DYNAMICAL THEORY FOR SIMULTANEOUS X-RAY DIFFRACTION

PART II: APPLICATION TO THE THREE-BEAM CASE

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Abstract

The results obtained in part I of this paper are applied to the case of simultaneous diffraction on three sets of reflecting planes. By normalizing the amplitudes of the plane-wave components and the wave vector, an explicit expression for the ω-surface is given, that contains only one structure-sensitive parameter. This parameter is zero if the crystal structure shows inversion symmetry. The ω-surface in the latter case is discussed in detail. There is a threefold and a twofold degenerate point. If one of the structure factors is zero in a crystal with inversion centre, there is a line of twofold degeneracy on the ω-surface. At all degenerate points the possible composition of the wave field is given. The absorption shows interesting behaviour in the case where one structure factor is zero. It is lower than in the limiting two-beam cases. For a few examples the minimum in attenuation coefficient has been calculated numerically. The only value of the absorption coefficient for a three-beam case that has been reported in literature agrees reasonably well with the calculated value.

1. Introduction

The three-beam case of simultaneous X-ray diffraction has been studied both experimentally and theoretically. Renninger 1) observed that a forbidden reflection may occur if a not-forbidden reflection is activated simultaneously. Borrmann and Hartwig 2) observed that in perfect germanium crystals the absorption of CuKα radiation is reduced below the absorption in the limiting two-beam cases if the third reflection is forbidden.

The three-beam case has been treated theoretically by Ewald 3) and Lamla 4). Ewald's treatment was reviewed in part I of this paper 5). Special cases have been investigated by others: Saccocio and Zajac 6) considered the case of simultaneous diffraction on three equivalent sets of planes; Hildebrandt 7) discussed the minimum in absorption in the case investigated experimentally by Borrmann and Hartwig.

In this paper we shall treat an arbitrary three-beam case by applying the general results obtained in part I. A simplification is obtained by normalizing the amplitudes of the plane-wave components and the wave vector, in such a way that only one structure-sensitive parameter plays a part instead of six without normalization. If the crystal structure shows inversion symmetry this remaining parameter is equal to zero. The shape of the normalized ω-surface

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(Ω-surface) is discussed in detail. Special attention is given to degenerate points. Of particular interest is the case where one of the three reflections is forbidden. The results are in reasonable agreement with the observations of Borrmann and Hartwig.

2. Normalization of the wave vector, amplitudes and ω-surface

In the three-beam case of diffraction the incident beam satisfies exactly or very closely the Bragg condition for two (and not more) sets of reflecting planes. The two reflected beams satisfy very closely the Bragg condition for a third set of planes. The wave vector of the wave in vacuum that satisfies two Bragg conditions exactly, is denoted by \( \mathbf{u}_j \omega/c \) where \( \mathbf{u}_j \) is a unit vector *. Hence

\[
\mathbf{u}_j = \mathbf{u}_t + \mathbf{b}_{ij} c/\omega = \mathbf{u}_k + \mathbf{b}_{kj} c/\omega,
\]

where \( \mathbf{u}_t \) and \( \mathbf{u}_k \) are unit vectors in the direction of the two reflected beams and \( \mathbf{b}_{ij} \) and \( \mathbf{b}_{kj} \) are the reciprocal-lattice vectors of the two sets of reflecting planes. The reciprocal-lattice vector of the third set of planes is given by

\[
\mathbf{b}_{kl} = \mathbf{b}_{kj} - \mathbf{b}_{ij} = -\mathbf{b}_{jk} \quad - \mathbf{b}_{ij}.
\]

Throughout this paper the subscripts \( i, j \) and \( k \) have in that order the values 1, 2 and 3 or a cyclic interchange thereof. In fig. 1 the relative orientations of \( \mathbf{u}_i \) and \( \mathbf{b}_{ij} \) are shown.

[Diagram showing the relative orientations of the unit vectors \( \mathbf{u}_i \) and reciprocal-lattice vectors \( \mathbf{b}_{ij} \).]

