

# General Formulation of the (111, $\bar{1}\bar{1}1$ ) Neutron Three Beam Case \*

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A formalism developed in a previous paper [1] is now applied in a general way to the special three beam case (111,  $\bar{1}\bar{1}1$ ). The restriction for the incoming wave to be located in the symmetry plane is abolished. The individual behavior of the dispersion surfaces and reflection curves are determined and discussed.

## Introduction

As is well known, absorption of diffracted X-rays in perfect crystals is governed by the so called “Borrmann-effect”, which was discovered first in the two beam case in 1941. In 1965 Borrmann and Hartwig proved that it also occurs in the case of simultaneous diffraction on the lattice planes (111) and ( $\bar{1}\bar{1}1$ ), e.g. in a three beam case [2]. Shortly later the details of the theoretical background of this experiment have been presented [3]. It is the aim of this paper to apply dynamical theory of diffraction to thermal neutron scattering and to study the properties of neutron waves under (111,  $\bar{1}\bar{1}1$ ) three beam case conditions. The general calculations of this special three beam case contain the basic ideas which can be applied to other very interesting many beam cases. In the first paper [1] the wave vector of the incoming beam  $\mathbf{k}^i$  fulfilled exactly the Bragg-condition; now  $\mathbf{k}^i$  is considered to be arbitrary relative to the reflecting planes i.e. to the surface of the crystal slab.

## Basic Equations and Dispersion Surface

From the basic equation of the dynamical theory

$$\left[ \frac{\hbar^2}{2m} |\mathbf{K}_0 + \mathbf{G}|^2 - E \right] u(\mathbf{G}) = - \sum_{\mathbf{G}'} V(\mathbf{G} - \mathbf{G}') u(\mathbf{G}'), \quad (1)$$

we obtain the following homogeneous system of linear algebraic equations for this three beam case

$$\begin{aligned} [2\varepsilon_0 + V_0] u(\mathbf{0}) + V_{-G} u(\mathbf{G}) + V_{-H} u(\mathbf{H}) &= 0, \\ [2\varepsilon_G + V_0] u(\mathbf{G}) + V_G u(\mathbf{0}) &= 0, \\ [2\varepsilon_H + V_0] u(\mathbf{H}) + V_H u(\mathbf{0}) &= 0. \end{aligned} \quad (2)$$

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The general equation of the dispersion surface is now written as

$$\begin{aligned} \varepsilon_0^3 + \frac{1}{2} \varepsilon_0^2 [a_G b_G + a_H b_H + V_0] \\ + \frac{1}{4} \varepsilon_0 [a_G b_G a_H b_H + V_0 (a_G b_G + a_H b_H) \\ - V_G^2 (b_G + b_H)] \\ + \frac{1}{8} [a_G b_G a_H b_H V_0 - V_G^2 b_G b_H (a_G + a_H)], \end{aligned} \quad (3)$$

where

$$\begin{aligned} a_G &= \alpha_G + V_0, \quad a_H = \alpha_H + V_0, \\ \alpha_G &= \frac{1}{k^2} [G^2 + 2\mathbf{k} \cdot \mathbf{G}], \quad \alpha_H = \frac{1}{k^2} [H^2 + 2\mathbf{k} \cdot \mathbf{H}], \\ \frac{1}{b_G} &= \left( 1 + \frac{1}{k \cos \gamma_0} \mathbf{n} \cdot \mathbf{G} \right), \\ \frac{1}{b_H} &= \left( 1 + \frac{1}{k \cos \gamma_0} \mathbf{n} \cdot \mathbf{H} \right). \end{aligned} \quad (4)$$

In the symmetrical case one saw that from the dispersion branch II no waves originated into the 0-direction, because the corresponding Poynting vector was directed along  $\frac{1}{2}(\mathbf{G} + \mathbf{H})$ . Figures 1 and 2 show two sections through the dispersion surface for different deviations of  $\mathbf{k}^i$  from the symmetry plane. In Fig. 1 the angle  $\alpha$  of deviation is  $5.2''$  whilst in Fig. 2 it is  $7.8''$ . The sensibility of the so called “three beam region” around  $\Delta\theta = 0$  leads to quick changes of its shape, so that fractions of sec. of arc of deviation are sufficient to create waves from the second dispersion branch which contribute into the 0-direction. The coordinate system is built up in such a way that  $\mathbf{k}^i$  ( $\mathbf{k}^i = k(x, y, z)$ ) defines the zero position when the Bragg condition is exactly fulfilled. The vector  $[01\bar{1}]$  is perpendicular to the surface of the crystal slab. The crystal material is silicon, the used neutron wavelength  $\lambda$  is at all figures  $1.623 \times 10^{-8}$  cm;  $V_0 = 1.7192 \times 10^{-6}$ ,  $\gamma_0 = 18.48^\circ$ .



