in Fig. 1(*b*) of this work ($Cz^+$). To allow for the observed intensity increase in the reflexions {021} and {040}, which are not allowed by $Cz^+$, Weitzel concludes that the magnetic structure at LHeT has an antiferromagnetic $x$ component. This component causes a symmetry reduction, and the magnetic space group is $Pn'c2'$.

It was shown in this work that, allowing for small parameter changes (conforming with the RT space group *Pbcn*), the most probable structure is $Cz^+$ (space group $Pbc'n'$) with or without an $x$ component of weak ferromagnetism, which is allowed by $Pbc'n'$. We propose this structure, using the established principle that the choice of the highest possible symmetry model is the logical choice (Cox, 1972).

The symmetry $Pbc'n'$ conforms also with the second-order phase-transition theory (Landau & Lifshitz, 1958; Mukamel, 1973). This theory in our case (orthorhombic symmetry, and no cell enlargement) allows only a symmetry reduction by a factor of two, through the loss of the time-inversion operator, as is the case with $Pbc'n'$ (whereas the reduction from *Pbcn* to $Pn'c2'$ is by a factor of four).

The reflexions {021} and {040} may include, according to this proposal, nuclear and ferromagnetic contributions (no contributions from $Fe_2O_3$ are detected in our patterns). A discrepancy in the intensity calculation of the reflexions {050} and {111} is not solved in Weitzel's work because these reflexions are not resolved in his pattern. These reflexions cannot be quantitatively resolved in our longer-wavelength pattern.

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# A General Property in Extinction Theories: the Relation between Incident Point Sources and Homogeneous Beams. Application to Mosaic and Perfect Crystals

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The integrated reflectivity from an incident homogeneous beam (or plane wave) is shown to be a volume integral involving the intensity diffracted by a source point located on the surface of incidence of the crystal. Owing to the boundary conditions, the solution of the equations for extinction (either kinematical or dynamical) is often simpler with point sources than plane waves. The property that is established extends the domain of solution of diffraction theories: it is applied to mosaic-crystal equations and to the case of perfect crystals. In the latter case, a physically meaningful solution is found for primary extinction.

## Introduction

Extinction can be treated through various models originating in either kinematical (intensity coupling) or dynamical (wave coupling) theories. Kato (1976) has partially reconciled the two approaches, solving Takagi's (1969) equations in a statistical way under definite conditions. For optical coherence length smaller than the extinction distance, he obtained intensity coupling equations which can be shown to be identical with those employed to describe mosaic theories (Becker, 1977). The solution to these equations has been looked for by Zachariasen (1967), Becker & Coppens (1974) and Werner (1974). Kato's demonstration is obtained *via* the relation that exists between spherical and plane-wave theories of diffraction.

Homogeneous beams (or plane waves) are of general use in diffractometry. It will be shown that the solution for any set of diffraction equations can be decomposed into the superposition of contributions from point sources that are located on the surface of the crystal. The integrated reflectivity is then transformed into a volume integral, where the function to be integrated is the intensity diffracted by a point source associated with the variable point in the crystal.

The method will be then applied to mosaic and perfect crystals, in the Laue geometry. A new solution is thus obtained for primary extinction, that is derived from dynamical equations.

## 1. Case of intensity-coupling equations to represent the diffraction process

Let $\mathbf{u}_0$ and $\mathbf{u}_h$ be the unit vectors along the incident and diffracted beam directions. Fig. 1 shows the cross-section of a convex-shaped crystal cut by a plane containing $\mathbf{u}_0$ and $\mathbf{u}_h$.

For an incident homogeneous beam (or a plane wave) the surface of incidence on the crystal is *ADB*, and the exit surface *CBD*. The incident and diffracted beam cross-sections are respectively *ab* and *cd*. Let $x$ and $y$ be the coordinates along these two segments.

Because of the intensity coupling, it is possible to decompose the incident beam into a superposition of narrow slits. The direction **z** perpendicular to the plane of diffraction is irrelevant and we can consider the slit as a superposition of independent point sources like *S*. For a unit power the incident intensity of source *S* is:

$$\mathscr{I}_0(S)=\delta(x-x_\Sigma)\,. \qquad (1)$$

Let $s_0$ and $s_h$ be the coordinates of a point along axes defined by the point *S* and the directions $\mathbf{u}_0$ and $\mathbf{u}_h$.

