Approximate calculation of multiple-diffraction patterns based on Renninger’s kinematical ‘simplest approach’

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1. Introduction

Multiple diffraction in the framework of the kinematical theory was first considered by Renninger (1937). In chapter 7 of his famous paper, two kinematical approaches are discussed, namely the ‘simplest approach’ (Einfachster Ansatz), which will be discussed in this paper, and a ‘more sophisticated approach’ (Verfeinerter Ansatz), which is similar to the approximate kinematical theories presented or used by Moon & Shull (1964), Zachariasen (1965), Coppens (1968), Caticha-Ellis (1969), Prager (1971), Parente & Caticha-Ellis (1974), Tanaka & Saito (1975), Post (1976), Chang (1982), Soejima et al. (1985), Bolotina et al. (1990), Parente et al. (1994) and Sasaki et al. (1996). All these authors considered multiple diffraction in imperfect crystals as an extension of the theory of secondary extinction by generalizing the power-transfer equations of two-beam cases. Interference effects as well as multiple diffraction (primary extinction) inside the coherent blocks of the mosaic crystal were neglected.

Kinematical multiple diffraction inside a perfect crystallite was recently considered by Woolfson & Fan (1995), taking into account the interference between the beam diffracted by the primary reflection and the Umweganregung beam.

In the early work of the author of this paper (program UMWEG; Rossmanith, 1985, 1986), interest in multiple diffraction was restricted to Umweganregung in the case of forbidden reflections. Clearly, neither Aufhellung nor interference effects are observable for these reflections. The main aim of the investigations was the determination of the weak intensities of ‘almost forbidden’ reflections caused by anharmonic thermal motion (Kumpat & Rossmanith, 1990) and space-group determination by means of systematically absent reflections (Rossmanith & Armbruster, 1995). To avoid intensity contributions caused by secondary reflections, in both cases measured Renninger scans (ω–Φ scan) were compared with theoretical multiple-diffraction patterns. The evaluation of these patterns requires the knowledge of the peak location (Cole et al., 1962), integrated intensities (Lorentz factors) and the width and shape of the intensity profiles obtained during a scan (Rossmanith, 1992; Rossmanith et al., 1990, 1994; Rossmanith & Bengel, 1995). Because of the fact that Aufhellung as well as interference effects are observable in the case of ‘almost forbidden’ reflections, the algorithm for the calculation of multiple-diffraction patterns was modified to account for these effects (Rossmanith, 1998, 1999). Aufhellung was considered in analogy to Umweganregung, i.e. the weakening of the incident beam caused by secondary reflections was neglected. The interference effect was considered following Woolfson & Fan (1995). Additionally, primary extinction was taken into consideration.

In this paper, the Aufhellung and Umweganregung terms will be calculated according to Renninger’s ‘simplest approach’. The interference term and primary extinction will be evaluated according to previous work (Rossmanith, 1998). It will be shown that using this concept, satisfactory agreement between experiment and theory can be obtained even for strong reflections for a mosaic crystal (diamond) as well as for a perfect crystal (silicon).

2. Kinematical approach for multiple diffraction

2.1. Renninger’s simplest approach

In Fig. 1 the geometry of multiple diffraction is shown. Intensity due to multiple diffraction is recorded in the counter if at least three reciprocal-lattice points lie simultaneously on the Ewald sphere. These are the zero point, O, of the lattice, the point A belonging to the primary reflection h_{\text{prim}} and the point B belonging to the operative reflection h_{\text{coop}}. The X-ray beam, incident parallel to s_0, is diffracted in the s_1 direction as well as in the s_2 direction. The sharing of the incident beam between the primary and the operative reflection causes weakening of the incident intensity with respect to the primary reflection. Furthermore, the reflected beam in the s_1 direction acts as the incident beam for the cooperative reflection −h_{\text{coop}}, which in turn reflects part of this beam in the s_2 direction. The corresponding intensity reduction of the primary reflection together with the weakening caused by the intensity sharing of
the incident intensity is called Aufhellung, $I_{\text{Auth}}$. On the other hand, the reflected beam in the $s_i$ direction acts as the incident beam for the cooperative reflection $h_{\text{coop}}$ which in turn reflects part of this beam in the $s_i$ direction. This intensity gain in $s_i$ direction is called Umweganregung, $I_{\text{Umweg}}$.

