introduced (Bauspiess, Bonse & Graeff, 1976).

$$A \equiv \pi T/\Delta_0$$

$$B \equiv \pi/4k\Delta_0^2 \sin^2 \theta_B$$

$$G(t) \equiv \cos[(\pi t/\Delta_0)(y^2 + 1)^{1/2}]$$

$$S(t) \equiv \sin[(\pi t/\Delta_0)(y^2 + 1)^{1/2}](y^2 + 1)^{-1/2}$$

$$y \equiv -[A\theta \sin 2\theta_v] \frac{\hbar k^2}{2m_0|V_h|}.$$ (8)

where $m_0$ is the mass of the neutron and $V_h$ the Fourier component of order $h$ of the crystal scattering potential, $y$ is proportional to the deviation $\Delta \theta = \theta - \theta_B$ from the exact Bragg angle $\theta_B$ (Zachariasen, 1967). Furthermore, in order to describe the spatial modulations of the interfering beams in a convenient way we introduce a coordinate $q$, which varies over the cross section of the beam as indicated in Fig. 6.

$$O \text{ beam: } q = (2z_A^1 + T - \Delta z) \sin \theta_B - v$$

$$= (2z_B^1 + T + \Delta z) \sin \theta_B - v;$$ (9)

$$H \text{ beam: } q = (w - v \cot 2\theta_B) \sin 2\theta_B$$

$$- (2z_f + 2z_B^1 + T + \Delta z) \sin \theta_B$$

$$= (w - v \cot 2\theta_B) \sin 2\theta_B$$

$$- (2z_f + 2z_B^1 + T - \Delta z) \sin \theta_B.$$ (10)
Introducing the appropriate thickness $t_S$, $t_M$, $t_A$ into (6) and (7) we next define:

\[ U^I_{0}(q_n) = \int_0^\infty dy \exp(-iBw_0 y^2) \times \{ C(t_S) \cos[A(q_n + \Delta z/T)y] \\
+ yS(t_S) \sin[A(q_n + \Delta z/T)y] \} S(t_M)S(t_A) \]

(12)

\[ U^I_{h}(q_n) = \int_0^\infty dy \exp(-iBw_0 y^2) \times \{ C(t_A) \cos[A(q_n - \Delta z/T)y] \\
+ yS(t_A) \sin[A(q_n - \Delta z/T)y] \} \]

(13)

Using (12) to (15) we finally obtain the required amplitudes $\varphi^I_{0,n}$, $\varphi^I_{h,n}$ over paths I and II for the $O$ and $H$ beams:

\[ \varphi^I_{o,h} = D^I_{o,h}(k\omega)^{1/2} \Delta_0 \sin \theta_B \]

(16)

where the $+$ sign is for the $H$ beam and the $-$ sign for the $O$ beam.

Furthermore, a remark concerning the waveform and the distance $z_f$ of the source to the interferometer (Fig. 6) should be made. The assumption that the incoming wave is spherical is justified for the following reason: By using a fine slit (0.2 mm) the angular width of the incoming neutron wave is of the same order as or larger than the angular width of acceptance of the crystal according to dynamical theory ($\Delta \theta = 3\degree$); a plane wave would have zero divergence. The effective distance of the source to the interferometer is determined also by the geometry used with the monochromator. We employed an asymmetric diffraction of Si 220. The angle between the diffracting plane and the crystal surface was $\alpha = 13\degree 26\arcmin$. Because of the asymmetry the effective distance between the neutron point source and the crystal surface is reduced by a factor of $b = 2.49$. For the same reason the beam from the monochromator becomes more spherical (factor $b^{1/2}$).

If we suppose the real distance of the source to the monochromator to be the length of the neutron guide (55 m) then the virtual source is only 22.1 m away. The calculations were done with this value. The emittance of a neutron by a nucleus is a localized event. Different atoms emit neutrons incoherently. Thus, the diffraction pattern is first calculated for a point source and then spatially smeared over the coordinates of all sources, e.g. over the width of the entrance slit of 0.2 mm. In principle, the diffraction by a slit should also be accounted for. To describe the diffraction effect of a slit it is usual to imagine that every point of the slit sends out a spherical wave and that separate waves are coherent. The amplitude of reflection in any direction will be determined by the product of the Fresnel integral taken between the proper limits and the transmittance factor of the interferometer for the corresponding direction. For our experiments practically no influence from diffraction by the entrance slit is noted. Calculation has shown that it will be of importance when the entrance slit is made narrower than about 0.1 mm.

3. Experiment

The spatial intensity profiles in the $O$ and $H$ beams were determined by the direct technique with a $^{157}$Gd conversion metal foil (11.6 µm) in the back-screen...
configuration (Fig. 7). The low-energy internal conversion electrons emitted from the Gd in capturing neutrons expose the emulsion of the X-ray film (Agfa D7 double-emulsion) facing the Gd. A spatial resolution of 0.03 mm is obtained with thermal neutrons. Simultaneously with the intensity profile of the interferometer a 'stair' of silver foil with seven steps of 0.03 mm is obtained with thermal neutrons. Neutrons expose the emulsion of the X-ray film (Agfa D7 double-emulsion) facing the Gd. A spatial resolution of 0.03 mm is obtained with thermal neutrons. The optical densities on the film could thus directly be related to absolute neutron intensity. During exposure of up to 70 h the interferometer was kept automatically between 85 and 90% of the LLL rocking curve (y = 0).

