ANOMALOUS TRANSMISSION OF X-RAYS IN ELASTICALLY DEFORMED CRYSTALS

by P. PENNING and D. POLDER

Summary
The anomalous transmission of X-rays in perfect crystals may be explained by the dynamical theory of X-ray diffraction, a summary of which is given in this paper. This theory is not directly applicable to deformed crystals, but it can be extended to treat this case by assuming that the lattice parameters vary slowly. The extended theory given in this paper is analogous to the theory of the propagation of light in a medium of slowly varying refractive index. The most important result obtained in this way is that the path of a narrow beam in a deformed crystal is curved. Calculations of beam intensities made for crystals deformed by a uniform temperature gradient or by elastic bending give good qualitative agreement with available experimental data.

Résumé
La transmission anormale des rayons X dans les cristaux parfaits est expliquée par la théorie dynamique de la diffraction des rayons X. Cette théorie est résumée succinctement. La théorie dynamique n'est pas directement applicable aux cristaux déformés. En admettant une variation lente des paramètres de réseau, on peut établir par analogie avec la propagation de la lumière dans un milieu à indice de réfraction lentement variable, des équations donnant une relation entre le comportement d'un faisceau de rayons X à l'intérieur du cristal et la déformation de ce cristal. Le plus important des résultats obtenus est qu'à l'intérieur d'un cristal déformé le trajet d'un étroit faisceau est incurvé. On donne des résultats quantitatifs pour des cristaux déformés à gradient de température uniforme et pour des cristaux déformés élastiquement par flexion. Ces résultats concordent qualitativement avec les données disponibles.

Zusammenfassung

1. Introduction
Anomalous transmission of X-rays is the phenomenon that in perfect crystals the apparent absorption coefficient of the X-rays is very small if the beam suffers a Bragg reflection during the passage through the crystal. It was first observed
on quartz 1) and later on calcite 2-4), germanium 5) and silicon 6). The X-ray energy transmitted through the crystal when emerging from the back face is distributed over two beams, one parallel to the incident beam (the transmitted beam) and one in a diffracted direction (the reflected beam). The intensities of the two beams are approximately equal. The explanation of this phenomenon is given in the dynamical theory of X-ray diffraction in perfect crystals 7.8). In this paper a review of the explanation is given in a presentation adapted to the further development of the theory.

Since the anomalous transmission is only observed in perfect crystals, Hunter 5) deformed a perfect germanium crystal by bending in order to investigate the influence of the deformation on the anomalous transmission. He observed a decrease in the anomalously transmitted intensities upon applying a bending moment. Borrmann and Hildebrandt 9)10) performed similar experiments on calcite, the deformation being introduced by application of a temperature gradient to the crystal. They also found a decrease of transmitted intensities with increasing deformation, but further observed a change in the ratio of the intensities of the transmitted and the diffracted beam. This last phenomenon was attributed to a curvature of the X-ray beam inside the crystal. Finally Okkerse 6) in this laboratory investigated in germanium the problem set by Hunter. He also observed that bending gave rise to a decrease in intensity and a variation of the ratio in intensity of the two emerging beams. Further he found the magnitude of the changes to be dependent on the amount of strain and on the orientation of the reflecting planes with respect to the front and back faces of the sample. His finding is that the larger the deviation from 90° in angle between the reflecting planes and the surfaces, the stronger the influence of a certain amount of strain on the transmitted and reflected intensities.

These last observations, together with the idea of "selfadjustment of internal radiation fields" in elastically strained perfect crystals as introduced by Cole and Brock 11) led us to make an attempt to extend the dynamical theory of X-ray diffraction to elastically deformed perfect crystals. The basic assumption is that in any small part of the crystal the dynamical theory still describes the behaviour of the X-ray beam. Due to the deformation of the lattice, however, the behaviour will be different from place to place and the remaining problem is to match the solutions prevailing at the different sites. Although the solution of our problem can be applied to the Bragg case of X-ray diffraction, in this paper it will be used only for the Laue case, i.e. where the diffracted beam penetrates into the crystal and emerges from the crystal only at the back face of the crystal slab.

In sec. 2 we give some results of the dynamical theory of X-ray diffraction. Section 3 deals with the matching of the wave fields inside and outside the crystals. In sec. 4 the theory for strained crystals is given. Two applications are discussed in sec. 5: crystals deformed by a uniform temperature gradient and crystals
strained by a bending moment. In sec. 6 the experimental results of Hildebrandt as mentioned above are compared with the theory.

2. Unstrained crystals

2.1. Qualitative discussion

The occurrence of X-ray diffraction is due to the forced vibrations of electrons bound to the cores of the lattice atoms. The forced vibrations give rise to a dielectric constant $\varepsilon$ smaller than the vacuum value $\varepsilon_0$. We introduce a quantity $\psi$ defined by

$$\psi = (\varepsilon - \varepsilon_0)/\varepsilon_0,$$

where $\varepsilon$ will be place-dependent with the periodicity of the crystal lattice. Usually it is a complex number of the order of $10^{-5}$, the imaginary part being still one or two orders of magnitude smaller. For a large perfect crystal $\psi$ may be expanded in a Fourier series:

$$\psi = \psi_0 + \sum_{h,k,l} \psi_{hkl} \exp(jk_{hkl} \cdot r),$$

where $k_{hkl}$ is $2\pi$ times the reciprocal lattice vector of the plane $(hkl)$. The indices $h$, $k$ and $l$ may be any integer, positive or negative. For the purpose of further discussion we introduce with the aid of the vector $k_{hkl}$ the planes $P_{hkl}$ in reciprocal space (k-space) on which the vector $k$ satisfies the Bragg equation

$$2k_{hkl} = |k_{hkl}|^2 = 0.$$

By definition these planes are perpendicular to $k_{hkl}$ and hence parallel to the planes $(hkl)$ in real space.