The exit surface associated with the incidence point *S* is *pq*, the projection of which is $\alpha\beta$ (on *cd*). One can write:

$$\mathscr{I}_0(S)=(\sin 2\theta)^{-1}\delta(s_h)\,. \qquad (2)$$

Let *M* be a point on the exit surface *pq*. We represent the intensity diffracted at *M*, originating from *S* as:

$$(\sin 2\theta)^{-1}I_h(M/S) \qquad (3)$$

where $I_h(M/S)$ refers to thc incident beam $\delta(s_h)$. The integrated diffracted intensity is:

$$P(S)=(\sin 2\theta)^{-1}\int_{pq} I_h(M/S)\mathrm{d}\mathbf{l}\,.\,\mathbf{u}_h \qquad (4)$$

where $l$ is the curvilinear coordinate on the surface *pq*. Thus:

$$P(S)=(\sin 2\theta)^{-1}\int_{\alpha\beta} I_h(M/S)\mathrm{d}y\,.$$

The integrated intensity of the entire homogeneous beam is given by:

$$P=\iint P(S)\mathrm{d}x\mathrm{d}z\,. \qquad (5)$$

*P* may be a function of $\varepsilon$, the departure angle from Bragg's law, and represents the rocking curve. The integrated diffracted power is finally given by:

$$\mathscr{P}=\int P\mathrm{d}\varepsilon\,. \qquad (6)$$

We now consider a point *M* on the exit surface *DBC* and look for the sources *S* that contribute to the diffracted intensity at *M*. We shall distinguish the cases where *M* belongs to the arc *DA'* or the arc *A'C*, *A'* being defined in Fig. 2.

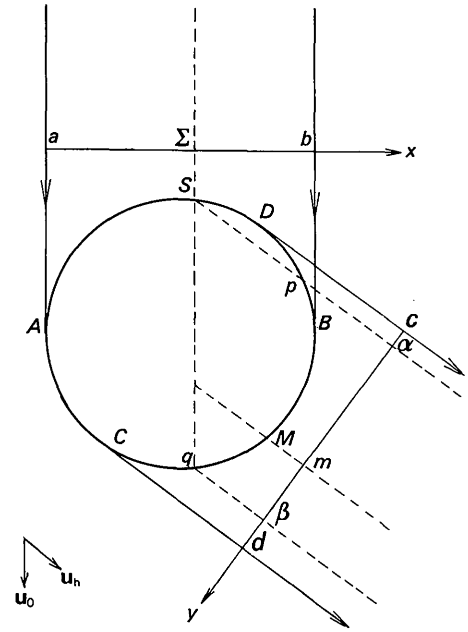


Fig. 1. Cross-section of the crystal on a plane parallel to the vectors $\mathbf{u}_0$ and $\mathbf{u}_h$.

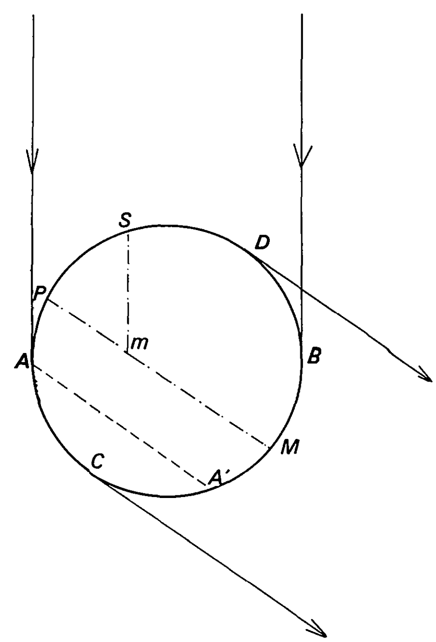


Fig. 2. The exit point *M* belongs to the arc *DA'*.

(*a*) $M \in DA'$. The relevant sources $S$ are associated with a given point $m$ along $PM$, as shown in Fig. 2. If we consider any point $m$ in the domain limited by the line $ADA'A$, we notice that:

$$Sm = T_0,\ mM = T_h'$$

where $T_0$ and $T_h'$ are the optical paths associated with $m$.