According to Renninger’s ‘simplest approach’ (Renninger, 1937, p. 161, ch. I, ‘Einfachster Ansatz’) the intensity (power) of the primary reflection in the three-beam case, $I_{\text{prim}}$, can be approximately expressed as

$$I_{\text{prim}} = I_0(k_{01} - k_{01}k_{02} - k_{01}k_{12} + k_{02}k_{21}),$$

(1)

where $I_0$ is the power of the incident beam and the $k_{ij}$ are dimensionless reflection coefficients for the reflection of the X-ray beam from the direction $s_i$ into the direction $s_j$ with $k_{ij} = k_{ji}$. The terms in the brackets in equation (1) correspond to the undisturbed primary reflection (first term), to the Aufhellung caused by the sharing of the incident beam (second term) as well as by the double diffraction (third term), and to the Umweganregung (fourth term). Following Renninger, the coefficient $k_{ij}$ is proportional to the integrated reflectivity $R_h^{(i)}$ of reflection $h$:

$$k_{ij} \approx R_h^{(i)}/\Delta \iota,$$

(2)

where $\Delta \iota$ is the width of the reflection with respect to the rotation axis $\iota$. Consequently, the total power received in the counter during the rotation about the $\omega$ and $\psi$ axes (Fig. 1), i.e. the intensities $I_{\text{prim}}(\omega, \psi)$, $I_{\text{Umweg}}(\omega, \psi)$ and $I_{\text{Auth}}(\omega, \psi)$, can be represented by

$$I_{\text{prim}}(\omega, \psi) = I_{\text{prim}}^{(\omega, \psi)} f(\omega),$$

(10)

$$I_{\text{Umweg}}(\omega, \psi) = I_{\text{Umweg}}^{(\omega, \psi)} f(\omega, \psi),$$

(11)

$$I_{\text{Auth}}(\omega, \psi) = I_{\text{Auth}}^{(\omega, \psi)} f(\omega, \psi),$$

(12)

Using the kinematical extinction length, $\Lambda_h$ defined by (Rossmanith, 2000, abbreviated Ro-00 hereinafter)

$$1/\Lambda_h = r_0 \lambda |F_h| K/V_{\text{cell}},$$

(4)

($r_0$ is the classical electron radius, $\lambda$ is the wavelength of the radiation used for diffraction, $F_h$ is the structure factor, $V_{\text{cell}}$ is the volume of the unit cell and $K$ is the polarization coefficient for the parallel and perpendicular component of the X-ray electric field), in the framework of the kinematical theory, the reflectivity integrated with respect to the rotation axis $\iota$ can be expressed as [von Laue, 1960, equation (18.38) therein]

$$R_h^{(\iota)} = I_h^{(\iota)}/I_0q_s = (\lambda L_s/\Lambda_h^2)q_s,$$

(5)

where $I_h^{(\iota)}$ is the intensity (power) of the reflection $h$ integrated with respect to $\iota$, $L_s$ is the Lorentz factor corresponding to the rotation about the $\iota$ axis and $I_0$ is the incident intensity (energy s$^{-1}$ cm$^{-2}$) and $q_s$ is the cross section of the crystal volume normal to the incident beam, i.e. $I_0q_s = I_0$, the incident power. The mean thickness of the crystal sample in the direction of the incident beam, $t_s$, is defined by

$$t_s = V_{\text{cry}}/q_s,$$

(6)

where $V_{\text{cry}}$ is the crystal volume and $q_s$ is the cross section of the crystal volume normal to the beam incident in the $s_i$ direction. Consequently, $I_{\text{prim}}^{(\omega, \psi)}$, $I_{\text{Auth}}^{(\omega, \psi)}$ and $I_{\text{Umweg}}^{(\omega, \psi)}$ are given by

$$I_{\text{prim}}^{(\omega, \psi)} = (I_0q_s)(\lambda L_s h_{\text{prim}}/\Lambda_h^2),$$