*) The same notation as in part I is adopted.
According to the dynamical theory of X-ray diffraction Maxwell's equations are satisfied in a first approximation by a mode of propagation of the following composition:

\[
D = \exp \left\{ j(\omega t - \Delta \cdot r) \right\} \sum_i D_i \exp (-j \mathbf{u}_i \cdot r \omega/c).
\]

(2.3)

It consists of three transverse plane-wave components with amplitude \(D_i\) and wave vector \(\mathbf{u}_i(\omega/c) + \Delta\). The magnitude of \(\Delta\) is small compared with \(\omega/c\) in the region of interest where more than two plane-wave components are predominant. The amplitudes and the wave vector \(\Delta\) of the mode of propagation have to satisfy the equations (see part I, eq. (3.4))

\[
(\psi_0 - 2\mathbf{u}_i \cdot \Delta c/\omega)D_i + \psi_{ij}^* \{D_j - \mathbf{u}_i(\mathbf{u}_i \cdot D_j)\} + \psi_{kl} \{D_k - \mathbf{u}_i(\mathbf{u}_i \cdot D_k)\} = 0.
\]

(2.4)

Here \(\psi_0\) is the average susceptibility of the crystal and \(\psi_{jk}\) the Fourier component associated with the reciprocal-lattice vector \(\mathbf{b}_{jk}\). Note that \(\psi_{ji} = \psi_{ij}^*\), where the asterisk indicates the complex conjugate. Absorption is left out of consideration for the time being.

Although solutions for \(\Delta\) can be obtained immediately by using the methods outlined in part I, it is convenient to normalize the wave vector and the amplitudes in such a way that as many structure factors as possible are eliminated from eq. (2.4). With the aid of eq. (2.2) it is easily shown that the product \(\psi_{ij}\psi_{jk}\psi_{kl}\) is independent of the choice of origin for \(r\). One may write:

\[
\psi_{ij}\psi_{jk}\psi_{kl} = \psi_0^3 M^3 \exp (j \varphi).
\]

(2.5)

In crystals with an inversion centre, \(\varphi\) is equal to zero and \(M\) either positive or negative. Normalization is now obtained by introducing

\[
D_i = n_i D_i,
\]

(2.6)

and

\[
y_i = (\psi_0 - 2\mathbf{u}_i \cdot \Delta c/\omega) m_i m_i^*/\psi_0 M^3,
\]

where

\[
m_i = \psi_{jk}/\psi_0, \quad m_i^* = \psi_{kj}/\psi_0, \quad n_i/n_j = r^2 m_i/m_j^*, \quad r = \exp (-j \varphi/3).
\]

(2.7)

The basic equations (2.4) are now easily transformed into

\[
y_i D_i + r D_j + r^{-1} D_k - \mathbf{u}_i \{\mathbf{u}_i \cdot (r D_j + r^{-1} D_k)\} = 0.
\]

(2.8)

All structure factors except \(\varphi\) have been eliminated. The expression for the normalized \(\omega\)-surface (which will be referred to as \(\Omega\)-surface) can now be found by applying the procedure indicated by Ewald and outlined in part I. One obtains
\( \Omega = (y_1 y_2 y_3 \gamma_1 y_2 y_3 y_3 + 2 \cos \varphi \gamma_1 y_2 y_3 a^2 y_1 y_1 - b^2 y_2 c^2 y_3 + 2 abc \cos \varphi) + \\
(1 - a^2 - b^2 - c^2 + 2 abc)(-2 y_1 y_2 y_3 \cos \varphi + y_1 y_2 + y_1 y_3 + y_2 y_3 - 1) = 0, \)

where \( a = u_2 \cdot u_3, b = u_3 \cdot u_1 \) and \( c = u_1 \cdot u_2 \), the cosines of the double Bragg angles involved. This result in a non-normalized form was also obtained by Lampl 4).