First we discuss the possible modes of propagation of electromagnetic radiation in such an infinite, periodic lattice. Unlike the vacuum case these modes cannot be represented by simple plane waves characterized by one single wave vector $k$. Generally speaking any mode of propagation will consist of a linear superposition of plane waves with vectors $k + k_{hkl}$ (all $hkl$); the relative amplitudes of the plane-wave components are a function of $k$.

The dynamical theory of X-ray diffraction shows that, for small values of $\psi$, in the majority of modes only one plane-wave component predominates, viz. if the $k$-vector of this component is not very near to one of the planes $P_{hkl}$ defined by the Bragg equation. In other modes, however, if the wave vector $k$ of one of the components is near to a plane $P_{hkl}$, two plane-wave components predominate: besides the plane-wave component with vector $k$ there is also a plane-wave component present with wave vector $k' = k - k_{hkl}$. Still more complicated modes occur for wave vectors in the neighbourhood of two or more different planes $P_{hkl}$. We shall not discuss these more complicated modes in this paper.
We now consider all possible modes \((k, k')\) with a given frequency \(\omega\). If \(k_0\) (fig. 1) is a point on a plane \(P_{hk0}\) such that \(\omega = |k_0|c\) (\(c = \) velocity of light in vacuum), the smallness of \(\psi\) certifies that modes \((k, k')\) exist with \(k\)-values in the neighbourhood of \(k_0\). The \(k\)-values of these modes for given \(\omega\) are found on a surface in \(k\)-space, which we shall call the \(\omega\)-surface. The actual shape of a \(\omega\)-surface in the region \(k \approx k_0\) is given by the dynamical theory of X-ray diffraction \(^*\). Its general form is given by an equation of the type

\[
\omega = \omega(k, b, \psi_0, \psi_1),
\]

where \(b, \psi_0\) and \(\psi_1\) are parameters in the function \(\omega(k); \psi_0\) has its usual meaning, \(\psi_1 = \psi_{hk0} = \psi_{-h, -k, -l} \)** and \(b = \frac{1}{2} \mathbf{k}_{hkl}\), for the reflection \((hkl)\) under consideration. Note that only these particular \(\psi_{hk0}\) and \(\mathbf{k}_{hkl}\) occur as parameters in eq. (1).

The typical form of the \(\omega\)-surface is indicated in fig. 1, which gives the intersection of the \(\omega\)-surface with the plane through \(k_0\) and \(b\). The surface itself shows cylinder symmetry with respect to the \(b\)-axis. The most interesting feature of the \(\omega\)-surface is that it consists of two branches. The distance between the branches is smallest in the plane \(P_{hk0}\) and is then of the order of \(\psi_1|k_0|\). Since \(\psi\) is very small (\(\approx 10^{-5}\)) the situation as drawn in fig. 1 in the region around \(k_0\) is completely out of proportion with respect to the rest of the figure.

To understand where the two branches come from we consider first what happens if \(\psi_1 \to 0\). The wave fields then propagate in a homogeneous medium with \(\varepsilon = \varepsilon_0(1 + \psi_0)\). The two branches degenerate in this case to the dashed

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\(^*\) A complete and rigorous description of the \(\omega\)-surface is possible with the aid of the concept of reduced wave vectors and the reduced Brillouin zone, analogous to the theory of electron bands in solids.

\(^*\) \(\psi_{hk0} = \psi_{-h, -k, -l}\) for crystal structures with an inversion centre.
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lines in fig. 1, crossing at the plane $P_{hkl}$. The modes $(k, k')$ corresponding to these lines degenerate into plane waves: on line $AB$: $\exp(\imath kr)$; and on line $A'B'$: $\exp(\imath k'r)$. The line $AB$ is part of the circle, representing the $\omega$-surface for a homogeneous medium with $\epsilon = \epsilon_0(1 + \psi_0)$; the line $A'B'$ is also part of the same circle: it is the line $\alpha \beta$ displaced by an amount $k_{hkl}$. The displacement of this part of the circle is due to our convention of expressing all modes $(k, k')$ in terms of the value $k = k' + k_{hkl}$, rather than that of $k'$. One could adopt $k'$ instead of $k$, but the entire picture would then have occurred around $k_0' = k_0 - k_{hkl}$; it would describe, however, precisely the same solutions and modes of propagation we have already discussed.

A qualitative discussion of the character of the modes along the branches $AB'$ and $A'B'$ of the $\omega$-surface for an actual crystal is also illuminating. In general the wave field consists of two plane-wave components of unequal strength, $C\{\exp(\imath kr) + \xi \exp(\imath k'r)\}$, where $k$ and $k'$ have their usual meaning; $\xi$ is the ratio in amplitude of the two plane-wave components. The magnitude of $\xi$ (*) varies continuously, going from $B'$ ($\xi \gg 1$) via $A$ ($\xi \to +0$), $B$ ($\xi \to -0$) to $A'$ ($\xi \ll -1$). Far away from the plane $P_{hkl}$ a mode consists mainly of one plane-wave component, i.e. $\exp(\imath kr)$ at $A$ and $B$ and $\exp(\imath k'r)$ at $A'$ and $B'$. For modes at the Bragg angle (k on the plane $P_{hkl}$) the two plane-wave components have equal amplitude ($\xi = \pm 1$); the modes are either $\exp(\imath kr) + \exp(\imath k'r)$ at $D$ or $\exp(\imath kr) - \exp(\imath k'r)$ at $E$. These wave fields have either nodes halfway between the reflecting planes of atoms (at $D$) or nodes at the reflecting planes of atoms (at $E$).