(7)

$$I_{\text{Umweg}}^{(\omega, \psi)} = (I_0q_s)(\lambda L_s h_{\text{Umweg}}/\Lambda_h^2),$$

(8)

and

$$I_{\text{Auth}}^{(\omega, \psi)} = (I_0q_s)(\lambda L_s h_{\text{Auth}}/\Lambda_h^2).$$

(9)

for all crystal shapes.

### 2.2. Phase dependence of the multiple-diffraction pattern

According to the previous section, the step intensities for particular $\omega$ and $\psi$ values during the rotation about the $\omega$ and $\psi$ axes (Fig. 1), i.e. the intensities $I_{\text{prim}}(\omega, \psi)$, $I_{\text{Umweg}}(\omega, \psi)$ and $I_{\text{Auth}}(\omega, \psi)$, can be represented by

$$I_{\text{prim}}(\omega, \psi) = I_{\text{prim}}^{(\omega, \psi)} f(\omega),$$

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$$I_{\text{Umweg}}(\omega, \psi) = I_{\text{Umweg}}^{(\omega, \psi)} f(\omega, \psi),$$

(11)

$$I_{\text{Auth}}(\omega, \psi) = I_{\text{Auth}}^{(\omega, \psi)} f(\omega, \psi),$$

(12)

and

$$\int f(\omega) d\omega = \int f(\omega, \psi) d\omega d\psi = 1.$$ 

(13)

In the case of multiple diffraction, i.e. when all three reflections are non-forbidden, there are two beams in the $s_i$ direction, the beam caused by the primary reflection $I_{\text{prim}}(\omega)$, reduced by $I_{\text{Auth}}(\omega, \psi)$, and the Umweganregung beam $I_{\text{Umweg}}(\omega, \psi)$. Because of the fact that for a particular $s_i$ direction the phase difference $\varphi(\omega, \psi)$ between the two beams in the $s_i$ direction is constant, they interfere with each other. The power recorded in the counter during the rotation about the $\psi$ axis can therefore be expressed as [Klein & Furtak, 1988].
\[ I_1(\omega, \psi) = I_{\text{prim}}(\omega, \psi) - I_{\text{Auth}}(\omega, \psi) + I_{\text{Umweg}}(\omega, \psi) + I_{\text{interfer}}(\omega, \psi), \]  
where the interference term \( I_{\text{interfer}}(\omega, \psi) \) is defined by

\[ I_{\text{interfer}}(\omega, \psi) = 2(1 - I_{\text{prim}}(\omega, \psi)) I_{\text{Umweg}}(\omega, \psi) \left( \frac{1}{2} \cos \varphi(\psi) \right)^{1/2}. \]  

The phase difference in (15) is defined by \( \varphi(\omega, \psi) \) and \( \varphi_0(\omega, \psi) \), which are the phases of the corresponding structure factors, and \( \varphi_{\text{coop}}(\omega, \psi) \) is the scattering phase shift deduced in the framework of the kinematical theory by Woolfson & Fan (1995).

The expressions given in this section are valid for all crystal shapes.

3. Approximations applied for comparison with experimental results

To simplify the mathematical treatment and the comparability with experimental results, approximations have to be applied to the evaluation of multiple-diffraction patterns.

