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Raytracing Code for
Crystal Optics

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Abstract

This report gives an overview about the BESSY software tools available for calculations of crystal optics. This library has been developed in the last months for the design of the BESSY II x-ray optics beamlines. This report is not intended to be a handbook for the available programs REFLEXE, DIXI1 and RAY, but summarizes the main features and equations of the dynamical theory of x-ray diffraction. Examples for the calculation of rocking curves for symmetrically and asymmetrically cut crystals are shown.

Introduction

The raytracing is one of the major and most powerful tools of up-to-date methods of synchrotron radiation beamline design. The cost and complicity of equipment and instrumentation involved is so high, that preliminary design studies under realistic conditions play an extremely important roll. At the BESSY GmbH in the last few years several useful programs for the design of synchrotron radiation beamlines have been developed. BESSY-I was constructed only for UV-, VUV and soft x-ray radiation employing mainly grating monochromators and only one crystal monochromator. BESSY-II, however, will provide not only VUV beamlines, but also some relatively high energy beamlines, probably up to 50 KeV. Thus, the need for hard X-ray optics has become considerable.

The goal of this work was to study X-ray optics, particularly from the point of view of developing a raytracing code for crystals as optical elements and X-ray diffraction as the physical process.

For this propose it was thought to be appropriate to apply the dynamic theory of X-ray scattering. This is a classic theory developed long time ago by Ewald and later elaborated by other workers. Only recently, with the advent of synchrotron radiation sources and good quality crystals, it has become possible and necessary as well to apply the dynamic theory of X-ray diffraction to actual experimental phenomena. The basic theory was reviewed and a unified formulation was prepared bringing together all the relevant formulae along with their limitations. This ground work was important as it can not only be of help in developing the raytracing code but also be useful for further theoretical developments.

Numerical programs for crystal diffraction rocking curve calculations have been kindly provided by the X-ray optics group at the University of Jena (PC code DIXI1) and by the Institute of Physics in Prague (VAX code REFLEXE). These programs were used and extensively studied from the point of integrating them into our raytracing code. Finally, incorporating the basic theory and using ideas from other programs as well as employing the basic structure of the RAY program our own program was developed and tested. It is now incorporated in the RAY program and can be used for simulating a synchrotron beamline with crystals as optical components in addition to other usual components such as mirrors, gratings, foils, slits etc. RAY is thus a real and quick alternative to the widely used synchrotron radiation raytracing program SHADOW.

Theoretical background. Dynamical theory of X-ray diffraction

Scattering of X-rays by a solid is essentially a perturbative phenomenon caused by interaction of incident electromagnetic radiation with the electrons in the scatterer. Diffraction can be thought of as a special case of scattering when the electron density in the scatterer is a periodic function of position. The scattering cross section is then non zero for directions satisfying the well known Laue equations, and, for a spatially very large scatterer, the angular distribution of scattered X-rays is given by a number of delta functions centred around the Bragg angles. This approach is known as the kinematic theory of diffraction and it usually ignores both absorption (at low energies mostly due to the photoelectric effect) and extinction (removal of intensity from the primary beam due to Bragg reflection) of X-rays in the scatterer. It is a very good first approximation for small crystals.

The intensity of scattered radiation from a crystal parallelepiped of edges $N_1\mathbf{a}_1, N_2\mathbf{a}_2, N_3\mathbf{a}_3$, where $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ are the basis vectors of the direct lattice unit cell and N_1, N_2, N_3 are positive integers characterising the size of the crystal, is obtained by using standard time dependent perturbation theory as

$$I_{sc} = I_0 |F|^2 \prod_i \frac{\sin^2[(N_i \mathbf{s} \cdot \mathbf{a}_i)/2]}{\sin^2[(\mathbf{s} \cdot \mathbf{a}_i)/2]}, \quad (1)$$

where I_0 is the intensity of radiation scattered by a single electron, F is the unit cell structure factor and \mathbf{s} is the scattering vector given by

$$\begin{aligned} \mathbf{s} &= \mathbf{k}_i - \mathbf{k}_s, \\ |\mathbf{k}_i| &= |\mathbf{k}_s| = \frac{2\pi}{\lambda}, \end{aligned} \quad (2)$$

