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Some Remarks on the Laue–Laue Interferometer

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Abstract

The two-crystal Laue arrangement has been utilized as a tool for diffraction focusing, as a spectrometer with rocking curves showing an extremely narrow central peak and as a LL interferometer. For these applications different approaches have been used independently, which are brought together in a description using spherical waves, plane waves and ray optics. It is shown that the frequently used ray optics fails in the focal region of the interferometer. The theory may be applied to neutron or (absorbing) X-ray interferometry.

Introduction

Two-crystal reflections have been considered by Indenbom, Slobodetskii & Truni (1974) and Indenbom, Suvorov & Slobodetskii (1976), who were particularly interested in the diffraction focusing in the center of the Borrmann fan of the second crystal plate. Somewhat later it was shown by Bonse, Graeff, Teworte & Rauch (1977) that the rocking curves of a two-crystal spectrometer should have an extremely narrow central peak, which has been observed for neutrons (Bonse, Graeff & Rauch, 1979) and for X-rays (Bonse & Teworte, 1980). A theoretical description was given by Petrascheck & Rauch (1984). Zeilinger, Shull, Horne & Squires (1979) presented the Laue–Laue (LL) interferometer as a ray optical device. According to the dynamical theory of diffraction an incident plane wave excites two wave fields which propagate in the first crystal slab along different directions of the (neutron) currents and meet at the focal point on the rear surface of the second plate. It is now our aim to investigate the conditions justifying ray optical considerations and to relate the phenomena of diffraction focusing to LL interferometry as well as to the extremely narrow peak in LL rocking curves.

Plane waves

Focusing and interference properties of a (monolithic) LL interferometer require equal thickness D for the two crystal plates within an accuracy of a small fraction of the *Pendellösung* length Δ_0. The LL interferometer, like other neutron (or X-ray) optical devices, is described on the basis of the dynamical theory of diffraction of plane waves. Avoiding too lengthy expressions, only symmetrical Laue reflections are considered.

For an incident plane wave

$$\psi_i = \exp[i\mathbf{k}(y)\mathbf{x}], \tag{1}$$

where the *Selektionsfehler* y (for the notation used here, see Rauch & Petrascheck, 1978) describes the deviation of the incident wave vector $\mathbf{k}(y)$,

$$\mathbf{k}(y) = \mathbf{k}_B + (\pi y/\Delta_0)[\hat{\mathbf{z}} + \hat{\mathbf{x}}/\tan\theta_B], \tag{2}$$

from $\mathbf{k}_B$, incident under the exact Bragg angle θ_B (see Fig. 1). A wedge between the two crystal plates deflects the beam by an angle v, expressed on the scale of y (Rauch, Kischko, Petrascheck & Bonse, 1983). The wave function of the double-diffracted beam, which is of most interest, is then given by

$$\begin{aligned}\psi_0 = &-\nu^2 \sin[A(\nu^2+y^2)^{1/2}]/(\nu^2+y^2)^{1/2}\\ &\times \sin\{A[\nu^2+(y+v)^2]^{1/2}\}/[\nu^2+(y+v)^2]^{1/2}\\ &\times \exp[-iAv - 2iA(y+v)(t+D)\\ &- ikV(0)D/2E\cos\theta_B]\exp[i\mathbf{k}(y+v)\mathbf{x}]\end{aligned} \tag{3}$$

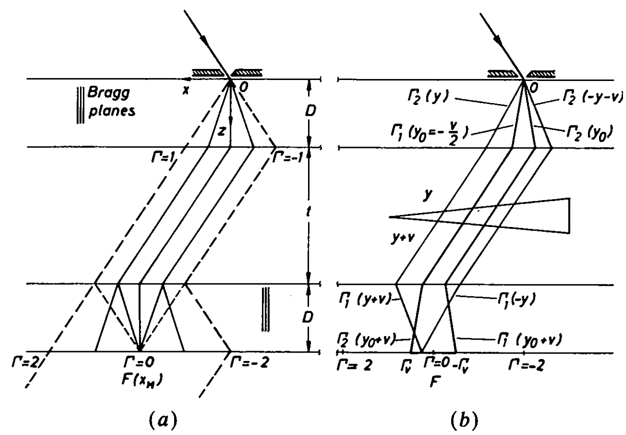

Fig. 1. Borrmann fan for a LL spectrometer. (a) An incident plane wave is split into two Bloch waves propagating in different directions in the first slab. If these rays change their direction according to the other wave field, they meet at the focus F and should interfere. (b) If the waves are deflected by v, the ray optical picture suggests a focal region $0 \le |\Gamma| \le \Gamma_v = v/(1+v^2/4)^{1/2}$ with enhanced intensity. However, for small v no plane waves of neighbouring y values meet at the back surface indicating that geometrical optics fail.

