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Abstract

The calculated intensities of the X-ray beam behind the exit surface of the Ge [440, 220] dispersive monolithic monochromator for Co Kα1 radiation are presented. The reflections 440 and 220 resulting from Ge {000, 440, 260, 220} coplanar four-beam diffraction were taken into account and the influence of the π/2 reflection 260 is discussed. The four-surface arrangement of Ge [440, 220] providing the resultant beam parallel to the incident beam is considered. For comparison Ge [440, 220] in the two-beam approximation is solved. The obtained results demonstrate that the four-beam basis of diffraction affects the resultant beam. The quality of the X-ray beam evaluated behind the examined monochromators also provided the conditions for the use of such monochromators as wavelength standards.

1. Introduction

On the surfaces of a dispersive monolithic monochromator (e.g. Deslattes, 1968; Hart, 1971; Beaumont & Hart, 1974; Petroff, Sauvage, Riglet & Hashizume, 1980) a many-beam diffraction occurs. In this paper we deal with the dispersive monolithic monochromator Ge [440, 220]. We chose the case when coplanar Ge {000, 440, 260, 220} four-beam diffraction (Fig. 1) on the surfaces of this monochromator takes place. Some introductory remarks referring to Ge {000, 440, 260, 220} can be found in Pacherová & Bubáková (1982). Here we shall give the basic information about our procedure for solving the case of Ge [440, 220] and its useful variant Ge [440, 440, 220, 220].

The basic expressions for the dynamic solution of many-beam diffraction have been taken from Penning & Polder (1968). Our calculation of the coplanar four-beam diffraction Ge {000, 440, 260, 220} is based on the following assumptions. The incident X-ray wave is monochromatic and plane. The diffracting crystal is assumed to be perfect, absorbing X-radiation and bounded by only one plane boundary. The boundary is oriented in two ways – parallel to the (440) or to the (220) diffracting planes [surface (110) or (1T0)]. The coplanar four-beam diffraction Ge {000, 440, 260, 220} is supposed to take place even if the Bragg condition is not exactly satisfied for all participating diffractions 440, 260 and 220 at the same time. Then the coplanar Ge {000, 440, 260, 220} holds not only for \( k_{\text{m}} \) (see Fig. 1), but also for an interval of values of \( k \) in the neighbourhood of the value \( k_{\text{m}} \). In our calculation we have employed some common practices used in solving problems in dynamic diffraction. They are recapitulated in Appendix A.

For a comparison we solved Ge [440, 220] also in the two-beam approximation. The diffraction participating in a dispersive monolithic monochromator is considered in this case as the usual two-beam diffraction. The purpose of this paper is to find the range of validity of this simpler calculation for description of the properties of the dispersive monolithic monochromator.

We used for the calculation the constants as follows (\( a_0 \) lattice constant, \( F_{\text{kl}} \) real part of the Fourier sum of the structure factor, \( m \) mass absorption coefficient, \( \psi_{\text{kl}} \) imaginary part of the term of the Fourier sum of the susceptibility):

\[
\begin{align*}
a_0 &= 0.565745 \text{ nm} \quad (\rightarrow k_{\text{m}} = 35.1203 \text{ nm}^{-1}) \\
F_0 &= 249.20 \quad (f' = -0.85; \text{Cromer, 1976}) \\
F_{220} &= 190.32 \\
F_{440} &= 129.84 \\
F_{260} &= 117.92
\end{align*}
\]

\( a_0 \) and \( k_{\text{m}} \) are the lattice constant and the radius of the Ewald sphere for the coplanar four-beam diffraction Ge {000, 440, 260, 220}.
The Ge [440, 220] monolithic monochromator works as a double-crystal spectrometer with the mutual adjustment of its two crystals. Both crystals of this double-crystal model are in a many-beam diffraction position. Nevertheless, the first view of solving the dispersive monolithic monochromator can provide the two-beam approximation thanks to the well-known graphical solution of DuMond (1937). Owing to the mutual adjustment of the two crystals of the double-crystal model the mutual position of the corresponding reflection bands is constant and therefore the so-called spectral window is also constant. When π/2 reflection* is involved in the many-beam diffraction, 'oscillation' of radiation between the two crystals occurs. Therefore, the double-crystal model has to be replaced in such a case by a series of many-crystal devices.