3.1. Intensity distribution and scattering phase shift

Because of mechanical shortcomings, with standard four-circle diffractometers it is nearly impossible to measure the intensity \( I_1(\omega, \psi) \) of perfect crystals by the \( \omega-\psi \) scanning technique with satisfactory precision. This will be demonstrated in a forthcoming paper. The ‘experimental multiple-diffraction pattern’ presented in the graphical output of UMWEG99 (a program for the calculation and graphical representation of multiple-diffraction patterns) is therefore obtained by integrating the measured step intensities \( I_1(\omega, \psi) \) with respect to \( \omega \) and plotting the integrated intensity against \( \psi \). For comparability, it is therefore assumed in a very first approximation that the two-dimensional distribution function \( f(\omega, \psi) \) used in equations (11) and (12) can be expressed as the product of two one-dimensional distribution functions, i.e. it is assumed that the distribution functions \( f(\omega) \) and \( f(\psi) \) are independent of each other:

\[ \int f(\omega, \psi) \, d\omega \, d\psi = \int f(\omega) \, d\omega \int f(\psi) \, d\psi = 1. \]  

Taking into account equation (17) and integrating (11) and (12) with respect to \( \omega \), one obtains

\[ I_{\text{Umweg}}^{(\omega)}(\psi) = I_{\text{Umweg}}^{(\omega)}(\psi), \]

and

\[ I_{\text{Auth}}^{(\psi)}(\psi) = I_{\text{Auth}}^{(\omega)}(\psi), \]

are obtained and equations (14) to (16) can be replaced by

\[ I_{\text{interfer}}^{(\psi)}(\psi) = 2(1 - I_{\text{prim}}^{(\omega)}(\psi)) I_{\text{Umweg}}^{(\omega)}(\psi) \left( \frac{1}{2} \cos \varphi(\psi) \right)^{1/2}. \]  

3.2. Intensity distribution and scattering phase shift for a perfect crystal in a real experiment

In a real experiment, the incident beam is neither exactly monochromatic nor exactly parallel. The shape, \( f(\psi) \), as well as the integral width, \( \Delta \psi_{\text{integral}} \), of the intensity profile therefore not only depend on the shape and magnitude of the perfect crystal sample but are additionally influenced by the divergence, \( \delta \), and wavelength spread, \( \Delta \lambda/\lambda \), of the incident beam. To simplify mathematical treatment, for the distribution functions \( f(\omega), f(\psi) \), normalized Gaussian-, Lorentzian- or pseudo-Voigt functions are used in UMWEG99:

\[ f(x) = \frac{1}{1 + \left( x - x_0 \right)^2 \Delta x_{\text{integral}}} + \frac{\eta}{1 + \left( \left( x - x_0 \right)^2 \Delta x_{\text{integral}} \right)^2} \]

where \( \eta \) is a measure of the Lorentzian contribution to the pseudo-Voigt distribution, \( x \) has to be replaced by the variables \( \omega \) and \( \psi \), respectively, caused by the divergence, \( \delta \), and wavelength spread, \( \Delta \lambda/\lambda \), of the incident beam and the size of the perfect crystal sample (Rossmanith, 1992). In UMWEG99, the corresponding scattering phase shift is approximated by (Ro-98):

\[ \varphi_{0-\pi}(\psi) = \pi/2 + \arctan[(\psi_0 - \psi)/\Delta \psi_{\text{integral}}]. \]

3.3. Mean path length and extinction correction

The expressions given in the previous sections are only valid for tiny crystals, i.e. for the case that \( l_s \ll \Lambda_a \). According to Ro-98 and Ro-00, in all other cases the mean path lengths \( l_s \) have to be replaced by \( l_s^{\text{eff}} = l_s (1 - c) \), where \( c \) is the crystal-shape- and reflection-dependent primary-extinction correction factor discussed in Ro-00. Approximations for the primary-extinction correction in the case of double diffraction, used in UMWEG99, are given in Ro-98.