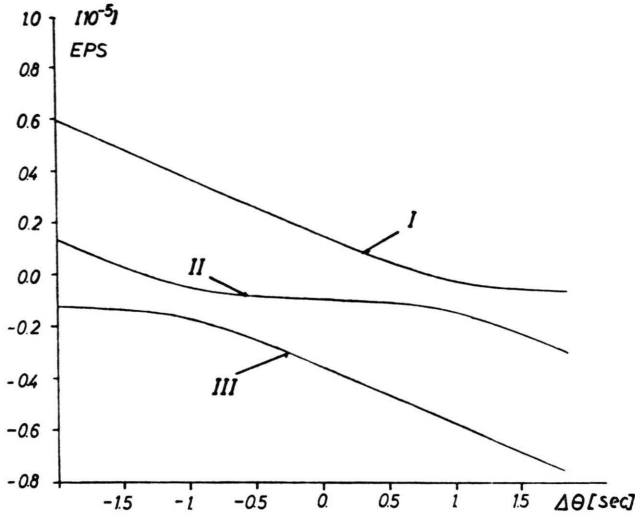


Fig. 1. Section through the dispersion surface,  $\alpha$  is 5.2 sec of arc. I, II and III denotes the particular branches.

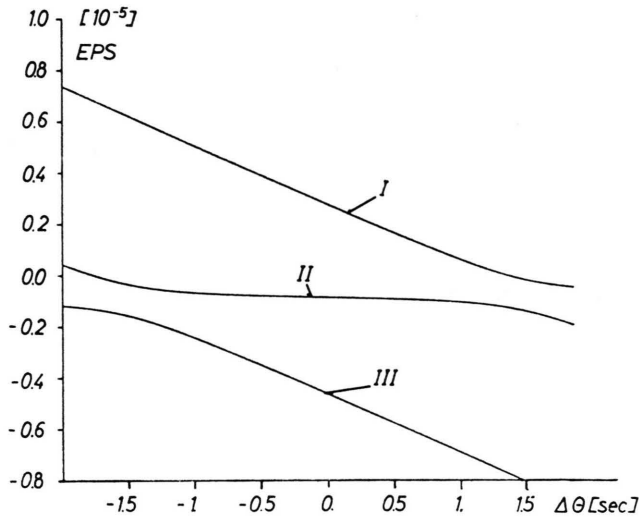


Fig. 2. Section through the dispersion surface,  $\alpha$  is 7.8 sec of arc.

### Intensities Behind a Perfect Crystal Slab and Reflection Curves

The general solution for the boundary conditions for the wave functions  $\Psi_0$ ,  $\Psi_G$  and  $\Psi_H$  yields the inhomogeneous system of equations

$$\begin{aligned} \sum_j u_j(0) &= u_0; \quad \sum_j X_j u_j(0); \\ \sum_j Y_j u_j(0) &= 0, \end{aligned} \quad (5)$$

for  $j = 1, 2, 3$  and  $\Psi_e = u_0 \exp(i \mathbf{k} \cdot \mathbf{r})$ .