Ge [440, 220] is of this type. It is schematically drawn in Fig. 2. The entrance surface is in this case (110) and the exit surface is (110). This choice of the adjustment to the incident wave has no importance for the results, so that they are valid also for the opposite case, namely Ge [220, 440]. The indexing of the resulting waves in Fig. 2 and in the text corresponds to the number of successive reflections inside the two-surface monochromator, i.e. corresponds to the number of crystals in the given many-crystal model.

Now the treatment of the resulting waves of Ge [440, 220] follows.

We have calculated two sets of reflection curves† for Ge {000, 440, 260, 220} for several values of Δk = k - k_m:

1. reflection curves corresponding to reflections 440 and 260 at the surface (110), namely 440 (θ_B4 + φ), 260 (θ_B2 + φ); and
2. reflection curves corresponding to reflections 220 and 260 at the surface (110), namely 220 (θ_B2 + φ), 260 (θ_B2 + φ). The symbols θ_B4 and θ_B2 stand for θ_B4_{440} and θ_B2_{220} and mean the Bragg angles for diffractions Ge {000, 440} and Ge {000, 220}. Their values for k_m are θ_B4_{440} and θ_B2_{220}. It can be seen from Fig. 1 that θ_B4_{440} + θ_B2_{220} = π/2. Generally, θ_B4 + θ_B2 = π/2 - δ = θ_B4 + θ_B2 - δ. i.e. δ = (θ_B4 - θ_B4_{440}) + (θ_B2 - θ_B2_{220}) = 2Δk/k_m + Δk/2k_m = 5Δk/2k_m.

The reflection coefficients belonging to the waves Qn and Rn resulting from Ge [440, 220] (see Fig. 2) are determined from the expressions given below (++, +). The change of the direction of the incident wave on a particular surface is expressed by the substitution of the quadruplet of the reciprocal-lattice points 000, 440, 260 and 220 by the equivalent quadruplets describing the same four-beam diffraction – see Fig. 3. The glancing angles of reflection of the resulting waves and the glancing angles of incidence of the participating successive reflections are given in parentheses.

We have derived the following from the geometrical considerations‡ (the glancing angle of the incident wave P is θ_B4_{440} + φ).

* The reflection curves in this paper present the reflection coefficient plotted as a function of the incident angle θ. See Appendix A, paragraph 3.

† The derivation of the expressions for the intensities of the waves R1, Q2, R3 and Q4 is given in Appendix B.

‡ The glancing angle of the incident wave P is θ_B4_{440} + φ.
**A. Double-crystal model** $N = 2$: (+)

\[ Q_2(\theta_{440}^m - \varphi) = 440(\theta_{440}^m + \varphi) \times 220(\theta_{220}^m - \varphi). \]

In the two-beam approximation this relation expresses $Q_2^{(2)}$.

**B. Many-crystal model**: (+ +)

For the waves $Q_N$, $N$ is even, $N = 4, 6, \ldots$, for the waves $R_N$, $N$ is odd, $N = 3, 5, \ldots$.

\[ Q_N[\theta_{440}^m - (N - 2)\beta - \varphi] = 440(\theta_{440}^m + \varphi) \times 220(\theta_{220}^m - \varphi) \]

\[ R_N[\theta_{220}^m - (N - 2)\beta - \varphi] = 440(\theta_{440}^m + \varphi) \times 220(\theta_{220}^m - \varphi). \]

For $R_3$, by definition,

\[ \prod_{M=3}^{1} [620 \times 620] = 1. \]

The beam $R$ is completed by the $\pi/2$ reflection of the incident wave $P$ on the entrance surface ($N = 1$):

\[ R_1(\theta_{440}^m + 0.4\beta - \varphi) = 260(\theta_{440}^m + \varphi). \]

**3. The evaluation of $Q_N$, $N = 2, 4, 6, \ldots$**

The mutual position of the reflection curves $440, 220, 620$ and $620$ participating in $Q_2^{(2)}$, $Q_2$ and $Q_4$ given by equations (+), (+ +) is shown for several values of $\Delta k$ in Figs. 4, 5.