There exist interesting relations between \( \Omega(y_1, y_2, y_3, \varphi) = 0 \) and the products \( D_i \cdot D_i^* \) and \( D_i \cdot D_j^* \), that play a part in the equations for the power flow and absorption coefficient (eqs (4.6) and (4.10) in part I). By using the same procedure as employed in deriving eq. (4.8) in part I, but now applied to the normalized basic equations, it can be shown that

\[
\sum_i D_i \cdot D_i^* \delta y_i - \frac{1}{2} j \delta \varphi \sum_i (rD_i^* \cdot D_j - r^{-1}D_j^* \cdot D_i) = 0.
\]

Since \( \Omega \) is a function of \( y_i \) and \( \varphi \) only, the following relation holds also in non-degenerate points:

\[
\sum_i \frac{\partial \Omega}{\partial y_i} \delta y_i + \frac{\partial \Omega}{\partial \varphi} \delta \varphi = 0.
\]

Comparison of these two equations shows that

\[
D_i \cdot D_i^* = C \frac{\partial \Omega}{\partial y_i} \quad (2.10)
\]

and

\[
\sum_i (rD_i^* \cdot D_j - r^{-1}D_j^* \cdot D_i) = 3jC \frac{\partial \Omega}{\partial \varphi} \quad (2.11)
\]

Multiplication of eq. (2.8) by \( D_i^* \) and its complex conjugate by \( D_i \) shows in the first place that the three terms in the sum of the left-hand side of eq. (2.11) are equal, so that

\[
rD_i^* \cdot D_j - r^{-1}D_j^* \cdot D_i = jC \frac{\partial \Omega}{\partial \varphi} \quad (2.12)
\]

Secondly it follows that

\[
rD_i^* \cdot D_j + r^{-1}D_i \cdot D_j^* = C \left( 2y_k \frac{\partial \Omega}{\partial y_k} - \sum_l y_l \frac{\partial \Omega}{\partial y_l} \right) \quad (2.13)
\]

Both results hold for any \( i \) and related values of \( j \) and \( k \).

In the next section the shape of the \( \Omega \)-surface is discussed. The axes for \( y_1, y_2 \) and \( y_3 \) are represented by orthogonal axes. In reality the \( y_i \) axis is perpendicular to \( u_j \) and \( u_k \). By introducing the reciprocal unit vectors \( \sigma_i \) in such a way that
\[ u_i \cdot \sigma_j = \begin{cases} 1 & \text{for } i = j, \\ 0 & \text{for } i \neq j, \end{cases} \]

it is easily shown that

\[ \Delta = \sum_i \frac{1}{2} \psi_0 \left( 1 - M^3 \frac{y_i}{m_i m^*} \right) \sigma_i \omega/c. \]

The transformation of the \( \Omega \)-surface into the \( \omega \)-surface involves a change in angle between the axes and a change in scale along the axes.

3. Discussion of the \( \Omega \)-surface

3.1. General three-beam case

The \( \Omega \)-surface in the three-beam case consists of six sheets. In order to give a rough idea of the shape of these sheets, we consider a cube in \( y \) space with sides parallel to the \( y_1, y_2 \) and \( y_3 \) axes and centred around \( y_1 = y_2 = y_3 = 0 \). The sides of the cube are considered to be so large that in the surfaces of the cube the situation for \( y_i = \infty \) is present. It is easily verified that there the limiting two-beam cases are found, with

\[ y_j y_k = 1 \quad \text{or} \quad y_j y_k = (u_j \cdot u_k)^2. \]

![Fig. 2. Intersections of three sheets of the "normalized" \( \Omega \)-surface with a cube centred around \( y_1 = y_1 = y_3 = 0 \) and with sides parallel to the three \( y \) axes. Sheet I passes through curve I and is curved downwards, sheet III is warped and sheet V is curved upwards. For the location of the other three sheets, see text.](image)
In fig. 2 the cube is drawn as seen along a line close to \( y_1 = y_2 = y_3 \) in the negative direction. In the faces of the cube some branches of the limiting hyperbolae are drawn. Three of the six sheets can now be visualized. Sheet I passes through the closed curve I, which consists of the branch \( y_j y_k = 1 \) with \( y_j > 0 \). It is curved downwards. Sheet V passes through curve V which consists of branches of the hyperbolae \( y_j y_k = (u_j \cdot u_k)^2 \) with \( y_j < 0 \). It is curved upwards. Sheet III is warped. It passes through curve III that consists alternately of branches of the hyperbolae \( y_j y_k = 1 \) (dashed parts) and \( y_j y_k = (u_j \cdot u_k)^2 \) (drawn parts). The intersections with the other three sheets have not been shown. These sheets are found in exactly the same way by using the remaining twelve branches of the hyperbolae. Sheet II is curved downward, sheet VI upward and sheet IV is warped. In general the six sheets have no point in common.