$\mathbf{k}_i, \mathbf{k}_s$ being the incident and the scattered wave vectors. The maximum value of the intensity occurs for directions corresponding to

$$\mathbf{s} \cdot \mathbf{a}_i = 2\pi H_i, i = 1, 2, 3. \quad (3)$$

Here H_i 's are three integers entirely independent of one another. Thus when the Laue equations (3) are satisfied the intensity of scattering becomes

$$I_{\mathbf{H}} = I_0 |F_{\mathbf{H}}|^2 N^2, \mathbf{H} \equiv (H_1, H_2, H_3). \quad (4)$$

We have shown the dependence of the scattered intensity on the direction by explicitly putting the subscript H. In eq.(4) $N = N_1 N_2 N_3$ is the number of unit cells in the crystal and $F_{\mathbf{H}}$ is the value of the structure factor for $\mathbf{s} = \mathbf{s}_{\mathbf{H}}$ satisfying eq.(3):

$$\begin{aligned} F_{\mathbf{H}} &= \sum_j f_j \exp(i\mathbf{s}_{\mathbf{H}} \cdot \mathbf{r}_j), \\ \mathbf{s}_{\mathbf{H}} &= 2\pi[H_1 \mathbf{b}_1 + H_2 \mathbf{b}_2 + H_3 \mathbf{b}_3], \end{aligned} \quad (5)$$

where f_j, \mathbf{r}_j refer to the atomic structure factor and position of the j th atom in the unit cell and the summation runs over all the atoms in the unit cell. $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ are the reciprocal lattice vectors defined by

$$\begin{aligned} \mathbf{b}_i &= \frac{\mathbf{a}_j \times \mathbf{a}_k}{\Omega}; i, j, k = 1, 2, 3 \\ \Omega &\equiv \mathbf{a}_i \cdot (\mathbf{a}_j \times \mathbf{a}_k). \end{aligned}$$

Consider the scattered intensity in the close vicinity of the Bragg angle θ_B corresponding to

$$\mathbf{s} = \mathbf{s}_{\mathbf{H}} + \mathbf{v}. \quad (6)$$

Then

$$I_{\mathbf{H}}(\mathbf{v}) = I_0 |F_{\mathbf{H}}|^2 \prod_i \frac{\sin^2\left(\frac{1}{2} N_i \mathbf{v} \cdot \mathbf{a}_i\right)}{\sin^2\left(\frac{1}{2} \mathbf{v} \cdot \mathbf{a}_i\right)}. \quad (7)$$

Smoothing out the oscillations in I_H by replacing the factor $\frac{\sin^2(Nx)}{\sin^2(x)}$ for large N by $N^2 \exp\left[-\frac{N^2 x^2}{\pi}\right]$ with the same maximum value and area under it, we have

$$I_H(\mathbf{v}) \approx I_0 |F_H|^2 N^2 \exp\left[-\frac{(\mathbf{v} \cdot \mathbf{A})^2}{4\pi}\right],$$

$$\mathbf{A} = N_1 \mathbf{a}_1 + N_2 \mathbf{a}_2 + N_3 \mathbf{a}_3. \quad (8)$$

The magnitude of \mathbf{s}_H is related to Bragg angle by

$$|\mathbf{s}_H| = \frac{4\pi}{\lambda} \sin \theta_B \quad (9)$$

and if \mathbf{v} corresponds to change φ in the scattering angle i.e. $2\theta_B \rightarrow 2\theta_B + \varphi$, then

$$|\mathbf{v}| = \frac{2\pi}{\lambda} \varphi \cos(\theta_B) \equiv \nu \quad (10)$$

and

$$\mathbf{v} \cdot \mathbf{A} \approx \nu D, \quad (11)$$

where D is the average linear dimension of the crystal. Then

$$I_H(\mathbf{v}) \approx I_0 |F_H|^2 N^2 \exp\left[-\pi \left(\frac{\varphi D \cos(\theta_B)}{\lambda}\right)^2\right] \quad (12)$$

and the angular full width at half maximum $\Delta\Theta$ is given by

$$\Delta\Theta = \frac{2\lambda}{D \cos(\theta_B)} \sqrt{\frac{\ell n 2}{\pi}}. \quad (13)$$