As to $Q_2^{(2)}$, the overlapping of the intensive parts of $440$ and $220$ (i.e. spectral window) occurs at $\Delta k \sim 1.2 \mu m^{-1}$, so that we can expect considerable intensities of $Q_2^{(2)}$ [$Q_2^{(2)} = 440 \times 220$] in this region. The same is true for the four-beam $Q_2$, too.

Now we deal with $Q_4$. We can estimate from Fig. 5 that there are some small contributions to $Q_4$ ($Q_4 = 440 \times 220 \times 220$) only for the values of $\Delta k \sim 0.8 \mu m^{-1}$ as a consequence of the considerable broadness of $440$ and $220$. However, in the region of the essential overlapping of $440$ and $220$ at $\Delta k \sim -1.2 \mu m^{-1}$ $Q_4$ is negligible because of very low values of $620$ and $220$.

It can be seen from the mutual position of the reflection curves participating in $Q_N$, $N = 6, 8, \ldots$, that the circumstances for obtaining them ($Q_N = 440 \times 620 \times 220$) are even more unfavourable than for $Q_4$. Therefore, the exit beam of Ge [440, 220] can be considered to be created only by wave $Q_2$ corresponding to the double-crystal model. The difference between the exit beams when the four-beam diffraction is taken into account and in the two-beam approximation is thus caused only by the different shape of the four-beam and two-beam reflection curves $440$ and $220$.

**4. The monolithic monochromator in the arrangement Ge [440, 440, 220, 220]**

It is apparent from Fig. 2 that the resulting beam $Q$ of Ge [440, 220] is directed against the incident wave $P$. The modification Ge [440, 440, 220, 220] of the examined monolithic monochromator outlined in Fig. 6 gives the exit beam parallel to the incident one. The expressions for $Q'$ and $R'$ behind the new exit surface and in front of the new entrance surface have the following forms:

\[ Q_4[\theta_{440}^m - (\beta - 1.4)\beta - \varphi] = 440(\theta_{440}^m + \varphi) \times 220(\theta_{220}^m - \varphi) \]

\[ R_4[\theta_{220}^m - (\beta - 1.4)\beta - \varphi] = 440(\theta_{440}^m + \varphi) \times 220(\theta_{220}^m - \varphi) \]

\[ \times 440(\theta_{440}^m + \varphi) \times C_4[ P \cdot \cdot \cdot C_2 Q_2 ] \]

\[ = Q_4[\theta_{440}^m - \varphi] \times C_4[ P ] \times C_2 Q_2 ] \]

\[ = Q_4[\theta_{440}^m - \varphi] \times C_4[ P ] \times C_2 Q_2 ] \]

*We can imagine pictures similar to Fig. 5. The position of the reflection curves $440$ is for all $Q_n$ the same as in Fig. 5. However, the position of the reflection curve $220$ participating in $Q_n - 2$ is shifted with respect to $220$ participating in $Q_n$ by the distance $2\varphi$. In the region $\Delta k > 0$, where the reflections $620$ and $620$ have considerable values, the reflection curves $220$ are shifted with increasing $N$ to the left. This is the reason why the distance between the intensive parts of the reflection curves $440$ and $220$ increases.

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**Fig. 4.** Graphic representation of the expression for $Q_2^{(2)}$ - the angular dependences for several values of $\Delta k$. — Two-beam reflection curve $440$; --- two-beam reflection curve $220$. The position of the significant angles of incidence: $\theta$, Bragg angle $\theta_{ba}^m$ - the fixed point of the angular scale; $\circ$, Bragg angle $\theta_{ba}^m$ and the angle $\theta_{ba} + \beta$ [Bragg angle $\theta_{ba}$ on the surface (110)]. The length of the horizontal axes is equal to 1.
\[ Q_N[\theta_{B4} - (N - 2)\theta - \varphi] = Q_N[\theta_{B4} - (N - 2)\theta - \varphi] \times 440(\theta_{B4} + \varphi) \times 220(\theta_{B4} - (N - 2)\theta - \varphi) \times C_4 |P| \times C_2 |Q_N| \times \prod_{M = 2, \text{even}}^{N-2} (c_2 |Q_M| \times c_4 |R_M + 1|) \]