The wave field for any mode of propagation consists of three plane-wave components. No solutions exist with one plane-wave component of zero amplitude, excluding the limiting two-beam cases. Furthermore the direction of polarization of the total dielectric displacement rotates as a function of time at arbitrary place.

3.2. Three-beam case in crystals with inversion centre

In crystals that show inversion symmetry the phase angle \( \varphi \) in the product
\[ \psi_{ij} \psi_{jk} \psi_{ki} \]
is equal to zero. All normalization factors are real if one chooses the origin in the inversion centre. The expression for the \( \Omega \)-surface reads:
\[
\Omega = (y_1 y_2 y_3 - y_1 - y_2 - y_3 + 2)(y_1 y_2 y_3 - a^2 y_1 - b^2 y_2 - c^2 y_3 + 2 abc) + (1 - a^2 - b^2 - c^2 + 2 abc)(-2 y_1 y_2 y_3 + y_1 y_2 + y_1 y_3 + y_2 y_3 - 1) = 0. \quad (3.1)
\]
The factor \((1 - a^2 - b^2 - c^2 + 2 abc)\) is equal to the volume squared of the parallelepiped on the three vectors \( u_i \).

On the \( \Omega \)-surface lie three straight lines (see fig. 3):
\[ y_i = y_j = 1, \quad y_k \text{ arbitrary.} \]
The composition of the wave field is very simple for these modes of propagation:
\[
D_i = -D_j; \quad D_k = 0. \quad (3.2)
\]
The direction of polarization of \( D_i \) and \( D_j \) must be normal to the plane through \( u_i \) and \( u_j \). In the inversion centre the amplitudes are in anti-phase. Since the normalization factors \( n_i \) and \( n_j \) are in general not equal, the total amplitude in the inversion centre is not equal to zero. The three straight lines are part of sheet I \((y_k > 1)\) and sheet III \((y_k < 1)\). They intersect at the point of threefold degeneracy \( y_1 = y_2 = y_3 = 1 \). Here, any linear combination of the three possible solutions given in eq. (3.2), is a solution also.

There is also a point of twofold degeneracy on the \( \Omega \)-surface. Its coordinates are given by
Fig. 3. Similar to fig. 2, but now for a crystal structure with inversion centre. There are three straight lines on the $\Omega$-surface. They lie in sheet I for $\gamma_k > 1$ and in sheet III for $\gamma_k < 1$. In the point $\gamma_1 = \gamma_2 = \gamma_3 = 1$, the intersection of the three straight lines, the sheets I, II (not indicated in the figure) and III come together. A point of twofold degeneracy is also present but not shown in the figure.

$$y_1 = 1 + \left\{1 - (u_i \cdot u_j)(u_i \cdot u_k)/(u_j \cdot u_k)\right\} [1 - \sum_i \left\{1 - (u_i \cdot u_j)(u_j \cdot u_k)/(u_k \cdot u_i)\right\}]^{-1}. \quad (3.3)$$

In this point either sheets I and II are connected or sheets V and VI. The first case is present if $(1 - ab/c)(1 - bc/a)(1 - ca/b)$ is negative; the second case if it is positive. In the point of twofold degeneracy the two sheets touch each other, so that the $\Omega$-surface is a cone in its immediate vicinity. The wave field consists of the following reduced components:

\begin{align*}
(1 - bc/a)D_1 &= bc(A + B)u_1 - bAu_2 - cBu_3, \\
(1 - ac/b)D_2 &= a(A + B)u_1 - acAu_2 - cBu_3, \\
(1 - ab/c)D_3 &= a(A + B)u_1 - bAu_2 - abBu_3, \quad (3.4)
\end{align*}

where $A$ and $B$ are arbitrary constants.