The above expression for the width of the diffraction peak is experimentally valid only for small crystals of the order of about 10^{-4} cm or so. It is not satisfactory for big good crystals presently employed in X-ray optics and instrumentation. Although the intensity formula of eq.(7) is a good first approximation, it does no more yield either the correct shape or the width of the diffraction peak. One can in principle include the effects of absorption in the kinetic approach by including them in the atomic (and hence crystal) structure factors. However, the extinction effects involve consideration of the reduction in the incident intensity due to Bragg reflection when the Laue equations are exactly or very nearly satisfied.. Thus the general theory should involve the interaction between the incident and the scattered radiation. When this coupling is taken into account one solves it for a self consistent solution involving the different diffracted and incident waves in the crystal. The problem essentially reduces to that of dispersion theory and it leads one to the general or dynamical theory of X-ray diffraction.

The fundamental equations of the dynamical theory essentially correspond to the Maxwell equations inside the scatterer - a single crystal. It is simpler to consider the wave equation for the displacement vector

$$\nabla \times (\nabla \times \frac{1}{\epsilon} \mathbf{D}) = -\frac{1}{c} \frac{\partial^2 \mathbf{D}}{\partial t^2}, \quad (14)$$

where ε is the dielectric constant of the crystal. In general; ε is a tensorial quantity, however, we shall treat it to be a scalar as is commonly done. This is essentially the Laue model of diffraction theory. ε can be put in terms of crystal polarisability α as

$$\varepsilon = 1 + 4\pi\alpha \equiv 1 + \psi. \quad (15)$$

For X-ray frequencies ψ is negative and

$$10^{-4} \approx |\psi| \ll 1. \quad (16)$$

The refractive index n is equal to the square root of the dielectric constant:

$$n = \sqrt{\varepsilon} \approx 1 + \frac{1}{2}\psi. \quad (17)$$

The polarisability α or rather ψ is related to the atomic scattering factor by

$$\begin{aligned} \psi &= -2\Delta - 2i\beta, \\ \Delta &= \frac{r_0}{2\pi} N\lambda^2 \sum_j f_{1j}, \\ \beta &= \frac{r_0}{2\pi} N\lambda^2 \sum_j f_{2j}, \\ r_0 &\equiv e^2 / (mc^2). \end{aligned} \quad (18)$$

In (18) N is the number of unit cells per unit volume in the crystal, the summation over j runs over all the atoms in the unit cell and $f_{1,2}$ are the real and imaginary parts of the atomic scattering factor given by

$$\begin{aligned} f_1 &= Z + Q \int_0^\infty \frac{\xi^2 \mu(\xi)}{E^2 - \xi^2} d\xi, \\ f_2 &= \frac{\pi}{2} QE\mu(E), Q \equiv (\pi r_0 hc)^{-1}. \end{aligned} \quad (19)$$

In (19) Z is the atomic number, E is the photon energy and μ is the photo absorption cross section

$$\mu = \frac{At}{N_0 \rho} \mu_l, \quad (20)$$

where At, N_0, ρ, μ_l refer respectively to atomic weight, Avagadro number, density and linear absorption coefficient. A better approximation for the atomic structure factor would replace Z by the form factor f_0 given by

$$f_0 = \int_0^\infty \frac{U(r) \sin(kr)}{kr} dr, k \equiv \frac{4\pi}{\lambda} \sin(\Theta) \quad (21)$$

$$\begin{aligned} &\cong Z \text{ for } \frac{\sin(\Theta)}{\lambda} \leq 0.05 \text{ \AA}^{-1} \\ &\cong 0.9Z \text{ for } \frac{\sin(\Theta)}{\lambda} \approx 0.1 \text{ \AA}^{-1}. \end{aligned}$$

In (21) $U(r), 2\Theta$ refer to the radial atomic charge distribution function and the scattering angle respectively.