\[ R'_1(\theta_{B4} + 0.4\theta - \varphi) = 620(\theta_{B4} + \varphi) \]

\[ R'_N[\theta_{B4} - (N - 1.4)\theta - \varphi] = R_N[\theta_{B4} - (N - 1.4)\theta - \varphi] \times 440(\theta_{B4} + \varphi) \times 440(\theta_{B4} - (N - 1.4)\theta - \varphi) \times C_4 |P| \times C_4 |R_N| \times c_2 |C_N - 1| \times \prod_{M = 3, \text{odd}}^{N-2} (c_2 |Q_M - 1| \times c_4 |R_M|) \]

The coefficients \( C_4 \) and \( C_2 \) originate from the oscillation of radiation due to the reflections 260 and 260 between the parallel surfaces of Ge \([440, 440, 220, 220]\), the wave in the brackets is the incident wave for this oscillation. They are:

\[ C_4 |R_N| = \sum_{M = 1}^{\infty} \{260[\theta_{B4} - (N - 1.4)\theta - \varphi] \times 260[\theta_{B4} + (N - 1)\theta + \varphi]\} + 1 \]

\[ C_2 |Q_N| = \sum_{M = 1}^{\infty} \{260[\theta_{B4} + (N - 0.4)\theta + \varphi]\}

Because of the symmetry of the reflection curves 260 around the values \( \theta_{B4} + 0.8\theta \) or \( \theta_{B4} + 0.2\theta \) the coefficients \( C_4 \) and \( C_2 \) can be written as

\[ C_4 |R_N| = \sum_{M = 1}^{\infty} \{260[\theta_{B4} + (N - 1)\theta + \varphi]\}^2 + 1 \]

\[ C_2 |Q_N| = \sum_{M = 1}^{\infty} \{260[\theta_{B4} + (N - 0.4)\theta + \varphi]\}^2 + 1 \]

The surfaces \((\overline{1}10)\) and \((\overline{1}10)\) of Ge \([440, 440, 220, 220]\) not only change the direction of the resulting beam but they also affect the wave field between the surfaces \((110)\) and \((\overline{1}10)\) because of reflections 260. The coefficients \( c_4 \) and \( c_2 \) express this additional action of the surfaces \((\overline{1}10)\) and \((\overline{1}10)\). They are:

\[ c_4 |R_N| = 440[\theta_{B4} - (N - 1.4)\theta - \varphi] \times 440[\theta_{B4} + (N - 1)\theta + \varphi] \times C_4 |R_N| + 1 \]

\[ c_2 |Q_N| = 220[\theta_{B4} - (N - 2)\theta - \varphi] \times 220[\theta_{B4} + (N - 0.4)\theta + \varphi] \times C_2 |Q_N| + 1 \]

Fig. 5. Graphic representation of the expressions for \( Q_2 \) and \( Q_4 \) – the angular dependences for several values of \( \Delta k \) and real four-beam reflection curves for \((a)\) \( \sigma \) polarization, \((b)\) \( \pi \) polarization. – reflection curve 444; – reflection curve 220 \((N = 2)\); – reflection curve 220 \((N = 4)\); – reflection curves 620 \((N = 4)\) and 620 \((N = 2)\). See Fig. 4 caption \((N = 4): \theta_{B4} - \delta \rightarrow \theta_{B3}\).
The quantitative analysis of the effect of $C_4$, $C_2$, $c_4$ and $c_2$ (all are $\geq 1$) shows that these coefficients are not large enough to influence the development of $Q_N$, $N \geq 4$. Therefore, we will also deal in the case of Ge $[440, 440, 220, 220]$ with $Q_2$ only.

The effect of $C_4[P]$ and $C_2[Q_2]$ on $Q_2$ is also very small. The influence is observable for $\Delta k \sim (0.5 - 0.8) \mu m^{-1}$ but only to the extent given in Fig. 7. For the purpose of this paper it is therefore sufficient to take for the resulting beam of Ge $[440, 440, 220, 220]$ the simple wave $Q_2^2 = 440 \times 440 \times 220 \times 220 = [Q_2]^2$.