4. Comparison with experiment

The experiments (Rossmanith et al., 1999) were performed at HASYLAB (DESY, Hamburg, Germany) in the manner described in Ro-99. Multiple-diffraction patterns of the strong 115 reflection (silicon, perfect spherical crystal with radius \( r = 84 \mu m \rightarrow l_s \gg \Lambda_a \), severe primary extinction, cell parameter \( a = 5.43 \AA \), wavelength of the synchrotron radiation \( \lambda = 1.4375 \AA, a/\lambda = 3.777 \)) and the strong 1 5 1 reflection (diamond, ideally imperfect octahedrally shaped crystal with a diameter...
of about 500 μm, a mosaic block radius $r = 0.15 \text{μm}$ and mosaic spread equal to $0.05^\circ \rightarrow I_e \ll \Lambda_h$, negligible primary extinction, cell parameter $a = 3.5646 \text{Å}$, wavelength of the synchrotron radiation $\lambda = 0.9440 \text{Å}, a/\lambda = 3.776$) are compared with theoretical patterns calculated with UMWEG99. It should be noted that the cell constant to wavelength ratios in the two cases are nearly equal. The patterns given in Figs. 3(a) and 3(b), as well as Figs. 4(a), 4(b) and 4(c), are therefore equivalent in the sense that the multiple-diffraction events are caused by equivalent pairs of operative/cooperative reflections (see Table 1), i.e. the corresponding $\psi-\lambda$ diagrams (lowest diagrams in the figures) are identical. The different shapes of the multiple-diffraction patterns obtained for silicon and diamond are mainly due to the different degrees of perfection of the two samples.

In Fig. 2, which presents the graphical output of UMWEG99 (see Ro-99 for details), the measured multiple-diffraction pattern of the strong 1Å 5Å 1Å reflection of diamond (upper scan) is compared with the theoretical pattern (lower scan). The dashed lines in the $\psi-\lambda$ diagram (lowest diagram of the figure) correspond to multiple-diffraction events with forbidden operative reflections. The weakening of the intensity of the primary reflection is therefore solely caused by the second term in the brackets of equation (9) (double diffraction $h_{\text{prim}}/h_{\text{coop}}$). The dash-dot lines in the $\psi-\lambda$ diagram correspond to multiple-diffraction events with forbidden cooperative reflections. For these multiple-diffraction events, the weakening of the intensity of the primary reflection is solely caused by the first term in the brackets of equation (9) (sharing of the incident intensity between the primary and operative reflection). In both cases, $I_{\text{Umweg}}(\omega, \psi)$ as well as $I_{\text{interf}}(\omega, \psi)$ are zero. Interference effects can therefore be expected solely for the solid lines in the $\psi-\lambda$ diagram corresponding to multiple-diffraction events with all three reflections being non-zero. Bearing in mind the many approximations used for the calculation of the theoretical pattern, as well as the inaccuracy of the $\omega-\psi$ scan caused by mechanical shortcomings of the four-circle diffractometer (this point will be discussed in detail in a forthcoming paper), the agreement between experiment and theory is satisfactory.

An enlargement of the intensity gap at $\psi_0 = 309.156^\circ$ in Fig. 2 (Aufhellung: $h_{\text{prim}}/h_{\text{coop}} = 1 5/1 1 0 4 2, F_{\text{prim}} = 7.10, F_{\text{coop}} = 16.92, F_{\text{coop}} = 0.0$) is shown in Fig. 3(a). The width of the gap is mainly due to the particle size effect (mosaic block radius = 0.15 μm) and mosaic spread of the cloudy natural diamond sample (see also Fig. 9 of Ro-99). The contribution caused by the wavelength spread and divergence of the synchrotron radiation is negligible. In Fig. 3(b), the equivalent gap of the Si sample is presented on the same $\psi$ scale ($h_{\text{prim}}/h_{\text{coop}} = 1 5/1 1 0 2 4, F_{\text{prim}} = 34.07, F_{\text{coop}} = 59.37, F_{\text{coop}} = 0.0$). In the case of the perfect spherical crystal, the contribution of the particle size effect to the width of the gap is small and the width is mainly caused by the wavelength spread and divergence of the synchrotron radiation.

Table 1

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<tr>
<th>$\psi_0$ ($^\circ$)</th>
<th>$h_{\text{coop}}$</th>
<th>$F_{\text{coop}}$</th>
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The solid lines in the $\psi-\lambda$ diagram corresponding to multiple-diffraction events with all three reflections being non-zero. Bearing in mind the many approximations used for the calculation of the theoretical pattern, as well as the inaccuracy of the $\omega-\psi$ scan caused by mechanical shortcomings of the four-circle diffractometer (this point will be discussed in detail in a forthcoming paper), the agreement between experiment and theory is satisfactory.