(*b*) $M \in CA'$. The situation is depicted in Fig. 3. If $m$ lies between $R$ and $M$, the conclusion is the same as in case (*a*). But source points located on $AQ$ also contribute to the diffracted intensity at $M$. If $m$ is taken along $RP$, a unique source $S$ can still be associated with $m$.

From this discussion, we must consider the domain limited by the line $ADBCEA$. With any point in this domain are associated a unique source $S$ and a unique point $M$ on the exit surface, with:

$$Sm = T_0,\ mM = T_h'\,.$$

Let $I(m)$ be the quantity:

$$I(m) = I_h(M/S)\,. \tag{7}$$

The positions of $\Sigma$ (or $S$) and $m$ are related by:

$$dx_\Sigma = (\sin 2\theta) ds_h(m)\,.$$

If $v'$ is the volume where $m$ is to be varied, the expressions (4)–(6) can be written in the final desired form:

$$\mathscr{P} = \int d\varepsilon \int_{v'} dv I(m)\,. \tag{8}$$

## 2. Case of amplitude-coupling equations to describe the diffraction process

This is a case for which perfect-crystal theory applies. The demonstration employs the relation between spherical and plane-wave theories. This has been discussed by Kato (1974, 1976) and we shall here only summarize his final discussion.

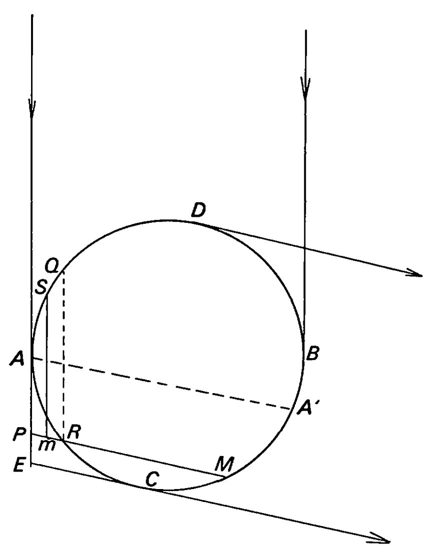


Fig. 3. The exit point belongs to the arc $A'C$.

An incident spherical wave is assumed to impinge on the crystal at $S$. The amplitudes of the incident and diffracted waves are $D_0$ and $D_h$, and the boundary condition is:

$$D_0 = \delta(s_h) \tag{9}$$

for a beam of unit power. Coordinates $x$ and $y$ along the directions $ab$ and $cd$ (which are the wave fronts for an incident plane wave) satisfy:

$$x = s_h \sin 2\theta,\ y = s_0 \sin 2\theta\,.$$

If an incident plane wave with a given departure angle, $\varepsilon$, from Bragg's law is considered, its wave vector $\mathbf{K}$ will have a component $K_x = K\varepsilon$. The $\varepsilon$-dependent part of the incident plane wave can be written as:

$$\exp(2\pi iK\varepsilon x) = \int \exp(2\pi iK\varepsilon x_\Sigma)\delta(x - x_\Sigma)dx_\Sigma\,. \tag{10}$$

The diffracted amplitude corresponding to the incident spherical wave is $D_h^s(s_0, s_h)$ or $D_h^s(x - x_S, y - y_S)$ where $x_S$ and $y_S$ are related by the equation of the surface of the crystal.

Relation (10) shows that the diffracted amplitude for an incident plane wave is given by:

$$D_h^p(x,y) = (\sin 2\theta)^{-1} \times \int \exp(2\pi iK\varepsilon x_S) D_h^s(x - x_S, y - y_S)dx_S\,.$$

The integrated diffracted intensity $\mathscr{P}^p$ for the plane wave is:

$$\mathscr{P}^p = \lambda \int\int dydz \int dK_x |D_h^p(M)|^2 = (\lambda/\sin^2 2\theta) \int\int dydz \int dx_S |D_h^s(x_M - x_S, y_M - y_S)|^2\,.$$

From arguments similar to those employed in § 1, one obtains the final relation:

$$\mathscr{P}^p = (\lambda/\sin 2\theta) \int_{v'} I^s(m) dv\,, \tag{11}$$

where $I^s(m)$ is the intensity diffracted at $M$ and originating from an incident spherical wave of unit power at $S$.