$X_j$  and  $Y_j$  are the amplitude's ratios

$$\frac{u_j(\mathbf{G})}{u_j(0)} = - \frac{V_G}{2\varepsilon_{0,j}/b_G + a_G} = X_j \quad (6)$$

and

$$\frac{u_j(\mathbf{H})}{u_j(0)} = - \frac{V_H}{2\varepsilon_{0,j}/b_H + a_H} = Y_j.$$

The abbreviations are defined in [1].  $\varepsilon_{0,j}$  is the individual Anregungsfehler (excitation error) which is determined from the dispersion surface (Equation (3)). Solving (5) the determinant of this algebraic system is

$$\Delta = X_1(Y_2 - Y_3) + X_2(Y_3 - Y_1) + X_3(Y_1 - Y_2), \quad (7)$$

and the amplitudes  $u_j(0)$  from the  $j$ -th dispersion branch are

$$u_j(0) = \frac{\varepsilon_{jkl} X_k Y_l}{\Delta} u_0 \quad (j = 1, 2, 3). \quad (8)$$

( $\varepsilon_{jkl}$  is the known  $\varepsilon$ -tensor; e.g.

$$u_1(0) = (X_2 Y_3 - X_3 Y_2) u_0 / \Delta, \text{ etc.})$$

These amplitudes can be calculated from (8) because the  $X_j$  and the  $Y_j$  are known from Equation (6). The wavefields originating from the dispersions branches, I, II, III, are independent solutions of the Schroedinger equation as

$$\Psi_j(\mathbf{r}) = \sum_{\mathbf{G}'} \exp \left\{ i \left( \frac{k \varepsilon_{0,j}}{\cos \gamma_0} \mathbf{n} + \mathbf{G}' + \mathbf{k} \right) \cdot \mathbf{r} \right\} \cdot u(\mathbf{G}'), \quad (j = 1, 2, 3; \mathbf{G}' = 0, \mathbf{G}, \mathbf{H}),$$

but one can combine the components of the wave functions  $\Psi_j$  in terms of the 0-,  $\mathbf{G}$ - and  $\mathbf{H}$ -directions. This can be done because all three wavefields propagate equivalently through the crystal due to the very small absorption of neutrons in crystals such as silicon or germanium.

The  $\Psi$ -functions classified in the 0-,  $\mathbf{G}$ - and  $\mathbf{H}$ -directions can then be written as follows

$$\begin{aligned} \Psi_0 &= \Psi_e \cdot \frac{1}{\Delta} \sum_j \varepsilon_{jkl} \exp \left\{ i \frac{k \varepsilon_{0,j} D}{\cos \gamma_0} \right\} X_k Y_l, \quad (9) \\ \Psi_G &= \Psi_e \frac{e^{i \mathbf{G} \cdot \mathbf{r}}}{\Delta} \sum_j \varepsilon_{jkl} \exp \left\{ i \frac{k \varepsilon_{0,j} D}{\cos \gamma_0} \right\} X_j X_k X_l, \\ \Psi_H &= \Psi_e \frac{e^{i \mathbf{H} \cdot \mathbf{r}}}{\Delta} \sum_j \varepsilon_{jkl} \exp \left\{ i \frac{k \varepsilon_{0,j} D}{\cos \gamma_0} \right\} Y_j X_k Y_l, \end{aligned}$$

so that  $\Psi^* \cdot \Psi$ , the intensities behind a slab of definite thickness  $D$ , are

$$\begin{aligned} I_0 &= \sum_{k,l} u_k(0) u_l^*(0) \cdot \cos \{A(\varepsilon_0, k - \varepsilon_0, l)\}, \\ I_G &= \sum_{k,l} X_k X_l u_k(0) u_l^*(0) \cdot \cos \{A(\varepsilon_0, k - \varepsilon_0, l)\}, \\ I_H &= \sum_{k,l} Y_k Y_l u_k(0) u_l^*(0) \cdot \cos \{A(\varepsilon_0, k - \varepsilon_0, l)\} \\ &\quad (l, k = 1, 2, 3). \end{aligned} \quad (10)$$

The Figs. 3 and 4 show a series of reflection curves for the 0,  $G$  and  $H$  beams for several thicknesses of a perfect crystal plate. Note that the oscillations

move together with increasing path lengths of the wave fields in the crystal. There are some peculiar events to be mentioned: the 0-beam intensity is always oscillating symmetrically around  $\Delta\theta = 0$ . This does not depend on the deviation of  $k^i$  from the symmetry plane or the crystal thickness, unlike the  $G$  and the  $H$  beams whose maxima and minima are situated asymmetrically around  $\Delta\theta = 0$ . This means that for a definite angular deviation of  $\alpha$  out of the symmetry plane and a certain deviation  $\Delta\theta$  from the exact Bragg angle e.g., one of the reflected beams receives more intensity than the 0- and the

