Limits of the X-Ray Collimation by One Asymmetrical Bragg Reflection

O. Brümmer and H. R. Höche

Sektion Physik, Martin-Luther-Universität, Halle-Wittenberg (DDR)

J. Nieber

Sektion Mathematik/Physik, Pädagogische Hochschule ,,N. K. Krupskaja'' Halle (Saale), DDR

Dedicated to Herrn Prof. G. Hildebrandt on the occasion of his 60th birthday

In connection with the production of highly collimated X-rays the study of extremely asymmetrical Bragg reflections became of interest. In this paper the so-called extended dynamical theory of X-ray diffraction will be tested experimentally. As a result of this investigations the optimum conditions for X-ray collimation by means of one asymmetrical Bragg reflection are being discussed.

1. Introduction

Due to the refraction index $n = 1 - \delta \approx 1 - 10^{-5}$ it is impossible to construct X-ray lenses in the usual sense. For the same reason the reflection power of X-rays is nearly zero ($R \approx 10^{-10}$) for perpendicular incidence on the mirror surface. That means the impossibility of the mirror optics for X-rays in the range of wavelength $\lambda \leq 0.2$ nm. Only in the range of total reflection, where the angle of incidence with respect to the surface is smaller than $1°$, the reflection power attains values of a relevant order of magnitude. But the construction of focusing devices for X-rays on the basis of the total reflection raises many problems resulting from the very small angular range of total reflection and the influence of the surface profile on the critical angle of total reflection θ_c. The utilization of Fresnel's zone plates is also limited by practical problems consisting in the preparation of the zone plates. Thereby one uses the phenomena of the well known X-ray diffraction to realize optical systems for X-rays. Bent crystals are applied in the spectroscopy to focus X-ray beams. In the last years some applications of highly collimated X-rays could be seen, especially in connection with the development of the so-called plane-wave topography for testing semiconductor crystals for microdefects. Asymmetrical Bragg reflections are a very simple way of collimating X-rays, cf.

Renninger [1], Bubákova [2], Kohra [3]. Unfortunately the conventional dynamical theory of X-ray diffraction given by v. Laue [4] expressively excludes the case of grazing incidence, which is important for X-ray collimation.

2. Results of the Extended Dynamical Theory of X-ray Diffraction

In the conventional treatment of the fundamental equations of the X-ray diffraction the dispersion surface is approximated by straight lines instead of the correct form of circles, cf. Rustichelli [5]. This so-called tangent approximation yields a quadratic equation for the determination of the excitation points. In the more correct extended treatment the corresponding equation is an equation of the fourth order, cf. Kishino and Kohra [6], Bedynska [7], Brümmer et al. [8], Mazkedian and Rustichelli [9]. For simplicity the following discussion will be restricted to the σ polarization with the electric field vector normal to the diffraction plane. As a result of the more correct solution of the fundamental equations one obtaines four excitation points on the dispersion surface for each incident σ-polarized X-ray beam. In order to solve the problem of matching the amplitudes of the four X-ray waves inside the crystal on the crystal surface one has to consider the continuity of the tangential components of the electric *and* magnetic field vectors. In the conventional treatment the continuity of the electric vector alone is sufficient.

The geometrical description of an asymmetrical Bragg reflection according to the conventional treatment is shown in Figure 1. In addition to the geometry in the real space the representation in the reciprocal space including the dispersion surface is given. In the zero absorption case the angular deviation of the incident wave from the Bragg law $\Delta\theta_{i(c)}$ can be given by the following analytic expression

$$\Delta\theta_{i(c)} = \frac{|\chi_0|}{2\sin 2\theta_B}\left(1 - \frac{\gamma_h}{\gamma_0}\right), \quad (1)$$

where

χ_0 = 0th Fourier coefficient of electric susceptibility,

θ_B = Bragg angle determined by the Bragg equation,

γ_0, γ_h = direction cosine of the incident and reflected wave, respectively ($\gamma_h < 0$ in the Bragg case),

b = γ_0/γ_h = factor of asymmetry used in the conventional dynamical theory.