In both kinematical and dynamical theories of extinction, an important difficulty in solving the models comes from the boundary conditions at the surface of the crystal. The exact solution is very difficult to find, unless the entrance and exit surfaces on the crystal do not overlap appreciably (Bonnet, Delapalme, Becker & Fuess, 1976). Equations (8) and (11) allow one to solve the problem in many cases, as will be shown below and in a separate article.

### 3. Application to mosaic crystals, Laue geometry

We shall illustrate the method in the case of mosaic crystals, under Laue geometry, as assumed in previous treatments (Becker & Coppens, 1974; Bonnet, Delapalme, Becker & Fuess, 1976; Kato, 1976), and obtain in a more elegant way the solution proposed by Becker & Coppens, which can be generalized to other geometries.

Let a source point be $S$, and $M$ be a point where one looks for the diffracted intensity $I_h(M/S)$. The situation is summarized in Fig. 4. The Laue-geometry assumption is equivalent to the fact that all points in the parallelogram $SaMb$ belong to the crystal. The coupling equations are:

$$\begin{aligned} \partial I_0/\partial s_0 &= -\sigma(I_0 - I_h)\,, \\ \partial I_h/\partial s_h &= -\sigma(I_h - I_0)\,. \end{aligned} \tag{12}$$

If we write:

$$\begin{aligned} I_0 &= J_0 \exp\left[-\sigma(s_0 + s_h)\right]\,, \\ I_h &= J_h \exp\left[-\sigma(s_0 + s_h)\right]\,, \end{aligned} \tag{13}$$

where $\sigma(\varepsilon)$ is the coupling function, (12) transforms to:

$$\begin{aligned} \partial J_0/\partial s_0 &= \sigma J_h\,, \\ \partial J_h/\partial s_h &= \sigma J_0\,. \end{aligned} \tag{14}$$

We assume the boundary condition:

$$I_0 = \delta(s_h)\,.$$

Thus, after a unique diffraction along the axis $Ss_0$, the diffracted intensity is given by:

$$\lim_{\eta \to 0} I_h(s_0, \eta) = \sigma \exp(-\sigma s_0)\,.$$

Integrating the second equation (14), one obtains:

$$J_h(s_0, s_h) = \sigma \int_0^{s_h} J_0(s_0, v)\,\mathrm{d}v + \sigma\,.$$

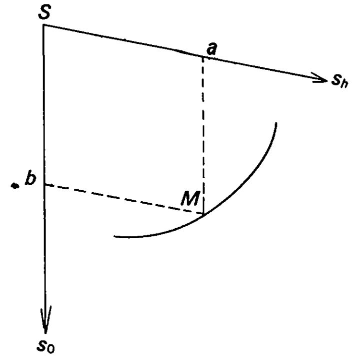


Fig. 4. Laue geometry for a point source.

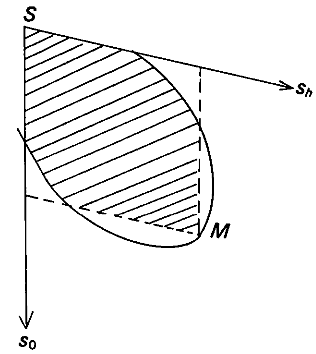


Fig. 5. Complex geometry for a point source (Laue–Bragg).

Since $I_0(0, s_h) = 0$, one has also:

$$J_0(s_0, v) = \sigma \int_0^{s_0} J_h(u, v)\,\mathrm{d}u\,.$$

Finally, one obtains:

$$J_h(s_0, s_h) = \sigma^2 \int_0^{s_0} \int_0^{s_h} J_h(u, v)\,\mathrm{d}u\mathrm{d}v + \sigma\,. \tag{15}$$

Defining $L$ as the integral operator:

$$Lf = \sigma^2 \int_0^{s_0} \int_0^{s_h} \mathrm{d}u\mathrm{d}v\, f\,, \tag{16}$$

(15) can be written formally (Werner, 1974):

$$(1 - L)J_h = \sigma\,. \tag{17}$$

It is important to observe that the Laue-geometry assumption only affects the limits of integration in (15) or (16). For more complicated geometries, as for example in Fig. 5, the domain of integration is the shaded area.