The development of the film was carried out in thermostatically controlled tanks with the film hung vertically. The recommendations of the manufacturer with respect to developer and developing temperature were followed. During development the films were gently moved up and down. After development, the films were rinsed in water for about 2 min, fixed in an acid fixing bath for 5 min, rinsed again in water for an hour and dried in air at room temperature. The reproducibility of chemical development thus obtained was determined as better than 5% for Agfa D7. With the aid of a microdensitometer (Mark 3CS Joyce & Loeb) the measured optical densities of the film could be directly transformed to absolute neutron intensities. Thus, a quantitative comparison between theory and experiment was achieved.

Distances and thicknesses of the wafers of the interferometer were measured with an Abbé comparator (Leitz; reproducibility: ± 0.0015 mm). Table 1 contains the complete set of geometrical data. For each step n = 1, 2, 3, 4, 5 there are two values; nL means the lower half of a step number n, nu the upper half. Δz is the defocus caused by geometrical aberrations of the distances of the wafers according to (1) as explained in Fig. 6.

### 4. Results

The intensity profiles in the O and H beams were calculated for eight different geometries of the LLL interferometer. The eight cases represent a considerable variety of geometrical conditions (t/ΔD = 38.50 to t/ΔD = 105.01). In a three-dimensional plot the intensity distribution in outgoing beams is shown as a function of the normalized coordinate a and the phase difference φ between the two interfering beams. The influence of a slit (0.2 mm) is included. In Figs. 8 to 11 examples of calculated and measured profiles will be compared. The measured profiles were obtained with a phase-shifting wedge in one of the interfering beams. The calculated O beam of the ideal geometry (Δz = 0) (Fig. 8) shows an asymmetric structure with a broad maximum and sharp peaks all vanishing simultaneously for φ = π as it should be. Most of the relative maxima are well separated, so one has the chance to detect them. The parameters chosen for the calculation are close to those of the real geometry of step 2 of the interferometer.

The experimental O beams in step 4u (Fig. 9) and step 4l (Fig. 11) have hardly anything in common with ideal geometry. In both cases two separated maxima are 'at gap' with varying φ. In agreement with these observations the theoretical profiles of steps 4u (Fig. 10) and 4l (Fig. 12) show maxima shifting across the beam with φ varying. There is no φ value for which the intensity falls to zero all across the beam. The different appearance of the theoretical profiles of steps 4u and 4l is caused by the different geometrical aberrations actually present within step 4, which is again confirmed by the different structures of the photographed profiles in Figs. 9 and 11.

---

Table 1. Geometrical data for the neutron step interferometer (Si 220) (data in mm)

<table>
<thead>
<tr>
<th>Geometry</th>
<th>Step</th>
<th>tL</th>
<th>tM</th>
<th>tU</th>
<th>T/ΔD</th>
<th>Δz</th>
</tr>
</thead>
<tbody>
<tr>
<td>t-2t-t</td>
<td>1L</td>
<td>1.937</td>
<td>3.862</td>
<td>1.935</td>
<td>104.88</td>
<td>0.002</td>
</tr>
<tr>
<td></td>
<td>1u</td>
<td>1.937</td>
<td>3.864</td>
<td>1.943</td>
<td>105.01</td>
<td>-0.016</td>
</tr>
<tr>
<td>t-t-t</td>
<td>2L</td>
<td>1.937</td>
<td>1.945</td>
<td>1.948</td>
<td>79.06</td>
<td>-0.006</td>
</tr>
<tr>
<td></td>
<td>2u</td>
<td>1.934</td>
<td>1.956</td>
<td>1.939</td>
<td>79.05</td>
<td>-0.018</td>
</tr>
<tr>
<td>t-2t-t</td>
<td>3L</td>
<td>0.962</td>
<td>1.955</td>
<td>0.981</td>
<td>52.86</td>
<td>-0.023</td>
</tr>
<tr>
<td></td>
<td>3u</td>
<td>0.967</td>
<td>1.943</td>
<td>0.980</td>
<td>52.75</td>
<td>-0.012</td>
</tr>
<tr>
<td>t-t-t</td>
<td>4L</td>
<td>0.961</td>
<td>0.929</td>
<td>0.981</td>
<td>38.93</td>
<td>-0.020</td>
</tr>
<tr>
<td></td>
<td>4u</td>
<td>0.951</td>
<td>0.924</td>
<td>0.964</td>
<td>38.50</td>
<td>-0.032</td>
</tr>
<tr>
<td>t-t-t</td>
<td>5L</td>
<td>0.315</td>
<td>0.303</td>
<td>0.334</td>
<td>12.91</td>
<td>-0.030</td>
</tr>
<tr>
<td></td>
<td>5u</td>
<td>0.305</td>
<td>0.284</td>
<td>0.315</td>
<td>12.26</td>
<td>-0.025</td>
</tr>
</tbody>
</table>

Definition: Δz = (zL + zU - zM - zO)/2; - before Δz means in the analyser.