It is also customary to introduce yet another response function χ through the definition

$$4\pi\mathbf{P} = \chi\mathbf{D} \quad (22)$$

so that

$$\chi = 1 - \epsilon^{-1} \cong 4\pi\alpha = \psi. \quad (23)$$

In the Laue model the polarisability as well as the dielectric constant and χ, ψ are periodic functions of the position and can be expanded in a Fourier series over the reciprocal lattice vectors:

$$\chi = \sum_{\mathbf{G}} \chi_{\mathbf{G}} \exp(i\mathbf{G} \cdot \mathbf{r}), \quad (24)$$

where

$$\begin{aligned} \mathbf{G} &= 2\pi[G_1\mathbf{b}_1 + G_2\mathbf{b}_2 + G_3\mathbf{b}_3], \\ G_i &\text{ integer, } i = 1, 2, 3. \end{aligned} \quad (25)$$

$\chi_{\mathbf{G}}$ is then seen to be proportional to the structure factor $F_{\mathbf{G}}$ given by eq.(5) with $\mathbf{s}_{\mathbf{H}} \rightarrow \mathbf{G}$ i.e.

$$\begin{aligned} \chi_{\mathbf{G}} &= -\frac{f_0}{\pi\Omega} \chi^2 F_{\mathbf{G}}, \\ F_{\mathbf{G}} &= \sum_j f_j \exp(i\mathbf{G} \cdot \mathbf{r}_j) \end{aligned} \quad (26)$$

Ω is the unit cell volume. The component corresponding to $\mathbf{G} = 0$ is the average response function

$$\chi_0 = -2 \Delta. \quad (27)$$

Fourier expanding the displacement vector and the polarisability, from eq.(14) we obtain

$$(\mathbf{k}_i^2 - \mathbf{k}_H^2)\mathbf{D}_H = \sum_{\mathbf{G}} [\chi_{H-\mathbf{G}}(\mathbf{k}_H \cdot \mathbf{D}_G)\mathbf{k}_H - \chi_{H-\mathbf{G}}\mathbf{k}_H^2\mathbf{D}_G]. \quad (28)$$

Eq.(28) is the fundamental system of equations of the dynamical theory. \mathbf{k}_i is the incident wave vector and \mathbf{k}_H is the diffracted wave vector from planes $\mathbf{H} = (H_1, H_2, H_3)$.

$$\mathbf{k}_H = \mathbf{k}_i + 2\pi[H_1\mathbf{b}_1 + H_2\mathbf{b}_2 + H_3\mathbf{b}_3]. \quad (29)$$

It is readily seen that

$$\mathbf{D}_H \cdot \mathbf{k}_H = 0 \quad (30)$$

so that all the waves are of transverse type and a particular Fourier component gets admixed with other components due to the response of the crystal.

The simplest application of eq.(28) corresponds to the situation when there is only one wave in the crystal, i.e. just the transmitted radiation, the geometry being such that for the particular incident wavelength under consideration Laue equations are not satisfied for any direction of scattering. Then the only non zero Fourier coefficient corresponds to $\mathbf{G} = 0$ Putting $\mathbf{G} = \mathbf{H} = 0$ in eq.(28) we have

$$\mathbf{k}_t^2 - \mathbf{k}_i^2 = -\chi_0 \mathbf{k}_i^2 \quad (31)$$

so that

$$\mathbf{k}_t^2 = \frac{\mathbf{k}_i^2}{1 - \chi_0} \quad (32)$$

or

$$k_t = k_i \left(1 + \frac{\chi}{2} \right) = k_i (1 - \Delta). \quad (33)$$

In (31) - (33) we have put the subscript t to indicate that the wave is the transmitted one corresponding to $\mathbf{H} = 0$, and it is clear that the refractive index for the incident wave corresponds to the average refractive index for the crystal.