In the two-beam approximation we have $Q_2^2 = [Q_2^{(2)}]^2$. So we come to the same result as in the case of Ge $[440, 220]$. The difference between the resulting beams when the four-beam diffraction is taken into account and in the two-beam approximation is caused only by the different shape of the corresponding reflection curves.

5. The resulting dependences for Ge $[440, 220]$ and for Ge $[440, 440, 220, 220]$

The exit beam of Ge $[440, 220]$ is in the two-beam approximation identical with the wave $Q_2^{(2)}$ and also in the four-beam case it is practically the wave $Q_2$. The values of $Q_2^{(2)}$ and $Q_2$ plotted as functions of incident angle $\theta$ are shown in Figs. 8 and 9. The similar dependences for the exit beam of Ge $[440, 440, 220, 220]$ are given by the mathematical operations $Q_2^{(2)} = [Q_2^{(2)}]^2$ and $Q_2^{(2)} = [Q_2]^2$.

When using Ge $[440, 220]$ and Ge $[440, 440, 220, 220]$ we can evaluate two extreme cases concerning the incident beam of white radiation.

In the first case the divergence of the incident beam is higher than that of the beams which are transmitted by the monolithic monochromators Ge $[440, 220]$ and Ge $[440, 440, 220, 220]$. The integrated intensities of $Q_2$ and $Q_2^{(2)}$ are shown in Fig. 10. For a comparison the integrated intensities of the reflection curves 440 and 220 resulting from Ge $[000, 440, 260, 220]$ are shown in Fig. 11 as well.

In the second extreme case the incident beam is parallel. The graphic representations of equation (+) for $Q_2^{(2)}$ and $Q_2$ are for several angles of incidence $\theta + \Delta \theta$ shown in Figs. 12 and 13. The wave distributions in the exit beams of Ge $[440, 440, 220, 220]$ $Q_2^{(2)}$ and $Q_2$ are evaluated in Figs. 14 and 15. The scale in $\Delta \lambda = \lambda - \lambda_m$ is given from the equation $\lambda = 2 \pi /k$.

6. Results

On the basis of the coplanar four-beam diffraction Ge $[000, 440, 260, 220]$ we have calculated the wave and angular dependences (the dependences on $k$, $\theta$ constant and the dependences on $\theta$, $k$ constant) of the intensity behind the two-surface monolithic mono-
chromator Ge [440, 220] and behind the four-surface monolithic monochromator Ge [440, 440, 220, 220]. The surfaces of these monolithic monochromators are supposed to be parallel with the lattice planes (110) and (110) (Ge [440, 220]) or with (T10), (110), (110) and (110) (Ge [440, 440, 220, 220]).

The examined monochromators are transmitting radiation with wavelengths from 0.178882 to 0.178906 nm (σ) and from 0.178889 to 0.178902 nm (π) and for angles of incidence from 63°25′35″ to 63°26′35″ (σ) and from 63°25′40″ to 63°26′0″ (π). We have set the properties of the examined monolithic monochromators in the two extreme cases: the incident beam of white X-ray radiation is divergent in the first case and parallel in the second case.

If the divergence of the incident beam is ≥ 1′, which is considerable, the wave dependence of the integrated intensity of the resulting beam gives the maximum value for the wavelength λ0 = 0.178895 nm (σ polarization) or λ0 = 0.178897 nm (π polarization). The decrease of the integrated intensity to 10% of its maximum value occurs for the values λ0 ± 7 × 10⁻⁶ nm (σ) and λ0 ± 5 × 10⁻⁶ nm (π). On the long-wavelength side of the peak the decrease is not monotonic, there is a local maximum for both σ and π polarizations.

If the incident beam is parallel, the wave dependence of the intensity of the resulting beam is different for various adjustments of the monolithic monochromator to the incident beam.