3.3. Three-beam case in crystals with inversion centre, one reflection forbidden

In view of the experimental results mentioned in the introduction, it is worth discussing the case where one structure factor is equal to zero in a crystal with inversion centre. We shall put $\psi_{23}$ equal to zero. The normalization offers a difficulty because $m_1$ and $n_1$ are zero. Furthermore the values of $y_1$, $y_2^{-1}$ and $y_3^{-1}$ go to zero for finite deviations from the Bragg angle. To overcome this difficulty new parameters $y_1'$ and $n_1'$ are introduced:
\[ y_1' = \frac{y_1}{m_1}, \quad y_2' = y_2m_1, \quad n_1' = n_1/m_1 = 1. \quad (3.5) \]

These parameters remain finite for finite values of \( \Delta \). Substituting eq. (3.5) in the expression (3.1) for the \( \Omega \)-surface and going over to the limit \( m_1 \rightarrow 0 \), one obtains

\[
\Omega = (y_1y_2y_3 - y_2 - y_3)(y_1y_2y_3 - b^2y_2 - c^2y_3) + 
\quad + (1 - a^2 - b^2 - c^2 + 2abc)y_2y_3 = 0. \quad (3.6)
\]

The primes have been omitted again since they are no longer necessary. The equations (2.10) and (2.13) still hold, although the definitions of \( y_i \) are changed.

A direct derivation of the expression for the \( \Omega \)-surface from the basic equations (with the newly defined \( y_i \) and \( n_i \)) is very simple. The basic equations read:

\[
y_1D_1 + D_2 + D_3 = u_1\{u_1 \cdot (D_2 + D_3)\},
\]

\[
y_2D_2 = -D_1 + u_2(u_2 \cdot D_1),
\]

\[
y_3D_3 = -D_1 + u_3(u_3 \cdot D_1).
\]

The vector \( D_1 \) must be perpendicular to \( u_1 \), so that

\[
D_1 = Au_1 \wedge u_2 + Bu_3 \wedge u_1.
\]

The other two amplitudes can now be shown to be:

\[
y_2D_2 = (-A + aB)u_1 \wedge u_2 + cBu_2 \wedge u_3,
\]

\[
y_3D_3 = (-B + aA)u_3 \wedge u_1 + bAu_2 \wedge u_3.
\]

Substitution of these expressions for \( D_1 \) in the first basic equation, and multiplying it by \( u_2 \) and \( u_3 \), respectively, leads to

\[
(y_1y_2y_3 - y_2 - c^2y_3)B = -y_2(a - bc)A,
\]

\[
(y_1y_2y_3 - b^2y_2 - y_3)A = -y_3(a - bc)B.
\]

Elimination of \( A \) and \( B \) gives eq. (3.6). The last two equations show that for given \( y_3/y_2 \), the ratio \( B/A \) is determined although \( y_1 \) remains free (with \( y_1y_3 \) fixed). Apparently the directions of polarization are constant along each line of intersection of the \( \Omega \)-surface with an arbitrary plane through the line \( y_2 = y_3 = 0 \). The intersection consists of six lines: the line \( y_2 = y_3 = 0 \) (twofold degenerate) and two hyperbolae. It can be shown that on the two branches of one hyperbola the polarization directions of \( D_1, D_2 \) and \( D_3 \) are the same, and that \( D_1 \) on one hyperbola is perpendicular to \( D_1 \) on the other.

Three of the six sheets are shown in fig. 4. On the line \( y_2 = y_3 = 0 \) the sheets III and IV touch each other. The wave field of the modes of propagation on this line have no plane-wave component 1. The amplitudes of the other two plane-wave components have as the only restriction that \( D_2 + D_3 \) must be
Fig. 4. Similar to figs 1 and 2, but now for the case where one reflection is forbidden in a crystal structure with inversion centre. The forbidden reflection gives rise to the crossing straight lines in two of the six faces of the cube. The $\Omega$-surface is twofold degenerate on the dash-dot line, where the sheets III and IV (not shown in the figure) coincide.

parallel to $u_1$. Note that the points of threefold and twofold degeneracy, found in the case of three non-zero structure factors, are no longer present.