Finally it must be mentioned in these qualitative considerations that the $\omega$-surface is different for the two main directions of polarisation of the electromagnetic field. There is a pair of branches for such a polarisation that the dielectric induction $D$ lies in the reflecting planes of atoms and hence is perpendicular to the plane of fig. 1 (TD-mode); $D$ follows then the exponential or combined behaviour indicated above. There is a second pair of branches where the magnetic field $H$ has these properties (TH-mode). These TH-modes propagate in a slightly different manner because of the fact that the dielectric induction $D$ has different directions in space for the two predominant plane-wave components. Even at the exact Bragg angle, where $\xi$ equals $-1$, the total dielectric induction, although minimum, is not equal to zero at the reflecting planes.

2.2. Quantitative discussion

In the dynamical theory of X-ray diffraction the actual shape of the $\omega$-surface is derived by solving Maxwell's equations for a medium of periodically varying dielectric constant. Under the assumption of small $\psi$, it may be shown (see /

*) The sign of $\xi$ depends on the sign of $\psi_1$. Here $\psi_1 < 0$. 
ref. 7, p. 117) that only two plane-wave components predominate, but that then their k-vectors have to satisfy the equations

\[ \omega^2/c^2 = |k|^2 - V_0 - V_1 \xi, \quad \omega^2/c^2 = |k - 2b|^2 - V_0 - V_1/\xi, \quad (2) \]

where \( V_0 = (\omega/c)^2 \psi \),

\[ V_1 = (\omega/c)^2 \psi_1, \text{ for TD-modes,} \]

\[ V_1 = (\omega/c)^2 \psi_1 \cos 2\theta, \text{ for TH-modes,} \]

with \( \sin \theta = b\alpha_0/k_0 \).

\( \theta \) being the Bragg angle. The parameter \( \xi \) is again the ratio in amplitude of the two components.

The shape of the \( \omega \)-surface is obtained from these two equations by eliminating \( \xi \):

\[ \omega^2/c^2 = |k|^2 - 2b(k - b) - V_0 \pm \{[2b(k - b)]^2 + V_1^2\}^{1/2}. \quad (3) \]

This equation is not quite of the form (1), because of the explicit \( \omega \)-dependence of \( V_0 \) and \( V_1 \), and the implicit \( \omega \)-dependence of \( \psi_0 \) and \( \psi_1 \). For our purpose we may neglect the \( \omega \)-dependence of \( V_0 \) and \( V_1 \) and regard them as constants. Equation (3) now represents an \( \omega \)-surface as discussed in the previous section. The upper sign corresponds to the left-hand branch of fig. 1, the lower sign to the right-hand branch. The asymptotes are reached for \( |b(k - b)| \gg V_1 \). In fig. 2 the region around \( k_0 \) is redrawn. The shape of the branches is calculated from eq. (3). The value of \( \xi \) for the different modes is given as parameter along the branches (\( \psi_1 < 0 \)).

Fig. 2. Enlargement of the region around \( k_0 \) of fig. 1. The \( \omega \)-surface is now drawn to scale. The magnification may be deduced from the fact that the smallest distance between the two branches is equal to \( |k_0|\psi_1/\cos \theta \), with \( \psi_1 \) of the order of \( 10^{-5} \).
The direction of energy flow (Poynting vector) is given by the group velocity of the mode. It has been shown (see, for example, ref. 12) that the group velocity is parallel to the normal of the \( \omega \)-surface and may be calculated from the equation

\[ \mathbf{v}_g = \nabla_k \omega. \]  

(4)

For modes far off the Bragg angle the direction of \( \mathbf{v}_g \) coincides with the phase velocity of the predominant plane-wave component. For modes near the Bragg angle the direction of \( \mathbf{v}_g \) changes rapidly with \( k \). It is parallel to the reflecting planes at the Bragg angle. The direction and magnitude of \( \mathbf{v}_g \) can be calculated from eqs (2), taking \( \nabla_k \) of both and eliminating \( \nabla_k \xi \). One obtains then

\[ \mathbf{v}_g \omega/c^2 = k - b + b (1 - \xi^2)/(1 + \xi^2). \]  

(5)

The amount of electromagnetic energy flowing in the direction of \( \mathbf{v}_g \) may be expressed by the magnitude of the Poynting vector, \( \mathbf{P} \), giving the energy flux per unit area perpendicular to \( \mathbf{v}_g \). In view of the discussions in the next sections, however, we shall introduce instead of \( \mathbf{P} \) the intensity, \( I \), of a beam. It is related to \( \mathbf{P} \) by the equation

\[ I = \int_S \mathbf{P} s \, dS, \]  

(6)

where \( s \) is a unit vector of arbitrary direction and \( S \) is the area of the beam perpendicular to \( s \). The quantity \( I \) is especially useful for diverging and curved beams, since \( I \) is constant in these cases (apart from absorption), whereas \( \mathbf{P} \) is not, neither in direction, nor in magnitude. For one mode of propagation it is easily shown that

\[ 2\epsilon I = D^2(1 + \xi^2)(v_g s) S, \]  

(7)

where \( D \) is the amplitude of the dielectric induction of the plane-wave component \( k \).