The most common application of eq.(28) corresponds to the case of two waves in the crystal, one transmitted or refracted and the other diffracted. Thus there are two non zero Fourier components, for $\mathbf{G} = 0, \mathbf{H}$ (say), and denoting the zeroth component as before by subscript t eq.(28) gives rise to following two coupled equations:

$$\begin{aligned} [\mathbf{k}_t^2 - \mathbf{k}_i^2 (1 - \chi_0)] \mathbf{D}_t &= \chi_{-\mathbf{H}} [(\mathbf{k}_i \cdot \mathbf{D}_\mathbf{H}) \mathbf{k}_i - \mathbf{k}_i^2 \mathbf{D}_\mathbf{H}], \\ [\mathbf{k}_i^2 - \mathbf{k}_\mathbf{H}^2 (1 - \chi_0)] \mathbf{D}_\mathbf{H} &= \chi_\mathbf{H} [(\mathbf{k}_\mathbf{H} \cdot \mathbf{D}_t) \mathbf{k}_\mathbf{H} - \mathbf{k}_\mathbf{H}^2 \mathbf{D}_t]. \end{aligned} \quad (34)$$

From eq.(34) it is clear that $\mathbf{D}_\mathbf{H}$ lies in the same plane as $\mathbf{k}_\mathbf{H}, \mathbf{D}_t$. These equations can be converted to two coupled scalar equations by taking the scalar products of the first equation with \mathbf{D}_t and the second equation with $\mathbf{D}_\mathbf{H}$. For further simplification put

$$\mathbf{k}_t^2 = k_i^2 (1 + 2\kappa_t), \mathbf{k}_\mathbf{H}^2 = k_i^2 (1 + 2\kappa_\mathbf{H}) \quad (35)$$

and keep only first order terms in polarisability. We then get

$$\begin{aligned} (2\kappa_t - \chi_0) D_t - \chi_{-\mathbf{H}} \sin(\Phi) D_\mathbf{H} &= 0, \\ -\chi_\mathbf{H} \sin(\Phi) D_t + (2\kappa_\mathbf{H} - \chi_0) D_\mathbf{H} &= 0, \end{aligned} \quad (36)$$

where Φ is the angle between \mathbf{D}_t and $\mathbf{k}_\mathbf{H}$. For s-polarisation \mathbf{D}_t is normal to the plane containing \mathbf{k}_i and $\mathbf{k}_\mathbf{H}$ so that $\Phi = \frac{\pi}{2}$. In p-polarisation $\Phi = \frac{\pi}{2} - 2\Theta$, where $2\Theta = 2\Theta_B$ is the scattering angle. Thus we shall consider only the case of s-polarisation and set $\sin(\Phi) = 1$. For p-polarisation replace $\chi_\mathbf{H}$ and $\chi_{-\mathbf{H}}$ every where with $\chi_\mathbf{H} \cos(2\Theta_B)$ and $\chi_{-\mathbf{H}} \cos(2\Theta_B)$.

The condition for existence of a solution of the simultaneous system of equations (36) is the vanishing of the determinant of the coefficients. Taking into consideration the linear relation

between κ_i and κ_H this leads to a quadratic equation for κ_i and its two solutions give rise to two transmitted waves and also correspondingly two diffracted waves. A linear combination of these waves is selected by application of the boundary conditions at the surface of the crystal. Let the external incident wave enter the crystal medium through the boundary $\hat{n} \cdot \mathbf{r} = 0$, where \hat{n} is the unit normal to the crystal surface pointing in the crystal. At this boundary it must join smoothly with internal incident wave. This requires

$$D_{t1} + D_{t2} = E_i,$$

where subscripts 1 and 2 refer to the two solutions for the transmitted waves respectively. This boundary condition does not, however, uniquely determine the internal incident and diffracted waves and an additional boundary condition needs to be imposed. This additional boundary condition is different for the Laue and Bragg cases, for the former there is no diffracted wave coming out of the crystal on the same side as the incident wave and for the latter there is no diffracted wave getting transmitted through the crystal. For the Bragg case of our interest the boundary condition is

$$c_1 x_1 D_{t1} + c_2 x_2 D_{t2} = 0 \text{ at } \hat{n} \cdot \mathbf{r} = T, \quad (37)$$

where T is the crystal thickness.