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with $A = \pi D/\Delta_0$ and

$$\nu^2 = V(\mathbf{G})V(-\mathbf{G})/|V(\mathbf{G})V(-\mathbf{G})| \simeq 1 - 2i\kappa.$$

$V(0)$ and $V(\mathbf{G})$ are the Fourier coefficients of the interaction potential and E is the energy of the incident neutron. The intensity derived from (3) can be separated into four contributions

$$I(y) = I_a(y) + I_p(y) + I_0(y) + I_t(y) \qquad (4)$$

using the addition formulas for the trigonometric functions. I_a is the average intensity, I_p gives rise to the central peak, I_0 and I_t are thickness dependent, but for I_0 the oscillatory structure dominates even the integrated intensity.

$$I_a = \exp(-\Sigma D_e)\cosh[2\kappa A/(1+y^2)^{1/2}] \times \cosh\{2\kappa A/[1+(y+v)^2]^{1/2}\} \times \{4(1+y^2)[1+(y+v)^2]\}^{-1} \qquad (5a)$$

$$I_p = \exp(-\Sigma D_e)\cos(2A\{[1+(y+v)^2]^{1/2} - (1+y^2)^{1/2}\})\{8(1+y^2)[1+(y+v)^2]\}^{-1} \qquad (5b)$$

$$I_0 = \exp(-\Sigma D_e)\cos(2A\{[1+(y+v)^2]^{1/2} + (1+y^2)^{1/2}\})\{8(1+y^2)[1+(y+v)^2]\}^{-1} \qquad (5c)$$

$$I_t = \exp(-\Sigma D_e)\cosh[2\kappa A/(1+y^2)^{1/2}] \times \cos\{2A[1+(y+v)^2]^{1/2}\} + \cosh\{2\kappa A/[1+(y+v)^2]^{1/2}\}\cos[2A(1+y^2)^{1/2}] \times \{4(1+y^2)[1+(y+v)^2]\}^{-1}. \qquad (5d)$$

Here Σ is the linear attenuation coefficient and $D_e = D/\cos\theta_B$ is the effective thickness. In neutron scattering $I_0 + I_t + I_p$ vanishes when averaged over the wavelength spread. In monolithic and nonabsorbing spectrometers I_p would produce a narrow peak for $y = -v/2$ if $Av < 1$. The usual diffraction pattern for a two-crystal spectrometer is obtained from I_a, which contains the anomalous weak attenuated intensity.

More relevant are the rocking curves

$$R(v) = \int_{-\infty}^{\infty} \mathrm{d}y\, I(y, v), \qquad (6)$$

which are obtained from (5) (see Petrascheck & Rauch, 1984). The average intensity

$$R_a = [\exp(-\Sigma D_e)/16(1+v^2/4)] \times \{1 + I_0[4\kappa A/(1+v^2/4)^{1/2}] + (1+v^2/4)I_2[4\kappa A/(1+v^2/4)^{1/2}]\} \qquad (7a)$$

is a crude interpolation between the results for $R_a(v = 0, \kappa)$ and $R_a(v, \kappa = 0)$. I_0 and I_2 are modified Bessel functions. For vanishing absorption one obtains from (7a) a Lorentzian.

$$R_p \simeq (\pi/8)\exp(-\Sigma D_e)J_1(2Av)/2Av \qquad (7b)$$

describes the central peak of the intrinsic rocking curves of a non-dispersive two-crystal spectrometer (see Fig. 2), where J_1 is a Bessel function of the first kind. Once more it should be mentioned that the shape of the peak with a half width $v_H = 2{\cdot}215/A$ ($\sim 10^{-3}$ s of arc) is not affected by the wavelength spread. Like R_p,

$$R_0 = (\pi/16A)\exp(-\Sigma D_e) \times \cos[4A(1+v^2/4)^{1/2} + \pi/4]/(1+v^2/4)^{5/4} \qquad (7c)$$

has no anomalous attenuation, but in addition it is smoothed by the wavelength spread. The thickness-dependent part

$$R_t \simeq (\pi/2A)\exp(-\Sigma D_e)\cosh[2\kappa A/(1+v^2/4)^{1/2}] \times \cos(2A + \pi/4)/(1+v^2), \qquad (7d)$$

which lowers or raises the broad average rocking curve, vanishes also with the wavelength spread. Thus, for neutrons only R_a and R_p have been observed (Bonse, Graeff & Rauch, 1979; Rauch *et al.*, 1983), whereas for X-rays even the oscillating terms could be observed (Bonse & Teworte, 1980).