Up till now we have completely neglected the absorption of the electromagnetic energy in the crystal. The absorption may be accounted for by adding small imaginary parts, \( jW_0 \) and \( jW_1 \), to the real quantities \( V_0 \) and \( V_1 \) respectively. Since \( \omega \) and \( b \) are real, one immediately sees that eq. (1) is only satisfied in the imaginary part if an imaginary vector \( jK \) is added to \( k \). \( K \) is not necessarily parallel to \( k \). Since all imaginary parts are small compared with their real parts, we may find \( K \) by expanding eq. (1) in a Taylor series, taking into account only the first-order terms of the increments \( jW_0 \), \( jW_1 \) and \( jK \), and setting the sum of all imaginary terms equal to zero. This procedure yields

\[ K \nabla_k \omega + W_0 \frac{\partial \omega}{\partial V_0} + W_1 \frac{\partial \omega}{\partial V_1} = 0. \]

According to this equation we can only determine \( K_g \), the component of \( K \) in
the direction of \( \mathbf{v}_g \) (\( \nabla_k \omega \)). Fortunately \( K_g \) is the only relevant component because it expresses the fractional decrease in the amplitude of the mode per unit length in the direction of energy flow, in so far it is caused by absorption. Since the decrease in \( I \) is only determined by the absorption, and both \( P \) and \( I \) are proportional to the square of the amplitude of the mode, the relative decrease in \( I \) per unit length in the direction of \( \mathbf{v}_g \) is equal to

\[
\frac{1}{I} \frac{dI}{dl} = -\frac{2}{|\mathbf{v}_g|} \left( \frac{\partial \omega}{\partial V_0} + \frac{\partial \omega}{\partial V_1} \right).
\]

Substitution of the actual dependence of \( \omega \) on \( V_0 \) and \( V_1 \) for a given \( k \) (eq. (3)), and eliminating \( k \) by the introduction \( \xi \) of \( \xi \) leads to:

\[
\frac{1}{I} \frac{dI}{dl} = -\mu_0 \left\{ 1 + \epsilon \frac{2\xi}{1 + \xi^2} \right\} c/|\mathbf{v}_g|,
\]

where \( \mu_0 = -W_0 c/\omega \), the absorption coefficient for waves far off the Bragg angle, and \( \epsilon = W_1/W_0 \). According to eq. (8) the effective absorption coefficient is not the same for every mode. For \( \xi > 0 \) (left-hand branch) it is larger than \( \mu_0 \), for \( \xi < 0 \) (right-hand branch) it is smaller than \( \mu_0 \). Extreme values occur for \( \xi = \pm 1 \):

\[
\frac{1}{I} \frac{dI}{dl} = -\mu_0 (1 \pm \epsilon)/\cos \theta.
\]

This behaviour may be understood as follows: The absorption of X-ray energy mainly takes place through the inner electrons of the atoms. Accordingly we may expect the imaginary parts of \( \psi_0 \) and \( \psi_1 \) to be almost equal (for point-shaped atoms they are exactly equal). Hence \( \epsilon \) is close to unity for TD-modes, whereas for TH-modes \( \epsilon \) will be smaller than unity because of the factor \( \cos 2\theta \) in \( V_1 \). The very small apparent absorption coefficient of the TD-mode with \( k \) at the Bragg angle and \( \xi = -1 \) is in agreement with the result given earlier that in this case the nodes of the dielectric induction are located on the atoms. If \( \xi = 1 \) the dielectric induction is maximum at the atoms and the absorption of energy will be stronger than far off the Bragg angle. For the TH-mode of propagation the dielectric induction will nowhere be zero even for \( \xi = -1 \) as mentioned above. The minimum absorption coefficient for TH-modes will hence be larger than for TD-modes. The small absorption coefficient for modes of propagation near to the plane \( P_{hkl} \) is essential to the explanation of the anomalous transmission of X-rays in perfect crystals.

*) We prefer \( \xi \) as parameter to characterize the mode rather than its k-vector. The variations of \( k \) in the region of interest are very small, whereas \( \xi \) may have any value between \(-\infty\) and \(+\infty\).

**) Not to be confused with the dielectric constant \( \epsilon \).
3. Matching at boundaries

For a finite crystal slab the wave fields inside the crystal have to be matched with those outside the crystal, in two respects: (a) the periodicity along the surface must be the same inside and outside; (b) the total amplitudes of the fields on both sides of the boundary have to be the same.

As incident beam we take a plane-wave field, propagating in vacuum, with wave vector $\mathbf{k}_1$, and polarized in either TD- or TH-mode. We assume further $\mathbf{k}_1$ to be in the neighbourhood of $\mathbf{k}_0$ (fig. 1). Although a strict treatment of the case $\mathbf{k} \approx \mathbf{k}_0 - 2\mathbf{b}$ is also possible, it is in that case a simpler procedure to reverse the sign of $\mathbf{b}$ (or $\theta$) in the treatment given below. Finally we will consider only the Laue case of diffraction, so that no reflected beam will be present in the vacuum at the front of the crystal. Matching condition (a) now requires

$$\mathbf{k} = \mathbf{k}_1 + \beta \mathbf{s},$$

where $\mathbf{s}$ is the front-surface normal (see fig. 3). The value of $\beta$ has to be adjusted so that $\mathbf{k}$, characterizing the mode propagating in the crystal, lies on the $\omega$-surface of the correct frequency. There are always two solutions for $\beta$ corresponding to points on the two different branches of the $\omega$-surface. The $\xi$-values of the two solutions are found by substituting eq. (9) in eqs (2) and eliminating $\beta$. The higher-order terms in $\beta$ may be neglected, because of the smallness of $\nu_0$ and $\nu_1$. Thus,

$$\xi - \gamma \frac{\nu_0}{\nu_1} = 2 \gamma \frac{2\mathbf{b} (\mathbf{k}_1 - \mathbf{b})}{\nu_1} + (\gamma - 1) \frac{\nu_0}{\nu_1}. \quad (10)$$