The index (c) refers to the conventional theory.

The second important quantity is the angular range of interference total reflection (width of the Darwin curve). For the incident wave the conventional theory leads to

$$w_{i(c)} = \frac{2|\chi_h|}{\sin 2\theta_B}\sqrt{\frac{|\gamma_h|}{\gamma_0}}, \quad (2)$$

where $\chi_h = h$-th Fourier coefficient of electric susceptibility. The corresponding angular range of the reflected beam is given by the equation

$$w_e = |b|\,w_i. \quad (3)$$

This relation is the consequence of the continuity of the tangential components of the wave vectors supposing pure elastic scattering, cf. Kuriyama and Boettinger [10]. The Eq. (3) is valid also in extremely asymmetric cases, although the quantities w_i and b used in the conventional theory are fictive in the range $\gamma_0 \lesssim \sin\sqrt{|\chi_0|} \approx \sin\theta_c$, cf. Brümmer et al. [11]. θ_c is the critical angle of the total reflection caused by the refraction.

The geometrical description of an asymmetrical Bragg reflection according to the extended dynamical theory of X-ray diffraction is shown in Figure 2. As in Fig. 1 the geometrical representation is given in the real and reciprocal space. The index (e) refers to the extended theory. In the zero absorption case the angular deviation of the incident wave from the
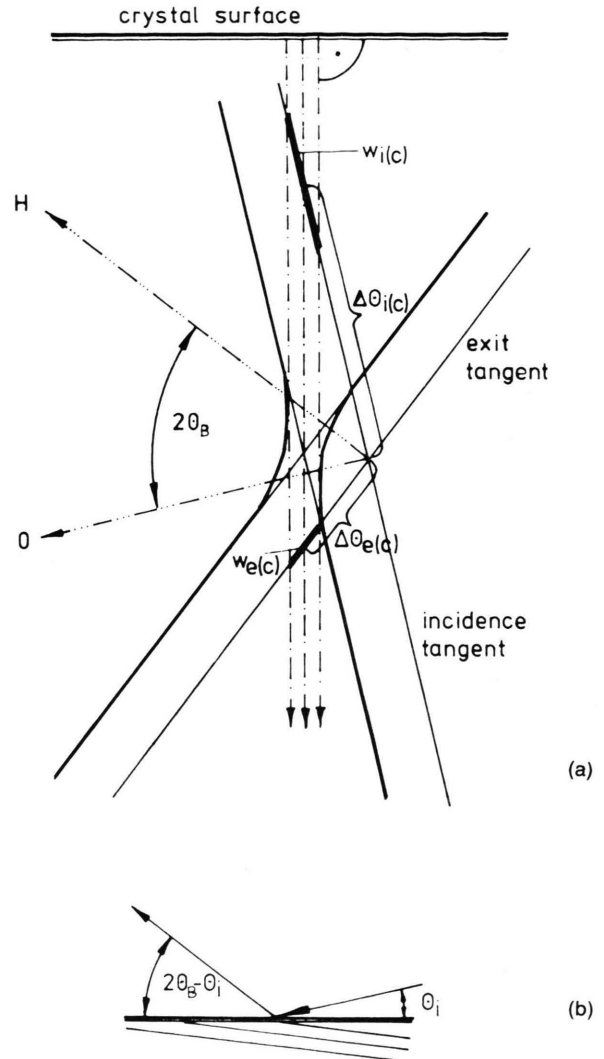

Fig. 1. Asymmetrical Bragg reflection according to the conventional treatment (tangent approximation). (a) dispersion surface; (b) real space.