LL Diffraction profiles

If a divergent beam is incident through a narrow slit it is generally sufficient to restrict the beam to a δ function whose argument vanishes along the Bragg direction of the subsequent crystal plate (see Fig. 1). Then the spatial intensity profile is obtained by the integration of the plane waves (3).

$$\varphi(\mathbf{x}) = (c_0/2)\exp(-\Sigma D_e/2) \times \int_{-\infty}^{\infty} \mathrm{d}y\, [\cos(A\{[\nu^2 + (y+v)^2]^{1/2} - (\nu^2 + y^2)^{1/2}\}) - \cos(A\{[\nu^2 + (y+v)^2]^{1/2} + (\nu^2 + y^2)^{1/2}\})] \times \exp(iA\Gamma y)/\{[\nu^2 + (y+v)^2]^{1/2}(\nu^2 + y^2)^{1/2}\} \qquad (8)$$

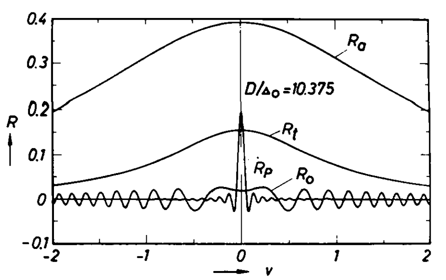

Fig. 2. The intrinsic rocking curves of a two-crystal spectrometer are composed of different contributions, where R_p is the central peak and R_a the average rocking curve. R_t and R_0 are thickness dependent and vanish with increasing thickness (after Petrascheck & Rausch, 1984).

at the back surface of the second crystal plate. c_0 is an unimportant constant, with $|c_0|^2=1$, and the geometrical factor $\Gamma=x/D\tan\theta_B$ describes the Borrmann fan for the two crystal slabs with $-2\le\Gamma\le 2$. As before, v describes the deflection of the beam by a wedge (see Fig. 1*b*). Removing the wedge from the spectrometer, *i.e.* $v=0$, one obtains diffraction focusing in the centre of the Borrmann fan (Indenbom, Slobodetskii & Truni, 1974; Indenbom & Slobodetskii, 1975; Indenbom, Suvorov & Slobodetskii, 1976; Aladzhadzhyan, Bezirganyan, Semerdzhyan & Vardanyan, 1977). Different methods have been used to approximate the integral (8) for $v=0$ and $D>\Delta_0$ and it should be mentioned that an exact solution of (8) is also available in the form of a convergent infinite series similar to a series for the LLL interferometer described by Petrascheck & Folk (1976).

But the most successful way to evaluate such oscillating integrals is given by the method of the stationary phase (Jeffreys & Jeffreys, 1966), which gives

$$\varphi(\mathbf{x})=\exp(-\Sigma D_e/2)(c_0\pi/2\nu)\times\{\exp(-A\nu|\Gamma|)-\theta(1-|\Gamma|/2)(\pi\nu A)^{-1}\times(1-\Gamma^2/4)^{1/4}\cos[2A\nu(1-\Gamma^2/4)^{1/2}+\pi/4]\}. \quad (9)$$

In the neutron case, where the *Pendellösung* oscillations are often smeared out, the average intensity is obtained as

$$\bar{I}_0(\Gamma)=(A\pi/8)\exp(-\Sigma D_e)\{\exp(-2A|\Gamma|)+(2\pi A)^{-1}\times(1-\Gamma^2/4)^{1/2}\cosh[4\kappa A(1-\Gamma^2/4)^{1/2}]\times\theta(1-|\Gamma|/2)\}, \quad (10)$$

shown in Fig. 3. It is in qualitative agreement with the intensity profile of the neutron LL interferometer of Zeilinger *et al.* (1979). The average reflectivity calculated from (10) is

$$\bar{R}(v=0)=(\pi/8)\exp(-\Sigma D_e)[1+I_1(4\kappa A)/4\kappa A], \quad (11)$$

where half of the first term can be related to the central peak R_p and the rest to R_a of (7).

For the rocking curves derived from (8), the absolute square of the first term yields R_p and (for zero absorption) half of R_a, whereas the absolute square of the second term contributes to R_0 and to the remaining parts of R_a. R_t describes the contribution of the interference between the central peak and the broad background of the intensity profile (see Figs. 2 and 3).

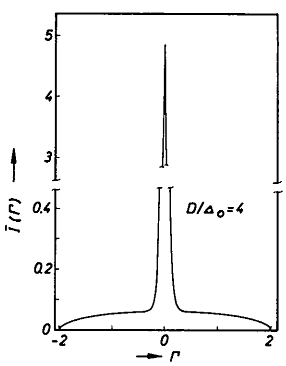

Fig. 3. The calculated (average) intensity profile showing the double-diffracted beam of the LL interferometer.