Here $\gamma$ determines the orientation of $\mathbf{s}$ with respect to $\mathbf{b}$ and $\mathbf{k}_1$:

$$\gamma = \frac{\mathbf{k}_1 \cdot \mathbf{s}}{(\mathbf{k}_1 - 2\mathbf{b}) \cdot \mathbf{s}}. \quad (11)$$

Note that in both equations $\mathbf{k}_1$ may be replaced by $\mathbf{k}_0$, obeying the Bragg
condition, without introducing a significant error. In the symmetrical Laue case \((s\parallel b)\) \(\gamma\) is equal to unity.

The amplitudes of the two modes follow from the amplitude matching at the surface:

\[
D_1 = -\frac{\xi_2}{\xi_1 - \xi_2} D_0,
\]

\[
D_2 = \frac{\xi_1}{\xi_1 - \xi_2} D_0.
\]

The subscripts 0, 1 and 2 refer to vacuum and the two different modes. If a beam of intensity \(I_0\) impinges on the surface, the two modes of propagation activated in the crystal give rise to two beams in the crystal, each with its own direction of propagation. The intensities of the two beams, \(I_1\) and \(I_2\), may be found from the matching conditions (12) by using further eqs (7), (10) and (11):

\[
I_1 = \frac{\gamma}{(\gamma + \xi_1^2)} I_0, \quad I_2 = \frac{\gamma}{(\gamma + \xi_2^2)} I_0, \quad I_1 + I_2 = I_0.
\]

From eq. (10) it follows immediately that the product of \(\xi_1\) and \(\xi_2\) is equal to \(-\gamma\), which is negative in the Laue case of diffraction. The beam with \(\xi > 0\) will be absorbed quickly. The other beam with \(\xi < 0\) will be attenuated only slowly.

At the exit face of the crystal slab quite similar boundary conditions hold. Each beam now resolves into two beams in vacuum; one almost parallel to \(k_0\) (transmitted direction) and one almost parallel to \(k_0'\) (reflected direction). We will consider slabs of such thickness that only the weakly damped beam with \(\xi < 0\) still gives an appreciable intensity, the other beam with \(\xi > 0\) being attenuated to a negligible intensity. The intensities of the beams emerging from the exit face in the transmitted direction \((I_T)\) and in the reflected direction \((I_R)\) are related to the intensity \(I_{\xi}\) of the weakly damped mode arriving at the exit face, by the equations

\[
I_T = \frac{\gamma}{(\gamma + \xi^2)} I_{\xi}, \quad I_R = \frac{\xi^2}{(\gamma + \xi^2)} I_{\xi}.
\]

In these equations the expression (11) for \(\gamma\) must be used with the values of \(k_1\), \(b\) and \(s\) corresponding to the situation at the back surface of the crystal slab.

4. Strained crystals

4.1. General considerations

The dynamical theory of X-ray diffraction as outlined above is only valid for perfect and unstrained crystals. The Fourier analysis of the dielectric constant gave as the only relevant component the vector \(b\) and the amplitude \(V_1\). In a strained crystal the lattice planes are curved and not parallel, so that it is now impossible to characterize the crystal by one value for \(b\) and one for \(V_1\). We will consider, however, only those cases where the strain varies slowly
from place to place. It should then be possible to describe the set of reflecting planes of a sufficiently small part of the crystal with one \( \mathbf{b} \) and a corresponding \( V_1 \). The entire crystal may then be considered as a medium of slowly varying \( \mathbf{b} \). The variation in \( V_1 \) will be neglected. At the same time we will split up the X-ray wave field inside the crystal into beams so narrow that within the width of the beam the crystal is characterized by one \( \mathbf{b} \) and, on the other hand, so wide that the corresponding uncertainty in the \( k \)-value is small compared with, for example, the minimum distance between the two branches of the \( \omega \)-surface in \( k \)-space. In this way we have gained the advantage that at least the local behaviour of the beam is given by the dynamical theory with the aid of the local values of \( \mathbf{b} \) and \( \mathbf{k} \).

A beam arriving at the location \( \mathbf{r} \) will propagate further over a distance \( dl \) in the direction of the group velocity. In vector terms:

\[
dr = a \, dl \, \nabla_k \omega ,
\]

where \( a = |\nabla_k \omega|^{-1} \). At the new location \( \mathbf{r} + dr \), \( \mathbf{b} \) will have changed by a small amount

\[
db = (dr \cdot \nabla_r) \mathbf{b} = a \, dl \, (\nabla_k \omega \cdot \nabla_r) \mathbf{b} .
\]

If this change takes place abruptly, each of the two plane-wave components of a single mode present at \( \mathbf{r} \) will activate two modes at \( \mathbf{r} + dr \), one on each branch (see sec. 3). In all, 4 modes are activated by one single mode. If \( db \) is only small the two modes on the other branch as the original one will have small amplitudes and the modes on the same branch will be close together.