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Figure 2

Graphical output of UMWEG99. Ideal imperfect diamond crystal: multiple-diffraction pattern of the strong 1Å 5Å 1Å reflection. The upper diagram is the observed $\psi$ scan, the lower diagram is the calculated $\psi$ scan, and the diagram at the bottom of the figure is the $\psi-\lambda$ diagram (peak-location plot).
beam case. It was pointed out in Ro-98 and Ro-99 that four-beam cases are handled in UMWEG99 in a first approximation as the sum of two three-beam cases. Umweganregung and Aufhellung corresponding to the two events at $\psi_0 = 287.032^\circ$ nearly cancel each other. Because of the mosaicity of the crystal, an interference effect is hardly observable in the measured scan, as well as in the scan predicted by UMWEG99.

The interference effect manifests itself in the very small gap at $\psi = 286.95^\circ$ and the shifting of the peak maximum to the right. The Aufhellung gaps at $\psi_0 = 287.197$ and $\psi_0 = 287.369^\circ$ are solely caused by double diffraction $h_{\text{prim}}/h_{\text{coop}}$.

Although caused by equivalent reflections, the pattern obtained for the perfect Si crystal (Fig. 4b) differs considerably from that obtained for the mosaic diamond (Fig. 4a). The theoretical pattern presented in Fig. 4(b) is calculated taking into account the interference effect. For comparison, in Fig. 4(c) the theoretical pattern is calculated according to equation (3), i.e. neglecting the interference term in equation (14). The calculated Aufhellung gaps at $\psi_0 = 252.710$ and $\psi_0 = 252.865^\circ$ agree well with the observation. On the other hand, the peak at $\psi_0 = 252.562^\circ$ in Fig. 4(c) is very small because of the cancellation of the corresponding Umweganregung and Aufhellung terms (Table 1). It can therefore be concluded from comparison of Figs. 4(b) and 4(c) that the pattern at $\psi_0 = 252.562^\circ$ is almost entirely determined by the interference term in equation (14). The overestimation of the corresponding intensity, $I_{\text{interfer}}$, is very probably caused by the approximations introduced in equations (17)–(24), i.e. using intensities integrated with respect to $\omega$ instead of the step intensities defined in equations (10)–(16). This can easily be deduced from contour plots of measured $\omega$–$\psi$ scans for perfect crystals. This point will be discussed in detail in a forthcoming paper where additional experimental results on diamond, silicon and germanium will be presented.

5. Conclusions

On the basis of Renninger’s kinematical ‘simplest approach’, expressions have been deduced for the simulation of multiple diffraction patterns, valid even for strong reflections. It is shown in this paper that, despite the many approximations made, satisfactory qualitative and even quantitative agreement is obtained between measured and evaluated $\psi$ scans for mosaic as well as for perfect crystal samples.
Figure 4
Graphical output of UMWEG99. (a) Ideal imperfect diamond crystal: multiple-diffraction pattern of the strong 1 5 1 reflection. (b) Perfect silicon crystal: multiple-diffraction pattern of the strong 1 1 5 reflection. In (a) and (b), the upper diagram gives the observed $\psi$ scan, the lower diagram is the calculated $\psi$ scan, and the diagram at the bottom is the $\psi-\lambda$ diagram (peak-location plot). (c) Perfect silicon crystal: multiple-diffraction pattern of the strong 1 1 5 reflection. The upper diagram is the observed $\psi$ scan, the lower diagram is the calculated $\psi$ scan neglecting the interference term, and the diagram at the bottom is the $\psi-\lambda$ diagram (peak-location plot).
Information about the availability of the program can be obtained via http://www.rrz.uni-hamburg.de/mpi/rossmanith. The project was funded by the Deutsche Forschungsgemeinschaft.

References