The intensity I_H of the Bragg reflected wave corresponding to diffraction from planes $\mathbf{H} = (H_1, H_2, H_3)$ in terms of the incident intensity I_0 is then obtained as

$$I_H = I_0 \left| \frac{x_1 x_2 (c_1 - c_2)}{c_2 x_2 - c_1 x_1} \right|^2. \quad (38)$$

In eq.(37), (38)

$$x_{1,2} = \frac{-z \pm \sqrt{q + z^2}}{\chi_{-H}}, \quad z \equiv \frac{1-b}{2} \chi_0 + \frac{b}{2} a, \quad q \equiv b \chi_H \chi_{-H}, \quad (39)$$

$$b = \frac{\hat{n} \cdot \hat{\ell}_i}{\hat{n} \cdot \hat{\ell}_d}, \quad (40)$$

$$a \equiv \frac{\mathbf{s}_H^2 + 2\mathbf{k}_i \cdot \mathbf{s}_H}{\mathbf{k}_i^2}, \quad (41)$$

$$c_{1,2} = \exp(-i\nu_{1,2}T), \quad \nu_{1,2} = \kappa_{t1,2} \left(\frac{2\pi k_i}{\hat{n} \cdot \hat{\ell}_i} \right), \quad (42)$$

$$\kappa_{1,2} = \frac{1}{2} \left[\chi_0 - z \pm \sqrt{q + z^2} \right]. \quad (43)$$

In the above equations $\hat{\ell}_i, \hat{\ell}_d$ are direction cosines for the incident and diffracted beams.

Eq.(38) is the basic equation for calculating the rocking curve of a crystal for the case of Bragg diffraction. It is customary to consider the reflecting power of the crystal which is the ratio of diffracted power to the incident power:

$$\frac{P_H}{P_i} = \frac{S_H I_H}{S_i I_i}, \quad (44)$$

where S_H, S_i refer to the cross section of the diffracted and incident beams respectively. If the linear width of the incident beam is large compared to the depth of penetration in the crystal

$$\frac{S_H}{S_i} \approx \frac{1}{|b|} \quad (45)$$

so that

$$\frac{P_H}{P_i} = \frac{1}{|b|} \frac{I_H}{I_0}. \quad (46)$$

For zero absorption Eq.(38) then becomes

$$\frac{P_H}{P_0} = \frac{\sin^2 \left[A \sqrt{y^2 - 1} \right]}{y^2 - 1 + \sin^2 \left[A \sqrt{y^2 - 1} \right]}, \quad (47)$$

where

$$A = a \sqrt{|b|} C |\chi_H|, y = \frac{z}{\sqrt{|b|} C |\chi_H|}, \quad (48)$$

$C = 1$ for s-polarisation and $|\cos(2\Theta_B)|$ for p-polarisation.

When the quantity under the radical sign in eq.(47) is negative the sine function gets replaced by a hyperbolic sine function. The centre of the diffraction pattern given by eq.(47) does not coincide with ideal Bragg angle Θ_B ; it occurs at

$$\Theta_B + \frac{1-b}{2b \sin(2\Theta_B)} \chi_0. \quad (49)$$

For the Bragg case of our interest since b is negative and so is χ_0 , this deviation implies that the glancing angle for the centre of diffraction pattern is always greater than the Bragg angle.

For the general case when absorption is not neglected the polarisability is complex and can be written as

$$\chi = \chi_1 + i\chi_2; \chi_{1,2} \text{ real}. \quad (50)$$

Expanding $\chi_{1,2}$ in Fourier series

$$\chi_{1,2} = \sum_{\mathbf{G}} \chi_{\mathbf{G}}^{1,2} \exp(i\mathbf{G} \cdot \mathbf{r}), \quad (51)$$

$$\chi_{-\mathbf{G}}^{1,2} = \chi_{\mathbf{G}}^{1,2*}.$$

The average refractive index is then given by

$$n = 1 + \frac{1}{2}\chi_0^1 + i\frac{1}{2}\chi_0^2$$

and is complex, the imaginary part being related to the true linear absorption coefficient by