In order to see what happens in a crystal with slowly varying \( \mathbf{b} \), we first inspect the somewhat analogous case of a beam of light passing through a medium of slowly varying index of refraction \( n \). There we know that the \( k \)-value of the beam varies slowly along the path of the beam; no spreading out of the \( k \)-value will take place if the variation in \( n \) is sufficiently slow. In that case, along the path of the beam the change \( dk \) in \( k \) is parallel to \( \nabla_r n \), the direction in space where \( n \) varies most rapidly.

We now assert that the propagation of an X-ray in a crystal with sufficiently slowly varying \( \mathbf{b} \) can also be described with slowly varying \( k \)- and \( k' \)-values along the path of the beam, without spreading out in \( k \)-space of the \( k \)-values. This implies that, along the path of the beam, a given mode remains on one branch of the \( \omega \)-surface. The question is now to what extent the crystal at a given point \( P \) must be considered as inhomogeneous. Let us consider \( \omega \) as a function of \( \mathbf{b} \) and \( \mathbf{k} \). For the crystal to be homogeneous as far as one plane-wave component is concerned, it is not necessary that \( \mathbf{b} \) is the same everywhere in the neighbourhood of \( P \). For one plane-wave component with wave vector \( \mathbf{k} \), the crystal may already be considered as homogeneous, if the variations in \( \mathbf{b} \) around \( P \) are such that \( d\omega \) is zero for constant \( \mathbf{k} \). Non-vanishing values of \( d\omega \)
occur only if the component of $b$ in the direction of $\nabla_b \omega$ shows variations around $P$. In that case the crystal must be considered as inhomogeneous as far as the propagation of the component $k$ of the mode is concerned. We now assert that the variation $dk$ along the path of the beam will be in the direction of the inhomogeneity, i.e. in the direction of the gradient of the component of $b$ just mentioned. Mathematically,

$$dk = \beta \nabla_r (b \cdot \nabla_b \omega).$$

The proportionality factor $\beta$ can be determined from the condition that along the path of the beam we must have

$$d\omega = dk \cdot \nabla_k \omega + db \cdot \nabla_b \omega = 0.$$  \hspace{1cm} (17)

Together with eq. (16) we find

$$dk = -a \frac{dl}{r} \nabla_r (b \cdot \nabla_b \omega).$$  \hspace{1cm} (18)

A similar argument must be given for the other plane-wave component of the mode. The variation $dk'$ is then found to be

$$dk' = -a \frac{dl}{r} \nabla_r (b' \cdot \nabla_b \omega),$$

where $\nabla_{b'} \omega$ represents the gradient of $\omega$ with respect to $b$, for constant $k' = k - 2b$. One now derives easily:

$$dk' = dk - 2a \frac{dl}{r} (b \cdot \nabla_k \omega).$$  \hspace{1cm} (19)

Finally we must check that the expressions for $dk$, $dk'$ and $db$ are consistent with the assertion that along the path one mode remains one mode on a branch of the $\omega$-surface, i.e. we still must prove that

$$dk' = dk - 2 db = dk - 2a \frac{dl}{r} (\nabla_k \omega \cdot \nabla_r) b.$$  \hspace{1cm} (20)

Equations (19) and (20) are identical if the vector $b$ is rotation-free. In the next section we shall show that this is always the case (eq. (21)).

4.2. Quantitative discussion

The deformation of the crystal is conveniently described by a displacement vector $v$. If the location of a lattice point prior to deformation is $R$ and after deformation $r$, then

$$r = R + v.$$  

By neglecting higher-order terms in $v$ (deformation is small) we may consider $v$ as a function of $r$ instead of $R$.

In the undeformed crystal the reflecting planes must be given by

$$Rb' = \pi m,$$
where \( m \) is an integer, and \( b' \) is \( \pi \) times the reciprocal lattice vector in the undeformed crystal. The strain deforms the lattice planes:

\[
r b' - v b' = \pi m.
\]

The new reciprocal lattice vector \( b \) is equal to

\[
b = b' - \nabla_r (v b').
\]  (21)

The variations in \( k \) and \( b \) can now be described in terms of the displacement vector:

\[
dk = adl \nabla_r (\nabla_b \omega \cdot \nabla_r)(v b'),
\]

\[
db = - adl \nabla_r (\nabla_k \omega \cdot \nabla_r)(v b').
\]

In these equations \( \omega \) has to be considered as a constant in regard to differentiation with respect to \( r \).

We are now able to calculate the change in the important parameter \( \xi \), characterizing the mode. Using eqs (2) we obtain

\[
d\xi = 4 \frac{\xi^2}{1 + \xi^2} \frac{adl}{V_1} [ (b \cdot \nabla_r)(\nabla_b \omega \cdot \nabla_r)(v b') - (k - 2b) \cdot \nabla_r)(\nabla_k \omega \cdot \nabla_r)(v b')].
\]

The introduction of the actual shape of the \( \omega \)-surface yields

\[
d\xi = -4 \frac{\xi^2}{1 + \xi^2} \frac{cl}{\omega} \{ (k_0 - 2b') \cdot \nabla_r \} (k_0 \cdot \nabla_r)(v b').
\]  (22)

In this equation the small variation of \( \xi \), after propagation of the mode over a distance \( dl \), is correlated to the small displacement vector \( v \). The small differences between \( k \)-vectors in the neighbourhood of \( k_0 \) (see fig. 1) have been neglected since they are of the same order or smaller than \( \nabla_r (v b') \).