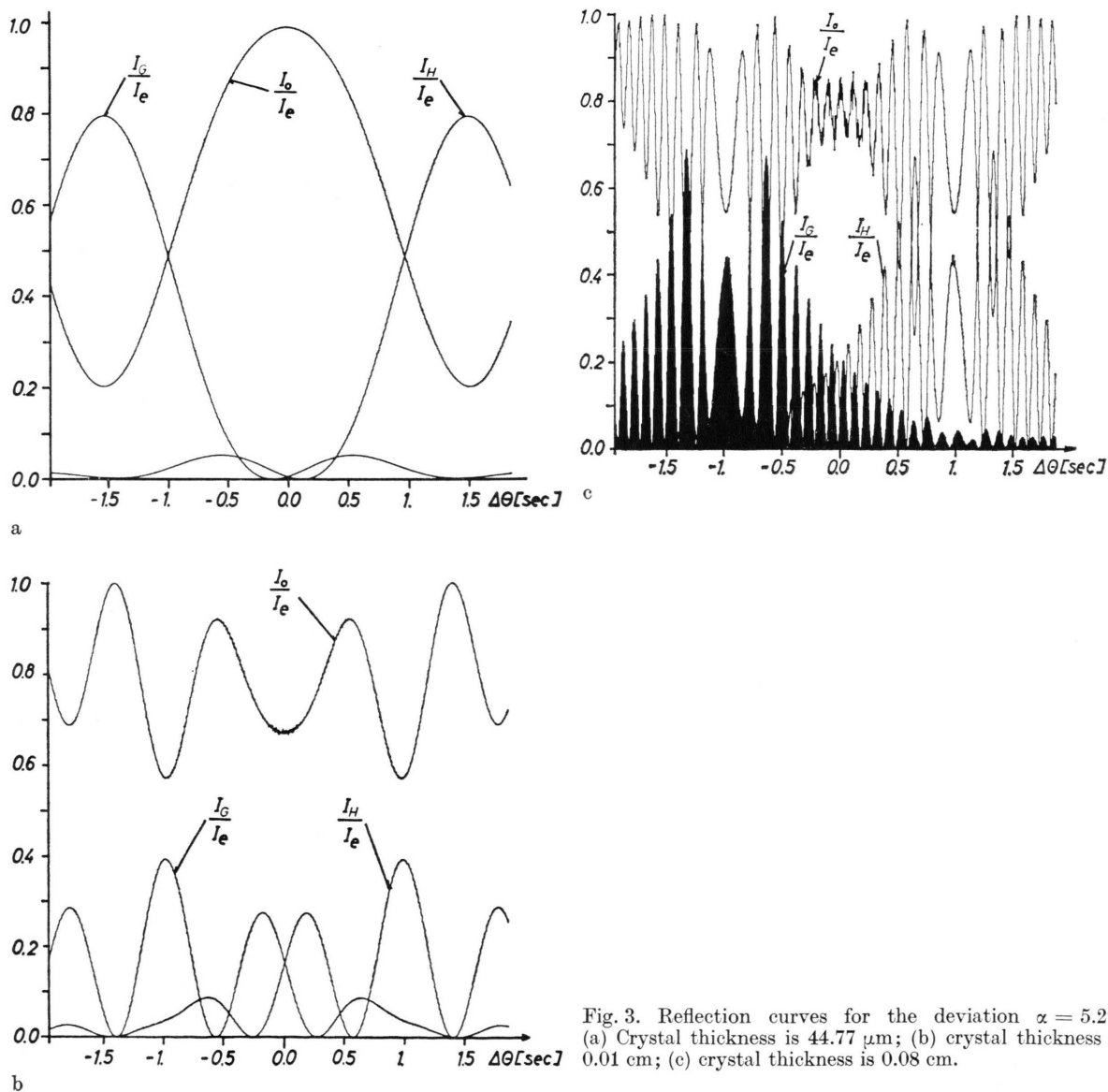
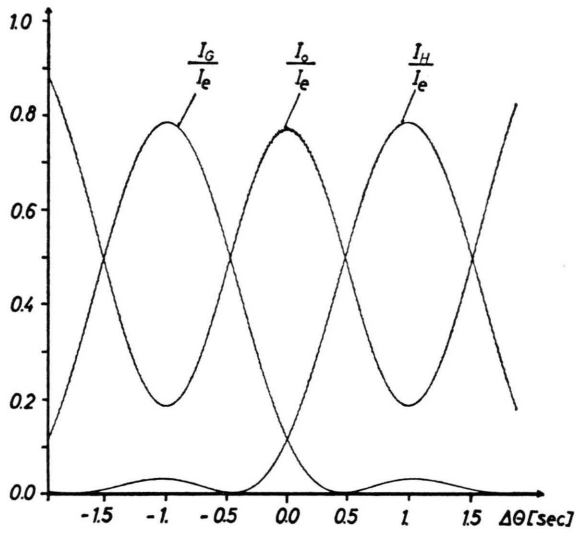
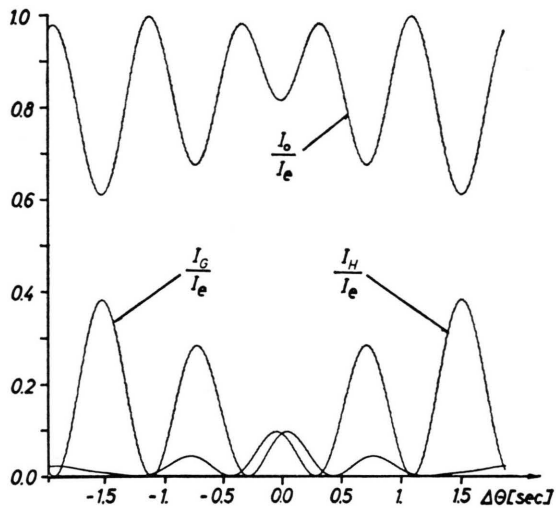