$$\mu_0 = -\frac{2\pi}{\lambda}\chi_0^2.$$

The reflected power for the Bragg case can then be written in a more convenient form as

$$\frac{P_{\mathbf{H}}}{P_0} = L - \sqrt{L^2 - (1 - 4\eta^2)}, \quad (51)$$

where

$$L = +\sqrt{(-1 + y^2 - g^2)^2 + 4(gy - \eta)^2} + y^2 + g^2, \quad (52)$$

$$\eta \equiv \frac{\chi_{\mathbf{H}}^2}{\chi_{\mathbf{H}}^1}, \quad g \equiv \frac{\text{Im}(z)}{C|\chi_{\mathbf{H}}^1|\sqrt{|b|}} = \frac{\left(\frac{1-b}{2}\right)\chi_0^2}{C|\chi_{\mathbf{H}}^1|\sqrt{|b|}}$$

When the true absorption is negligible, i.e. in the limit of $\eta = g = 0$ we get the famous Darwin solution:

$$\frac{P_{\mathbf{H}}}{P_0} = M - \sqrt{M^2 - 1}, \quad M \equiv |y^2 - 1| + y^2. \quad (53)$$

Thus

$$\frac{P_{\mathbf{H}}}{P_0} = 1 \text{ for } |y| \leq 1 \quad (54)$$

and

$$\frac{P_{\mathbf{H}}}{P_0} = \left[|y| - \sqrt{y^2 - 1}\right]^2 \text{ for } |y| \geq 1. \quad (55)$$

From eq.(51) it follows that the diffraction pattern is asymmetrical with respect to its centre at $y=0$ unless $\eta = 0$. The diffracted intensity is maximum at $y = \frac{\eta}{g}$ and the corresponding glancing angle is

$$\Theta_B + \frac{\left(\frac{1+|b|}{2}\right)|\chi_0^1| - \frac{\eta}{|g|}C|\chi_{\mathbf{H}}^1|\sqrt{|b|}}{|b|\sin(2\Theta_B)}. \quad (56)$$

Thus there is an additional shift of the Bragg angle as compared to eq.(49). The total angular width of the reflection is then seen to be given by

$$\Delta\Theta = \frac{\lambda}{\Lambda \sin(\Theta_B)}, \quad \Lambda \equiv \frac{\pi\Omega \cos(\Theta_B)}{r_0 \lambda C |F_{\mathbf{H}}|}. \quad (57)$$

It is interesting to compare the kinematical expression for the angular width eq.(13) with the dynamical expression of eq.(57). The former tends to zero as the crystal size increases. This of

course cannot occur in practice due to attenuation of X-rays in the crystal. According to the dynamic theory the maximum attenuation distance is about $(1/\pi)\Lambda \tan(\Theta_B)$.

Test of the computer code

A computer code for raytracing has been developed using the formulation described above. The program is integrated in the general raytracing code RAY at BESSY.

Typical X-ray reflectivity curves obtained using our program are attached herewith for illustration. The program allows for asymmetrical Bragg reflection from plane crystals and gives the profile of the reflected X-ray intensity. The raytracing code was applied for the calculations of Si(311) asymmetrically and symmetrically cut crystals. The angle of asymmetry was chosen to 15 and -15 degrees. In the figure 1 the comparative results between RAY and DIXI1 codes for the two polarisation states σ and π are shown. RAY results in this figure are represented by the noisy curve. The statistics is determined by the number of rays calculated. (1.000.000 incident rays, distributed into 100 channels).