The behaviour of a narrow X-ray beam in a finite deformed crystal is now completely determined. Equation (10) gives the \( \xi \)-values for the two modes activated in the crystal by the incident beam, eq. (13) their intensities. The path of the beam inside the crystal is determined simultaneously by the group velocity, eq. (5), tangent to the path, and the variation of \( \xi \) along the path, eq. (22). In general the path will be curved. The attenuation of the beam is determined by eq. (8), and is place-dependent through \( \xi \). At the exit face the transmitted and diffracted beams are formed; their intensities are given by eq. (14) where the local values of \( \xi, \gamma \), and the intensity of the beam arriving at the back surface have to be used.

5. Numerical calculations

In numerical calculations it is convenient to introduce a coordinate system based on the boundaries rather than the lattice planes. We define the \( XZ \)-plane as the plane of incidence, and the \( Z \)-axis as the normal to the front and back...
faces of the sample. We will neglect the difference between \( b' \) and \( b \), \( k_0 \) and \( k \), and accordingly assume the lattice planes to be flat and parallel, except of course for the influence of the curvature on the behaviour of the X-ray beam as expressed in the equations derived in the previous sections. Further we introduce the unit vectors \( l, m \) and \( n \) as follows:

\[
k_0 = l \omega/c, \quad k_0 - 2b = m \omega/c, \quad b = n(\omega/c) \sin \theta.
\]

Finally we will use as partial alternative for \( \xi \) the parameter \( \eta \):

\[
2\eta = \xi - (\gamma/\xi).
\]

The parameter \( \eta \) is a measure of the deviation of the incident X-ray beam \( (k_1) \) from the orientation for exact Bragg reflection, as follows from eq. (10). The equations reduce to

\[
d\eta = \frac{\xi^2 + \gamma}{2\xi^2} \, d\xi = -2 \frac{\sin \theta}{\psi} \gamma \frac{dz}{ls} (l \cdot \nabla_r) (m \cdot \nabla_r) (nv),
\]

\[
\frac{dI}{I} = -\frac{1 + \xi^2 + 2\xi \gamma}{\gamma + \xi^2} \frac{dz}{ls},
\]

\[
\frac{dx}{dz} = \frac{1 - \gamma \xi^2 - (\gamma - \xi^2) \cos 2\theta}{(\gamma + \xi^2) \sin 2\theta}.
\]

In experimental techniques it is common practice to determine the "integrated intensities", i.e. the total power transmitted through the sample either in the transmitted or reflected direction, when the sample is "rocked" through the Bragg angle with constant angular speed. In our terms these correspond to the integrals

\[
T = \int_{-\infty}^{\infty} \gamma I_T \, d\eta, \quad R = \int_{-\infty}^{\infty} \gamma I_R \, d\eta.
\]

5.1. Crystals deformed by a uniform temperature gradient

A crystal subjected to a uniform temperature gradient is deformed although no internal stresses are present. The lattice planes perpendicular to the temperature gradient \( \nabla_r T \) are curved with a radius \( R \), where

\[
1/R = \nabla_r (aT),
\]

with \( a \) the coefficient of linear thermal expansion. The lattice planes parallel to \( \nabla_r T \) remain flat, but become tapered with respect to each other. The displacement vector is given by *)

\[
v = r \{r \cdot \nabla_r (aT)\} - \frac{1}{2} (rr) \nabla_r (aT).
\]

*) Valid only if \( \nabla_r (aT) \) is constant in direction and magnitude. In other cases stresses will build up, giving rise to extra terms in \( v \). Do not confuse \( T \) and \( R \) with those of eq. (27)!
We will consider the symmetrical Laue case: reflecting atom planes perpendicular to front and back faces (see fig. 4a). The thickness, \( t \), will be taken so large that the heavily damped mode gives only a negligible contribution to \( I_T \) and \( I_R \).

Fig. 4. The geometry of the crystal as studied in sub-section 5.1. The reflecting planes are perpendicular to the front and back faces of the crystal. A temperature gradient gives the crystal another shape. Two exaggerated examples are shown in b and c. Possible X-ray beams are given: drawn lines for the slowly damped mode, dashed lines for the heavily damped mode.

For the variation in \( \eta \) we find according to eq. (24)

\[
d\eta = 2 \frac{\tan \theta}{\psi_1} n \cdot \nabla_r (aT) \, dz.
\]

Since the temperature gradient is constant, \( \eta \) varies linearly with \( z \),

\[
2\eta = \xi - 1/\xi = \xi_i - 1/\xi_i + 2 \beta z,
\]

with

\[
\beta = 2 \left( \tan \theta / \psi_1 \right) n \cdot \nabla_r (aT).
\]

The subscript \( i \) refers to values at the face of entrance. From this equation we may conclude immediately that if \( \nabla_r (aT) \) is perpendicular to \( n \), i.e. parallel to the reflecting planes, the parameter \( \eta \) is independent of \( z \). There is no change in character of the mode during passage through the crystal. The behaviour of the beam is as if no strains were present, although the reflecting planes are not parallel. The path of the beam is a straight line as indicated in fig. 4b.