Bragg law can be calculated by

$$\Delta\theta_{i(e)} = \frac{-\gamma_0 + \sqrt{\gamma_0^2 + \dfrac{\gamma_0|\chi_0|}{\sin 2\theta_B}\left(1 - \dfrac{\gamma_h}{\gamma_0}\right)\sqrt{1-\gamma_0^2}}}{\sqrt{1-\gamma_0^2}}. \quad (4)$$

The width of the Darwin curve is given by

$$w_{i(e)} = \frac{\gamma_0}{\sqrt{\gamma_0^2 + \dfrac{\gamma_0|\chi_0|}{\sin 2\theta_B}\left(1 - \dfrac{\gamma_h}{\gamma_0}\right)\sqrt{1-\gamma_0^2}}} \cdot \frac{2|\chi_h|}{\sin 2\theta_B}\cdot\sqrt{\frac{|\gamma_h|}{\gamma_0}}. \quad (5)$$
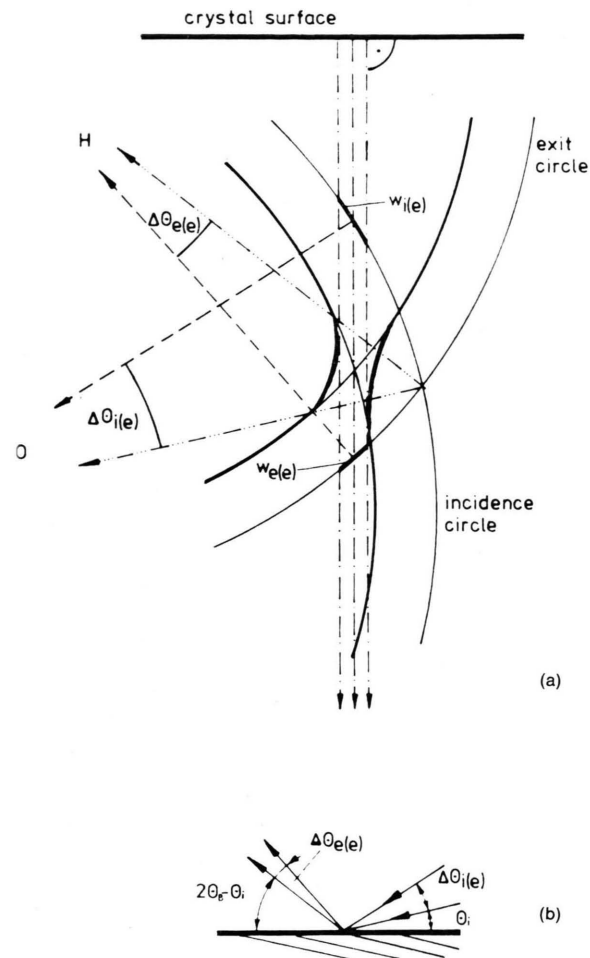
Fig. 2. Asymmetrical Bragg reflection according to the extended treatment. (a) dispersion surface; (b) real space.

limation. The graphic representations are better distinguishable, if the corresponding expressions are presented as functions of the asymmetry ratio $\beta = (1+b)/(1-b)$, introduced by Renninger [12] and Otto [13]. The advantage of this variable consists in the fact that the symmetrical Bragg reflection appears in the centre of the graph $(\beta = 0)$. The limit $\beta = 1$ corresponds to the geometry with grazing incidence of X-rays; $\beta = -1$ means grazing exit of the reflected beam. In Fig. 3 $\varDelta\theta_{i(c)}(\beta)/\varDelta\theta_s$ and $\varDelta\theta_{i(e)}(\beta)/\varDelta\theta_s$ are shown. $\varDelta\theta_s = |\chi_0|/\sin 2\theta_B$ is the angular deviation from the Bragg law in the symmetrical Bragg case. The value of the angular deviation of the reflected beam from the Bragg position can be obtained by exchange of γ_0 and γ_h in (2) and (4), respectively. In terms of β this means that β has to be replaced by $-\beta$. The conventional treatment leads to the function