It is possible to find such an adjustment of the monochromator that the wavelength λ0 = 0.178900 nm for σ polarization significantly rises from a broad maximum at shorter wavelengths. The maximum of the intensity in this special adjustment is, in the case of Ge [440, 440, 220, 220], 50% of the incident intensity, the intensity of the broad maximum reaches 35%

![Fig. 8](image_url)  
**Fig. 8.** The angular dependences of \( Q(2\theta) \) for several values of \( \Delta k \). The scale of \( Q(2\theta) \) is given on the curve for \( \Delta k = 0.75 \mu m^{-1} \) and σ polarization.

![Fig. 9](image_url)  
**Fig. 9.** The angular dependences of \( Q_2 \) for several values of \( \Delta k \). The scale of \( Q_2 \) is given on the curve for \( \Delta k = 0.55 \mu m^{-1} \) and σ polarization.

![Fig. 10](image_url)  
**Fig. 10.** The integrated intensities of \( Q_2 \) and \( Q(2\theta) \): --- \( Q_2 \); --- \( Q(2\theta) \). The scale of \( A \) (arbitrary units) is designated by the area under a Darwin reflection curve approximated to a rectangle plotted to the right.
of the incident intensity. The value of 10% of the maximum value is reached at the wavelength equal to \( \lambda_0 + (0.5 \times 10^{-6}) \) and \( \lambda_0 - (7 \times 10^{-6}) \) nm, the decrease of the intensity to the broad maximum level occurs at \( \lambda_0 - (1.5 \times 10^{-6}) \) nm.

For comparison we have solved Ge [440, 220] and Ge [440, 440, 220, 220] in the two-beam approximation. The difference between the exit beams when the four-beam diffraction is taken into account and in the two-beam approximation is practically expressed by the different shapes of the four-beam and two-beam reflection curves 440 and 220, only.

In this approximation the maximum of the integrated intensity for \( \sigma \) and \( \pi \) polarizations is shifted to the longer wavelengths by about \( 2.7 \times 10^{-6} \) and \( 1.0 \times 10^{-6} \) nm, respectively, and the peak is smooth. The resulting dependences in the case of parallel radiation are free from the broad maximum on the short-wavelength side and the maximum values are higher (up to 85% of the incident intensity). Apart from these differences the characteristic features of the resulting dependences are similar as in the four-beam case.

The results obtained describe the quality of the X-ray beam behind the monochromators examined as do their conditions of use as a wavelength standard for \( \lambda = 0.17890 \) nm.

In conclusion, we note that the monolithic monochromators Ge [440, 220] and Ge [440, 440, 220, 220] are also transmitting radiation with wavelengths \( \approx \lambda_0/2 \) owing to the eight-beam coplanar diffraction Ge \( \{000, 440, 840, 880, 4.12.0, 0.12.0, 480, 440\} \). We did not study this many-beam diffraction. This fact does not influence the conclusions listed above concerning the wavelengths around \( \lambda_0 \).

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**APPENDIX A**

1. The fundamental equations of the dynamical solution of \( n \)-beam diffraction (Penning & Polder, 1968, equation 3.8) can be arranged for a coplanar diffraction as follows:

\[
\sum_{j=1}^{n} A_{ij} Y_j = 0; \quad \sum_{j=1}^{n} A_{ij}(u_j, u) X_j = 0, \quad i = 1, 2, ..., n.
\]

\( X_j \) is the amplitude of the \( \sigma \) polarization component of the dielectric displacement \( D_j \) inside the diffracting crystal; \( Y_j \) is the amplitude of the \( \pi \) polarization polarizations. The wave dependences for several values of the angle of incidence \( \theta \), \( \Delta \theta = \theta - \theta_{\text{inc}} \). Two-beam wave dependence of reflection 440; \( \cdots \) two-beam wave dependence of reflection 220.
component of $D_{ij}$: $A_{ij} (i \neq j) = \psi_{ij}; A_{ii} = \psi_0 - 2(u_i, \Delta)/k_m$.

$\psi_{ij}$ is the term in the Fourier sum of the susceptibility corresponding to the reciprocal-lattice vector $b_{ij} = k_j - k_i$; $u_i$ is the unit vector parallel to the vacuum wave vector $k_i$, $k_i = k_m u_i$; $\Delta$ is the deviation of the centre of the sphere of reflection from the Laue point.