Fig. 3. Reflection curves for the deviation  $\alpha = 5.2''$ . (a) Crystal thickness is  $44.77 \mu\text{m}$ ; (b) crystal thickness is  $0.01 \text{ cm}$ ; (c) crystal thickness is  $0.08 \text{ cm}$ .



a



b

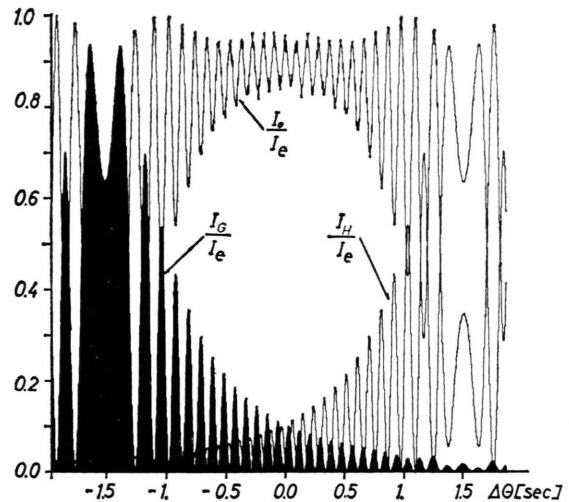


Fig. 4. Reflection curves for the deviation  $\alpha = 7.8''$ . (a) Crystal thickness is  $44.77 \mu\text{m}$ ; (b) crystal thickness is  $0.01 \text{ cm}$ ; (c) crystal thickness is  $0.08 \text{ cm}$ .

other reflected beam. Because of this asymmetry an enhanced sensitivity on lattice deformation is found for the wave vector  $\mathbf{k}^i$  in all three dimensions. Moving  $\mathbf{k}^i$  farther out of the symmetry plane the intensities of the reflected beams decrease and move to the edges of the three beam region. At  $\Delta\theta = 0$ ,  $I_0$  becomes dominant. As mentioned in [1] there is a region where pendellösung can be observed for each beam at given positions of the reflection curve, i.e. where the intensities change from one beam into the others. This region now is split and moves to the edges of the considered region, so that each reflected beam "gets its own region of pendellösung".

The position of this region (on the  $\Delta\theta$ -scale) depends on the deviations  $\alpha$  as well as on  $\Delta\theta$ . These behaviors are entirely different from those of the two beam cases, where the region of observable pendellösung lies always around  $\Delta\theta = 0$ . The strong three dimensional dependence seems therefore very important for the study of deformed lattices, especially in cases where the deformation is not too large.

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