$$\frac{\varDelta\theta_{i(c)}}{\varDelta\theta_s} = \frac{1}{1-\beta}.$$

For grazing incidence the conventional expressions (1) and (2) give the physically meaningless values

$$\lim_{\gamma_0 \to 0} \varDelta\theta_{i(c)} = \infty \quad \text{and} \tag{6 a}$$

$$\lim_{\gamma_0 \to 0} w_{i(c)} = \infty , \tag{6 b}$$

whereas the corresponding expressions according to the extended treatment tends to the finite values

$$\lim_{\gamma_0 \to 0} \varDelta\theta_{i(e)} = \sqrt{|\chi_0|} = \theta_c \quad \text{and} \tag{7 a}$$

$$\lim_{\gamma_0 \to 0} w_{i(e)} = 0 . \tag{7 b}$$

Of course the more exact expressions (4) and (5) are valid in symmetrical and slightly asymmetric cases. The differences to the conventional expressions (1) and (2) are significant in a small angular range only, but this is the important range for X-ray col-
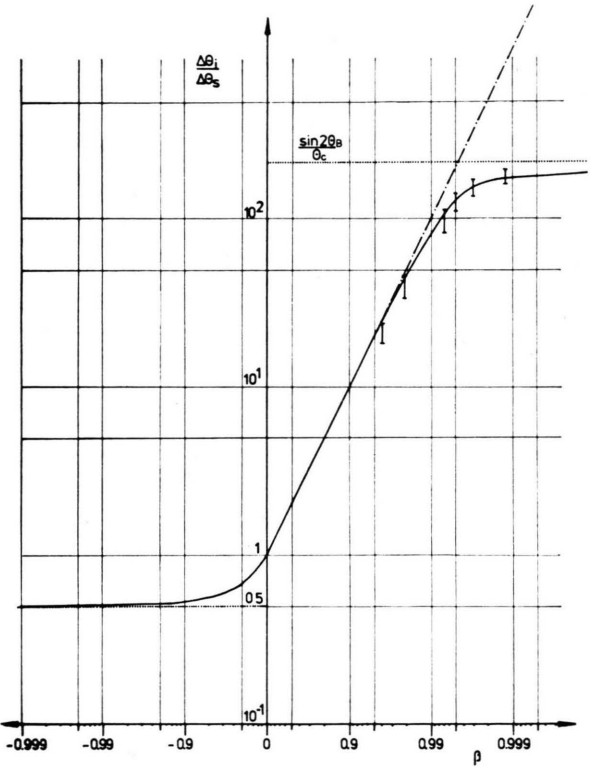

Fig. 3. Angular deviation from the Bragg law versus the asymmetry ratio β according to the extended treatment (solid curve) and according to the conventional treatment (broken curve). The experimental values are given with the error limits.

The corresponding curve (broken line in Fig. 3) is divergent for grazing incidence, i. e. $\beta \to 1$. The function $\Delta \theta_{i(e)}(\beta)/\Delta \theta_s$ approaches $(\sin 2\theta_B)/\theta_c$, if $\gamma_0 \to 0$ or $\beta \to 1$.

In Fig. 4 the graph of $w_i(\beta)/w_s$ is shown. In the symmetrical Bragg case the width of the Darwin curve can be calculated by $w_s = 2|\chi_h|/\sin 2\theta_B$. In the conventional theory $w_{i(c)}(\beta)/w_s$ is given by the function $\sqrt{(1+\beta)/(1-\beta)}$, which becomes infinite for β tending to one. In the extended treatment the corresponding expression $w_{i(e)}(\beta)/w_s$ passes through a maximum at the position

$$\beta = \frac{\sin(2\theta_B - \theta_c) - \sin \theta_c}{\sin(2\theta_B - \theta_c) + \sin \theta_c}.$$

This corresponds to an asymmetrical Bragg reflection with an angle of incidence θ_i, which is equal to θ_c, if θ_i is calculated without the dynamical deviation from the Bragg law. The maximum width of the Darwin curve resulting from (5) is

$$w_i = \sqrt[4]{\frac{2}{|\chi_0|}} \sqrt{\frac{\sin 2\theta_B}{3}} \, w_s. \tag{8}$$