---

Fig. 8. Calculated spatial intensity profile of the O exit beam for assumed ideal geometry (Δz = 0); tL = tM = tU = 1.940 mm, as a function of an overall phase difference φ between interfering beams I and II. zL = zU = 27 200 mm. T/ΔD = 78.9.
The $O$ beam of step 4 was particularly suitable as a test for quantitative comparison of calculated and measured profiles. Source distance $w_0$ and slit width $b$ were varied in the calculation. For $w_0 = 20$ m and $b = 0.3$ mm it was not possible to discern a clear separation of two maxima in the theoretical profile; for $w_0 = 50$ m and $b = 0.3$ mm or 50 m and 0.2 mm, respectively, the calculated profiles were not or only incompletely in agreement with those in the photographs of Figs. 9 and 11. So the values taken for the source distance (22.1 m) and the slit width 0.2 mm were justified.

It is found that $H$ beams are generally characterized by sharp peaks at the limits of the 'inner' Borrmann triangle, i.e. at $q_n = \pm 1/3$ for $t_S = t_M = t_A$ geometry and at $q_n = \pm 1/2$ for $2t_S = t_M = 2t_A$ geometry. As an example we show the $H$ beam of step 2u (Fig. 13). Furthermore, an interesting feature is the weak maximum in the middle. With increasing $\varphi$ this splits like a plait. The theoretical profile Fig. 14 explains just this behaviour: for $\varphi = 0$ there is a relative maximum at $q_n = 0$; on the other hand, at $\varphi = \pi$ the previous relative maximum splits into at least two. In the photograph of Fig. 13 there is clearly discernible a vertical ribbon structure, in accordance with the theoretical profile.

An example with $2t_S = t_M = 2t_A$ geometry gives Fig. 15, where the $O$ beam of step 3u is shown. In addition to the strong periodic intensity modulation in the focus range the previously mentioned chessboard pattern is visible in the photograph. The calculated profile (Fig. 16) behaves correspondingly: just when a subsidiary maximum occurs in the area $0.5 < q_n < 1$, another disappears in the $-0.5 < q_n < 0$ area. The intensities are almost 'on gap', as with a chessboard.
For this and all other steps the absolute intensities in $O$ and $H$ beams are in good agreement with theory (Figs. 17 and 18).

5. Conclusion

It has been found that spherical wave theory, as developed by Bauspiess, Bonse & Graeff (1976) for the absorption-free neutron interferometer, gives a good quantitative and qualitative description of the experimental intensity profile. In particular, the theoretically predicted focusing was confirmed for the $2t_S = t_M = 2t_A$ geometry. For the $H$ beam the intensity profile is symmetrical and limited to the central region $|q_n| < 0.6$ of the outgoing beam. The $O$ beam is asymmetrical with intensities gradually diminishing towards the edge. Geometrical differences within individual stages lead to definite changes in the intensity profiles. The plait pattern, which was something of a riddle in the past, has been explained by the effect of geometrical defocusing on the phase shift.

![Fig. 13. Photograph of $H$-beam profile of step 2u. Note the weak relative maximum in the centre and its plait-like behaviour with varying $\phi$. $\Delta q_n = 1/3$ corresponds to 1 mm in the picture.](image1)

![Fig. 14. Calculated $H$-beam profile with the actual geometry of step 2u: $\Delta z = -0.018$ mm, $t_S = 1.934$ mm, $t_M = 1.956$ mm, $t_A = 1.939$ mm, $z_2 = 27.021$ mm, $z_4 = 27.029$ mm, $T/d_0 = 79.1$. Note the correspondence with the measured profile of Fig. 13.](image2)

![Fig. 15. Photograph of $O$-beam profile of step 3u: $2t_S = t_M = 2t_A$ geometry. Note the focusing near $q_s = 0$. At larger $|q_n|$ a faint chessboard pattern is seen. $\Delta q_n = 1$ corresponds to 1.95 mm in the picture.](image3)

![Fig. 16. Calculated $O$-beam profile with the actual geometry of step 3u: $\Delta z = -0.012$ mm, $t_S = 0.967$ mm, $t_M = 1.943$ mm, $t_A = 0.980$ mm, $z_2 = 27.033$ mm, $z_4 = 27.041$ mm, $T/d_0 = 52.75$. Note the correspondence with the measured profile of Fig. 15, see text.](image4)
We are pleased to thank D. Richard and G. Greenwood for their help in the computation and G. Schmid for his technical assistance. A grant by the Bundesministerium für Forschung und Technologie, Bonn, Az. 03-B56Ao1 P is gratefully acknowledged.

References