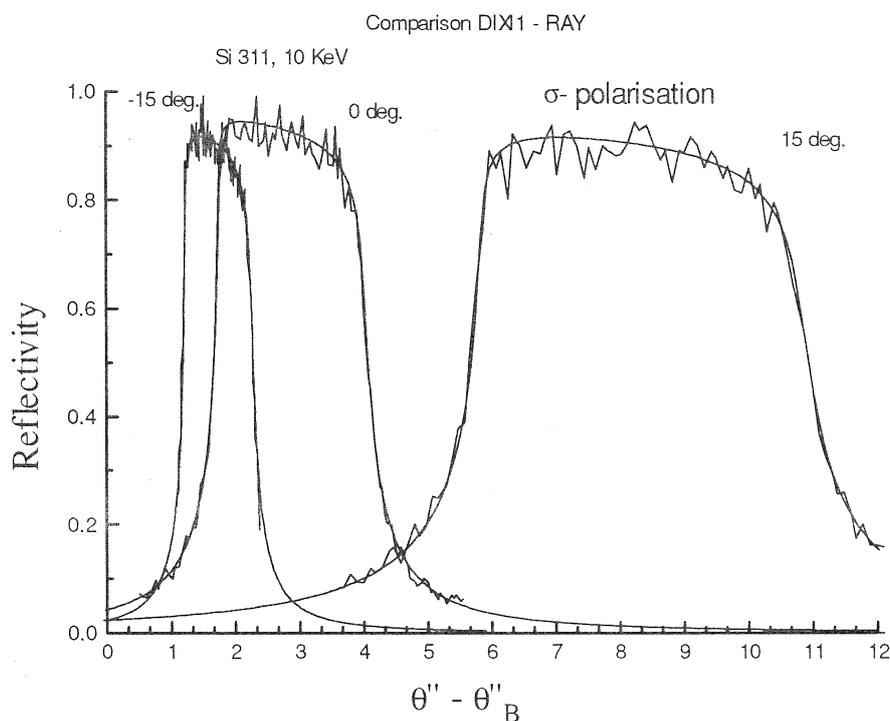


Fig.1a Rocking curves of Si(311) crystal with asymmetric cut (15° and -15° and symmetric cut (0°) for σ -polarisation. RAY code: statistical curve, DIXI1 code: solid line.

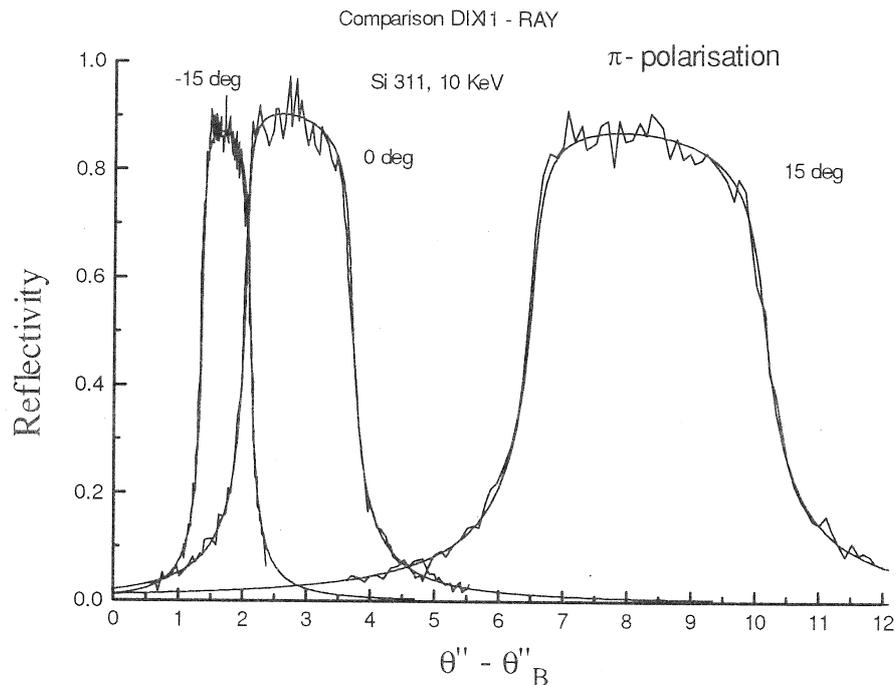


Fig.1b Rocking curves of Si(311) crystal with asymmetric cut (15° and -15° and symmetric cut (0°) for π -polarisation. RAY code: statistical curve, DIXI code: solid line.

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