Since the expressions for $w_{i(e)}$ and $\Delta \theta_{i(e)}$ are functions of χ_0 and θ_B (dependent on the material and X-ray wavelength), the extended dynamical theory can not give general expressions as the conventional theory does. Therefore the curves in Figs. 3 and 4 were calculated for the Si 311 reflection of CuK$_\alpha$ radiation.
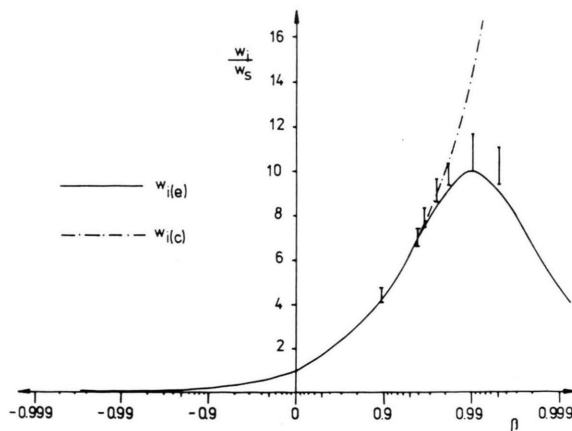

Fig. 4. Width of the Darwin curve versus β according to the extended treatment (solid curve) and according to the conventional treatment (broken curve). The experimental values correspond to the Si 311 reflection of CuKα radiation.

Beside the theoretical results some experimental values obtained by measurements with a double crystal arrangement were added. The measurements of $\Delta \theta_i$ were performed with a skew 311 reflection. Then it is possible to carry out the investigations with a single silicon slice with (111) surface orientation. In this way the influence of the surface profile of the specimen on the results can be kept constant. For the experimental determination of $w_{i(e)}$ the second crystal of the double crystal diffractometer was a skew 311 reflection, too. The corresponding Kossel cone intersects the crystal surface. The change of the asymmetry was realized by a rotation around the normal to the reflecting lattice planes, cf. Bubákova et al. [14]. The reason for the systematic difference between the theoretical curve and the experimental values in Fig. 4 is the absorption, which can not be neglected in the experiments, although (5) was derived on the assumption of zero absorption.

3. Conclusions

On the basis of the theoretical considerations supported by the experiments the optimum conditions for X-ray collimation, using one asymmetrical Bragg reflection can be given. The maximum of the width of the Darwin curve (see (8)) means that the maximum angular range of the incident radiation is reflected. On the other hand it can be seen from (4) that the real angle of incidence of the primary beam (middle of the Darwin curve) is greater than the corresponding one, calculated by means of the Bragg law. The maximum of $w_{i(e)}$ is found on the scale of the real angles of incidence at the value $\sqrt{2|\chi_0|} = \sqrt{2}\,\theta_c$. The discussion of the change of the beam cross-section, first published by Fankuchen [15], must be performed with the real angle of incidence. In the case discussed above this gives a reduced spreading of the beam in relation to the classical treatment. All applications of X-rays, highly collimated by asymmetrical Bragg reflections, have the disadvantage that the available intensity is low. Therefore the experiments should be carried out under this optimum condition. Then the divergence of the reflected beam is equal to $w_e = (\sqrt{|\chi_0|}/\sin 2\theta_B)w_s$. For the Si 311 CuK$_\alpha$ reflection the divergence of the reflected beam is nearly 0.2″. A second result of this work is the knowledge of the limit of the applicability of the conventional dynam-

ical theory of X-ray diffraction in the case of asymmetrical reflections. This limit is dependent on the material of the crystal, the reflecting plane and the wavelength of the X-rays. In general it can be stated that for angles of incidence smaller than $1°$ the extended theory has to be applied.

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