A very simple situation arises in the case where $a = bc$. The plane through $u_1$ and $u_2$ is then perpendicular to the plane through $u_1$ and $u_3$. The expression for the $\Omega$-surface can then be expanded into two factors:

$$\Omega = (y_1y_2y_3 - b^2y_2 - y_3)(y_1y_2y_3 - y_2 - c^2y_3) = 0. \quad (3.7)$$

If the first factor is equal to zero, then $D_1$ and $D_2$ are polarized in a direction perpendicular to both $u_1$ and $u_2$:

$$D_1 = -y_2D_2 = Au_1 \wedge u_2,$$

$$y_3D_3 = bA(cu_3 \wedge u_1 + u_2 \wedge u_3).$$

If the second factor in eq. (3.7) is equal to zero, $D_1$ and $D_3$ are both perpendicular to $u_1$ and $u_3$:

$$D_1 = -y_3D_3 = Bu_3 \wedge u_1,$$

$$y_2D_2 = cB(bu_1 \wedge u_2 + u_2 \wedge u_3).$$

In this special case there are two other lines of twofold degeneracy where the sheets I and II, and the sheets V and VI come together:
(1 - b^2)y_2 = (1 - c^2)y_3 = (1 - b^2 c^2)/y_1.

Along these lines the direction of \( D_1 \) may be chosen freely. The amplitudes of the other components follow from

\[
\begin{align*}
y_2 D_2 &= -D_1 + u_2 (u_2 \cdot D_1), \\
y_3 D_3 &= -D_1 + u_3 (u_3 \cdot D_1).
\end{align*}
\]

4. Absorption coefficient

In sec. 4.2 of part I it has been outlined how the absorption is introduced as a small perturbation of the solutions in non-absorbing crystals. At regular points of the \( \Omega \)-surface the absorption coefficient \( \mu \) can be calculated from eq. (4.10) of part I by determining the amplitudes of the plane-wave components or by determining the first derivatives of \( \Omega \) and making use of eqs (2.10), (2.12) and (2.13). At degenerate points, as found in the \( \Omega \)-surface for crystals with inversion centre, the latter method is not possible since all first derivatives are zero at degenerate points. The first method gives an answer, but it may be doubted whether the answer is correct, since it leads, in general, to results that are inconsistent from a physical point of view. At a point of twofold degeneracy there remains one degree of freedom in the composition of the wave field, for example the direction of polarization of one plane-wave component. The calculated absorption coefficient is in general dependent on this degree of freedom. A particular direction of polarization that gives rise to a well-defined value of \( \mu' \) can be considered as a linear combination of two wave fields with other directions of polarization. These two wave fields, however, have other values of \( \mu \). This inconsistency is not present when the attenuation coefficient is independent of the choice of polarization, for example along the line \( y_2 = y_3 = 0 \) mentioned in sec. 3.3 with \( \mu = \mu_0 |v_e| \) and at the point \( y_1 = y_2 = y_3 = 1 \) mentioned in sec. 3.2 if the three reflections are equivalent.

It seems likely that the assumption on which the determination of \( \mu \) is based, viz. that the absorption can be treated as a correction on the behaviour in non-absorbing crystals, is no longer valid at degenerate points. The degeneracy may be expected to be removed by the small imaginary parts in \( \psi \) that must be introduced to account for absorption. A more detailed analysis is necessary to determine the behaviour of the wave fields in the \( \Delta \) regions close to degenerate points.

The wave field that suffers minimum absorption is of special interest, since it plays an important part in the anomalous transmission. Its wave vector can be determined numerically by calculating \( K \) (eq. (4.9) of part I) as a function of \( y_1, y_2 \) and \( y_3 \). We do not expect any difficulty in the case of crystals without inversion centre. In the case of three allowed reflections in a crystal with inversion centre the minimum in \( K \) might lie close to or at the point of threefold
degeneracy. In view of the difficulties outlined above, one must abandon detailed calculations until the behaviour of the wave fields in that region is better known.

In the case of a crystal with inversion symmetry and one reflection forbidden, it is fairly easy to determine the value of \( y_1 \), with variable \( y_3/y_2 \), for which \( K \) is minimum. But the value of \( y_3/y_2 \) that gives the absolute minimum in \( K \) has to be determined numerically. Only in the case where the two not-forbidden reflections are equivalent and the surface normal \( s \) is parallel to the three sets of reflecting planes, can the vector \( \Delta \) that gives the absolute extremum in \( K \) be given in explicit form:

\[
u_i \cdot \Delta = \frac{1}{2} (\psi_0 + \psi_{12} \sqrt{H_0}) \omega/c,
\]

where \( H_0 \) may have the following values:

\[H_0 = 1 + b^2 \pm (a - b^2)\]