Ray optics

Interferometric experiments with the two-crystal spectrometer are usually performed with a narrow incident beam, as necessary for diffraction focusing. But, other than for diffraction focusing, the theoretical description of the interferometer was initially based on ray optical considerations (Zeilinger *et al.*, 1979).

According to the dynamical theory of diffraction a plane wave excites within the crystal two Bloch waves. Each Bloch wave is considered as a ray travelling along its direction of (neutron) current

$$\Gamma_{1,2}(y)=\mp y/(1+y^2)^{1/2}=x_{1,2}/D\tan\theta_B. \quad (12)$$

Fig. 1 shows that rays, belonging to the same wave field in both slabs, reach the back surface between $-2\le\Gamma\le 2$ and cause the broad intensity profile of Fig. 3. They contain the weak absorbed contributions to the intensity and are related to the second term of (8)-(10). Rays belonging to different wave fields in the two plates leave the spectrometer at the focus $\Gamma=0$ and are of main interest for the interference properties of the interferometer. In the simplest approximation the different incident plane wave components are assumed to be incoherent (Zeilinger *et al.*, 1979; Atwood, Horne, Shull & Arthur, 1984). Thus the total intensity of the central peak calculated for plane waves reflects the fact that the integrated intensities are equal for spherical as well as for plane waves.

If a wedge is brought into the interferometer one may argue that the two interfering rays have covered different optical path lengths, producing a phase shift $\pm Av\Gamma$. The resulting intensity

$$R=(\pi/16)[1+J_1(2Av)/Av] \quad (13)$$

is simply the integrated intensity obtained from the first term of (8). It should be kept in mind that a wedge only deflects both waves and their position-dependent phase shift $Av\Gamma$ is derived by expanding the phase factors of the plane waves to first order in

v. In a more rigorous treatment the deflection of the currents would separate the initially interfering rays, as shown in Fig. 1(b), indicating that something fails in our ray optical picture.

Thus it seems useful to reflect on the conditions necessary for ray optics by considering the diffraction by a single-crystal plate. We will assume that different wave components are coherent. Such a condition is inevitable for the construction of a localized wave packet at the entrance slit. Then one obtains for the diffracted intensity

$$I(\Gamma)=\sin^2[A(1-\Gamma^2)^{1/2}](1-\Gamma^2)^{1/2} \qquad (14)$$

(Petrascheck, 1975). The intensity oscillations are caused by the interference of rays with $\Gamma_1(-y)$ and $\Gamma_2(y)$ from different incident partial waves [see (12) and Fig. 1] and are, apart from a constant phase $\pi/4$, in agreement with the spherical theory for thick crystals. Since in thick crystals the wave functions of the spherical theory are obtained from the integration over rapidly varying functions, only a small portion of y contributes to the wave functions around the points of stationary phase, which are equal to the directions of the neutron currents (12). Thus the validity of ray optics presumes that for a given direction Γ only a small range of y contributes essentially and therefore the applicability of the method of stationary phase can be used for the justification of ray optics. For the LL spectrometer, the broad intensity distribution can be evaluated to a good approximation by geometrical optics but for the central part this is not possible and indicates the breakdown of the ray optical picture for the focal region. Thus the derivation of the reflectivity (13) (Atwood *et al.*, 1984) has to be explained from the plane-wave theory rather than from ray optics.

Discussion

We have considered the LL spectrometer under idealized conditions, which result from an incident monochromatic beam with the shape of a δ function.

In the crystal the beam spreads within the Borrmann fan, but after two equally thick crystal plates diffraction focusing occurs at the centre of the Borrmann fan. The calculated width of the central peak, $\Delta_0/\pi \tan\theta_B$, which is a few micrometres, is experimentally not easy to obtain (Suvorov & Polovinkina, 1974). The required fine slit leads to corrections due to the diffraction broadening at the entrance slit (Indenbom, Suvorov & Slobodetskii, 1976; Klein, Martin & Opat, 1977). In some cases a large source distance may lead to additional corrections (Bauspiess, Bonse & Graeff, 1976). At least the wavelength spread is, especially for neutrons, responsible for further broadening of the central resonance. But if we are interested in the convoluted rocking curves, then we are not forced to use an extremely narrow entrance slit and our idealized model is sufficient in a wide range of experimental conditions.

It has been shown that for geometrical optics one should be able to attach to a spatial range $\delta\Gamma$ (or δx) an angular range δy of the incident beam. This is fulfilled if the partial plane waves become extinguished except for a small range δy around the stationary phase for a fixed Γ. Moreover, the results of the spherical theory, approximated by the method of stationary phase, and the results of geometrical optics are equal if phase factors $\pm i\pi/4$ are added to each ray.

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