The calculation was performed in the plane of reflection only, i.e. $\Delta$ is supposed to lie in this plane. So we use the plane concepts of the dispersion curve etc.

The quantity $A_{ii}$ is a linear function of $u_i, \Delta$. Therefore, the calculation makes an approximation that the dispersion curve asymptotically approaches straight lines instead of the circles with centres at the reciprocal-lattice points lying on the Ewald sphere.

2. The boundary conditions were set as in two-beam diffraction (see e.g. James, 1963) and we therefore work with the same assumptions. The boundary conditions for the wave vectors have the practical consequences that the possible wave points of the dispersion curve lie on the surface normal.

In the four-beam diffraction four wave fields are the result of the fundamental system of equations but in the case studied (Ge \{000, 440, 260, 220\} in a thick crystal) only two are physically possible. We define the indexing as follows: the two wave fields $\alpha, \beta$; reciprocal-lattice point 000 $\rightarrow$ 1, 440 $\rightarrow$ 2, 260 $\rightarrow$ 3 and 220 $\rightarrow$ 4.
We set the boundary conditions for the amplitudes by the following equations:

(a) surface (110)  
\[ Z_{1a} + Z_{1b} = Z_1 \]  
\[ Z_{2a} + Z_{2b} = Z_2 \]  
\[ Z_{3a} + Z_{3b} = Z_3 \]  
\[ Z_{4a} + Z_{4b} = 0 \]

(b) surface (110)  
\[ Z_{1a} + Z_{1b} = Z_1 \]  
\[ Z_{2a} + Z_{2b} = 0 \]  
\[ Z_{3a} + Z_{3b} = Z_3 \]  
\[ Z_{4a} + Z_{4b} = Z_4 \]

where \( Z_j = X_j \) for \( \pi \) polarization and \( Z_j = Y_j \) for \( \sigma \) polarization.

Two excited wave points were determined by the help of the Poynting vector (see e.g., Kato, 1958):

\[ S_x = \sum_{i=1}^{n} |Z_{ix}|^2 u_r. \]

The wave point \( z \) is excited if \( (S_x, \mathbf{n}) > 0 \) (\( \mathbf{n} \) is the inward facing surface normal). We know in advance that \( S_x \) is, in a nonabsorbing crystal, perpendicular to the dispersion curve at the wave point \( z \) (Kato, 1958). The magnitude of \( S_x \) is known at the end of the calculation but the sense of \( S_x \) is known immediately after the resolution of the fundamental system of equations.

3. The reflection curves used in the paper are the angular dependences of the reflection coefficient \( R_j = |Z_{j1}|^2/|Z_{j2}|^2 \). The ratio \( |\gamma_1|^2/\gamma_2^2 \) (see James, 1963, equation 37.1) arising from the general relation of the reflection coefficient for the symmetrical reflections 440 and 220 and for the \( \pi/2 \) reflection 260 is equal to 1.

4. For \( k = k_m \) the term \((u_i \cdot \Delta)/k_m\) in \( A_{ii} \) is the so-called resonance error. For \( k = k_m + \Delta k \) the resonance error of the same point represented by \( \Delta \) is given by \((u_i \cdot \Delta - \Delta k)/k \) (the unit vectors \( u_i \) are assumed to be constant in the neighbourhood of \( k = k_m \)). All equations solving Ge \{000, 440, 260, 220\} for \( k = k_m \) hold also for \( k \neq k_m \) when the quantity \( \psi_0 \) is substituted by the effective value \( \psi_{eff} = \psi_0 + 2 \Delta k/k \) for \( k = k_m \) and \( k = k_m + \Delta k \).

5. Absorption was introduced into the calculation via the complex value of the susceptibility \( \psi \). This procedure is described in detail by Pacherová & Bubáková (1982).