The absolute extremes in \( K \) are found to be

\[-2K \cos \alpha/\mu_0 = 1 \mp \epsilon_{12} \sqrt{H_0},\]

where \( \alpha \) is the angle between \( s \) and any of the three wave vectors \( k_i \). Which one of the two \( H_0 \) values gives the lowest attenuation depends on the sign of \( a - b^2 \). These four modes with extreme values \( K \) all travel in the same direction. Their velocity of energy transport is not parallel to the intersections of the reflecting planes. According to eq. (4.12) of part I, one finds for the fractions of power flow travelling parallel to \( k_1, k_2 \) and \( k_3 \), respectively:

\[R_1 = \frac{1}{2}, \quad R_2 = R_3 = \frac{1}{4}.\]

This result is in close agreement with the observations of Borrmann and Hartwig.

5. Examples

To illustrate the results obtained above a few examples of simultaneous diffraction of CuK\(\alpha \) radiation in germanium were treated. The numerical values underlying the calculations are given in table I.

<table>
<thead>
<tr>
<th>reflecting planes</th>
<th>( m ) (^8)</th>
<th>( 1 - \epsilon ) (^9)</th>
</tr>
</thead>
<tbody>
<tr>
<td>220</td>
<td>0.728</td>
<td>0.0406</td>
</tr>
<tr>
<td>11(\bar{1})</td>
<td>0.598</td>
<td>0.3037</td>
</tr>
<tr>
<td>113</td>
<td>0.483</td>
<td>0.3324</td>
</tr>
</tbody>
</table>

\(^8\) Note that if \( a = b^2 \) the extremes in \( K \) occur on the two extra lines of degeneracy as discussed in the latter part of sec. 3.3. The value of \( K \), however, does not depend on the remaining degree of freedom.
We consider only plane-parallel crystal plates with surfaces perpendicular to
the three sets of reflecting planes. In view of the anomalous transmission the
extremes in attenuation coefficient are determined. In table II the results are
given for a number of possible three-beam cases with one reflection forbidden.
The values of $-2K \cos \alpha/\mu_0$ for the two minima are given. For other examples,
see also ref. 10.

**TABLE II**

The two minima in the attenuation coefficient $-K$ for simultaneous diffraction
of CuKα radiation in germanium. The angle between the incident beam and
the surface normal is $\alpha$ and $\mu_0$ represents the absorption coefficient off Bragg
angle

<table>
<thead>
<tr>
<th>reflecting plane</th>
<th>surface</th>
<th>$-2K \cos \alpha/\mu_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(111) (111) (200)</td>
<td>(011)</td>
<td>0.0525</td>
</tr>
<tr>
<td>(113) (113) (200)</td>
<td>(011)</td>
<td>0.0916</td>
</tr>
<tr>
<td>(311) (111) (222)</td>
<td>(011)</td>
<td>0.0893</td>
</tr>
<tr>
<td>(311) (113) (222)</td>
<td>(011)</td>
<td>0.168</td>
</tr>
<tr>
<td>(131) (113) (024)</td>
<td>(521)</td>
<td>0.198</td>
</tr>
</tbody>
</table>

The first case mentioned in table II was examined experimentally by Borr-\nmann and Hartwig 2). They compared the *integrated* intensity transmitted
through two crystals 0.8 and 1.2 mm thick. From a ratio of 6 : 1 they derived
a value for $-2K \cos \alpha/\mu_0$ of approximately 0.13. A comparison of this result
with the theory, however, is not immediately possible, because of the integration
over the divergent incident beam. With decreasing thickness more and more
modes off the minimum contribute substantially to the integrated intensity. In
the two-beam case this effect gives an additional factor of $1/t$ in the transmitted
intensity 9). It seems reasonable to use here a factor $1/t$. Introducing this factor
and using the lowest value of $K$ given in table II, leads to an expected intensity
ratio of 7.5 : 1 instead of 6 : 1 for the two crystals used by the authors. The
agreement is reasonable. The idea that integration plays a part here may also
be concluded from the observation made by Borrmann and Hartwig that the
distribution of intensity over the emerging beams depends slightly on the
direction of the incident beam, parallel to either $k_1$, $k_2$ or $k_3$. If only one wave
field survived, the distribution over the three emerging beams ought to be the
same for all three directions of incidence.

*Eindhoven, January 1967*
REFERENCES