(17) may be expanded as:

$$J_h = \sum_n L^n \sigma\,. \tag{18}$$

Each term in (18) corresponds to the contribution from the $(2n+1)$-times scattered beam. Obviously:

$$\begin{aligned} L\sigma &= \sigma^3 s_0 s_h\,, \\ L^n\sigma &= \sigma^{2n+1}(s_0 s_h)^n/(n!)^2\,. \end{aligned}$$

Thus $J_h$ is given by:

$$J_h(s_0, s_h) = \sigma \mathbf{I}_0[2\sigma(s_0 s_h)^{1/2}]\,, \tag{19}$$

where $\mathbf{I}_0$ is the zero-order modified Bessel function of the first kind.

Using equations (8) to obtain the homogeneous-beam solution, and noticing that the volumes $v$ and $v'$ are the same in the Laue case, we obtain:

$$\mathscr{P} = \int \mathrm{d}\varepsilon\sigma \int_v \mathrm{d}v \exp\left[-\sigma(T_0 + T_h')\right]\mathbf{I}_0[2\sigma(T_0 T_h')^{1/2}] \tag{20}$$

for the integrated power, and the extinction coefficient $y$ is given by:

$$y = \mathscr{P}/Qv \tag{21}$$

$$Q = \left(\frac{e^2}{mc^2}\frac{F_hC}{V}\right)^2 \frac{\lambda^3}{\sin 2\theta},$$

with $C$ being the polarization factor (Becker & Coppens, 1974).

The solution is thus the same as obtained previously. But we see from the derivation that geometrical conditions only arise in the limits of integration and the method can be employed for more general cases.

### 4. Application to perfect crystals, Laue geometry

We shall follow the arguments of Kato (1974). Takagi's equations are written:

$$\partial D_0/\partial s_0 = i\chi_{\bar{h}} D_h$$
$$\partial D_h/\partial s_h = i\chi_h D_0 \tag{22}$$

where $\chi_h$ is the Fourier coefficients of the electrical susceptibility of the crystal:

$$\chi_h = \frac{e^2}{mc^2}\frac{\lambda C}{V} F_h .$$

We take as a boundary condition for $S$:

$$D_0 = \delta(s_h) .$$

Following the same derivation as for mosaic-crystal equations, we obtain:

$$D_h = \sum_n L^n(i\chi_h)$$

where

$$Lf = -\chi_h\chi_{\bar{h}} \int_0^{s_0}\int_0^{s_h} f \,\mathrm{d}u\mathrm{d}v . \tag{23}$$

Thus one obtains:

$$D_h = i\chi_h \mathbf{J}_0[2(\chi_h\chi_{\bar{h}} s_0 s_h)^{1/2}] \tag{24}$$

as also derived by Kato. Applying (11) we obtain for the integral reflectivity:

$$\mathscr{P} = |\chi_h|^2 \lambda/\sin 2\theta \int_v \mathrm{d}v |\mathbf{J}_0[2(\chi_h\chi_{\bar{h}} T_0 T'_h)^{1/2}]|^2 ,$$

where $\mathbf{J}_0$ is a zero-order Bessel function. We obtain for the extinction in a perfect crystal:

$$y = v^{-1} \int_v |\mathbf{J}_0[2(\chi_h\chi_{\bar{h}} T_0 T'_h)^{1/2}]|^2 \mathrm{d}v . \tag{25}$$

Equation (25) is a rigorous derivation for primary extinction. (20) has been shown to be a very satisfactory approximation for secondary extinction in the case of small diffraction angles. Similarly, (25) is to be considered as a reasonable representation of primary extinction.

Generalization to other geometries will be considered separately. In the case of anomalous transmission, the argument of the Bessel function in (25) is complex and this corresponds to the Borrmann effect, which will be also discussed separately.

### Conclusion

Even under the limitations of Laue geometries, the property that has been derived allows one to calculate in a physical sense the primary extinction coefficient, which was not possible before.

The author is indebted to Professor Kato for several enlightening discussions.

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