6. The reflection curves were calculated in the interval of the angle of incidence \( \theta \), \( <\theta_M - 30^\circ, \theta_M + 30^\circ> \), where \( \theta_M \) is the middle of the range of total reflection of the two-beam diffractions Ge \{000, 440\} or Ge \{000, 220\} computed to tenths of seconds of arc. The calculation was performed in steps of 0.2° or in some cases 0.1 or 0.05°. No particular attention was paid to the singularities of the dispersion curve. Of course, for some values of \( \Delta k \) the calculation was made very near to the singularity. No anomalies of the reflection curves were observed in any case. In Fig. 16 the dispersion curves and the corresponding reflection curves for two values of \( k \) are shown.

A more detailed analysis of the calculation is given by Pacherová (1979). It will be published elsewhere.

**APPENDIX B**

Here the derivation of the relations for the resulting waves \( R_1, Q_2, R_3 \) and \( Q_4 \) of a Ge \{440, 220\} monochromator is given.

In Fig. 17 the situation in the neighbourhood of the Laue point La is drawn for \( \Delta k > 0 \). I corresponds to the incident wave from the source of X-rays, II and III to the waves inside Ge \{440, 220\}. The lines \( c_i \) (\( i = 1, 2, 3, 4 \)) are circles with centres at the reciprocal-lattice points \( i \) and with radius \( k = k_m + \Delta k \). These circles are
the starting points of the vacuum wave vectors of the incident and reflected waves. In our calculation they are substituted by the straight lines. The arrows below $c_i$ indicate the increasing glancing angle of incidence or of reflection. The waves inside Ge [440, 220] are the reflections on one of the two surfaces of Ge [440, 220] and at the same time the incident wave on the second surface. Therefore, the wave points of those waves find themselves in two parts of Fig. 17. The wave point for the reflected wave is designated as $S_j (j=1, 2, ...)$, and the wave point for the same wave but considered as the incident one is designated as $T_j (j=1, 2, ...)$.

In accordance with the boundary conditions for the wave vectors all the wave points excited when the incident wave is falling on the surface are lying on the surface normal.

In Fig. 17 the glancing angle of incidence of the incident wave $P$ is $\theta_{B4}^m + \phi$ ($\phi<0$). The quantities $\delta'$ and $\phi'$ are proportional to $\delta$ and $\phi$ of equations (+), (+ +). The succession of the excited wave points can be written as follows:

\[
P \Rightarrow R_1, S_1 \rightarrow T_1
\]
\[
T_1 \Rightarrow Q_2, S_2 \rightarrow T_2
\]
\[
T_2 \Rightarrow R_3, S_3 \rightarrow T_3
\]
\[
T_3 \Rightarrow Q_4, S_4 \rightarrow T_4
\]
\[
T_4 \Rightarrow R_4, \text{etc.}
\]

Schematically we can write the relations for the intensities of the waves participating in Ge [440, 220] ($R_{HKL}$ is the reflection coefficient of the reflection $HKL$ – see Appendix A):

\[
I(R_1) = I(P) \times R_{260}
\]
\[
I(S_1) = I(P) \times R_{440}
\]
\[
I(T_1) = I(S_1)
\]
\[
I(Q_2) = I(T_1) \times R_{220} = I(P) \times R_{440} \times R_{220}
\]
\[
I(S_2) = I(T_1) \times R_{620} = I(P) \times R_{440} \times R_{620}
\]
\[
I(T_2) = I(S_2)
\]
\[
I(R_3) = I(T_2) \times R_{440} = I(P) \times R_{440} \times R_{620} \times R_{620}
\]
\[
I(S_3) = I(T_2) \times R_{620} = I(P) \times R_{440} \times R_{620} \times R_{620}
\]
\[
I(T_3) = I(S_3)
\]
\[
I(Q_4) = I(T_3) \times R_{220} = I(P) \times R_{440} \times R_{620} \times R_{620} \times R_{220}
\]
\[
I(S_4) = I(T_3) \times R_{620} = I(P) \times R_{440} \times R_{620} \times R_{620} \times R_{620}
\]
\[
I(T_4) = I(S_4) \text{ etc.}
\]

When the intensities of the resulting waves are evaluated, the values of the corresponding angles of incidence must be added to the relations above. In equations (+), (+ +) these angles are written in parentheses and a shortened version is used: $R_{HKL} \rightarrow HKL$, $I(R_N, Q_N)/I(P) \rightarrow R_N, Q_N$.

**References**