If the temperature gradient is perpendicular to the lattice planes the parameter \( \beta \) is not equal to zero. The character of the mode will vary along the path of the beam. In fig. 5 it is shown how the local \( k \)-value of one mode will move along the \( \omega \)-surface as the beam passes through the crystal. It should be noted that in fig. 5 the \( \omega \)-surface is kept in the same position; in reality it will move in \( k \)-space because of the change in \( b \). The incident beam activates in...
Fig. 5. The movement of the \( \mathbf{k} \)-vector characterizing a mode, along the \( \omega \)-surface, when the reflecting planes are curved by a uniform temperature gradient (see fig. 4c). At the entrance face \( \mathbf{k} \) is located at \( \xi_1 \) or \( \xi'_1 \). At the exit face \( \mathbf{k} \) has moved upwards to \( \xi_2 \) or \( \xi'_2 \). Note the change in direction of the energy flux \( \mathbf{P} \).

the crystal two modes, one on each branch, characterized by, for example, \( \xi_1 \) and \( \xi'_1 \). According to eq. (10) the parameter \( \eta \) is directly proportional to the distance between \( \mathbf{k} \) and the plane \( P_{hkl} \). Equation (28) now indicates that this distance varies linearly with \( z \). In the situation drawn in fig. 4c \( (\nabla_r(\alpha T) \cdot \mathbf{n} > 0) \) the vectors \( \mathbf{k} \) for the two activated modes will move upwards along the \( \omega \)-surface until they reach points indicated by \( \xi_2 \) and \( \xi'_2 \) when the beam reaches the exit face. The total distance travelled by the \( \mathbf{k} \)-vectors in a vertical sense is independent of \( \xi_1 \) and is determined only by \( \beta t \). The most interesting consequence of this behaviour is that the direction of \( \mathbf{v}_g \) changes considerably during the propagation through the crystal. In the example given in fig. 5, \( \mathbf{v}_g \) is pointing upwards at the entrance face and pointing downwards at the exit face, at least for the slowly damped mode on the right-hand branch. For the heavily damped mode \( \mathbf{v}_g \) is first pointing downwards and at the end of the path in the crystal pointing upwards. Since the vector \( \mathbf{v}_g \) is always parallel to the path of the beam, this behaviour must lead to curved paths. Examples of such curved paths are shown in fig. 4c and fig. 6. Path 1 of fig. 6 corresponds

Fig. 6. Three possible paths of an X-ray beam in a crystal with curved reflecting planes. The absorption of energy in the crystal is minimum for such an angle of incidence that the beam follows path 2.
to the case $\xi_e = -1$; the path is parallel to the reflecting planes at the exit face. For path 2, $\xi = -1$ in the centre of the crystal and for path 3, $\xi_i = -1$. Note that for path 2 the beam leaves the crystal at the same lattice planes as it entered the crystal, although it did not follow these planes while passing through the crystal. The mathematical expression for the path corresponding to an arbitrary value of $\xi_i$ may be obtained by integrating eq. (5), taking into account the dependence of $\xi$ on $z$:

$$[2\beta x / \tan \theta + \xi_i + 1/\xi_i]^2 - [2\beta z + \xi_i - 1/\xi_i]^2 = 4.$$  (30)

For the slowly damped mode ($\xi_i < 0$) the path is curved in the same direction as the reflecting planes, whereas for the heavily damped mode the path is curved the other way. The curvature is maximum at that point where $\xi = -1$ and is then equal to $2\beta$. This maximum curvature is hence directly proportional to the curvature of the lattice planes, the proportionality factor being of the order of $1/\psi_i (= 10^5)$.

The attenuation of the intensity of the beam is also dependent on the value of $\xi$ (eq. (8)). It is minimum for $\xi = -1$, i.e. when the path is parallel to the reflecting planes. The more the path deviates from this direction, the stronger is the absorption of energy. It is clear that of all possible paths, path 2 of fig. 6 will cause minimum damping. The overall absorption in this case, however, will be larger than the minimum absorption in the unstrained case. The relative decrease in intensity of the beam may be calculated by integrating eq. (8), remembering that $\xi$ varies with $z$.

At the exit face the beam resolves into two beams, the transmitted and the reflected beam. The intensities of these two beams will depend on the intensity of the beam arriving at the exit face and on the direction ($\xi$-value) of the beam there. For path 1 (fig. 6) $I_T$ will be equal to $I_R$, but for paths 2 and 3 $I_R$ will be larger than $I_T$. Note that if $\nabla_r(aT)$ had the opposite sign, the curvature would have been in the other way and $I_R$ would have been smaller than $I_T$ for paths 2 and 3. Applying the boundary conditions (13) and (14), and taking into account the absorption in the crystal, one obtains the following relations between $I_T$, $I_R$ and $I_0$:

$$\frac{I_T}{I_0} = \frac{1}{1 + \xi_i^2} \frac{1}{1 + \xi_e^2} \exp \left\{ -\mu_0 t \left( 1 + \frac{\varepsilon}{\beta t} \ln \frac{\xi_e}{\xi_i} \right) / \cos \theta \right\},$$

$$\frac{I_R}{I_0} = \frac{1}{1 + \xi_i^2} \frac{\xi_e^2}{1 + \xi_e^2} \exp \left\{ -\mu_0 t \left( 1 + \frac{\varepsilon}{\beta t} \ln \frac{\xi_e}{\xi_i} \right) / \cos \theta \right\}. \quad (31)$$

In these equations we have neglected the contribution of the heavily damped mode. The subscript $e$ refers to values at the exit face. The relation between $\xi_i$ and $\xi_e$ (both $< 0$) may be derived from

$$\xi_e - 1/\xi_e = \xi_i - 1/\xi_i + 2\beta t.$$  (32)
Fig. 7. Plot of the intensities of the transmitted and reflected beams as a function of $\eta t$ which is directly proportional to the deviation of the incident beam from the exact Bragg condition. The incident beam (intensity $I_0$) is assumed to be polarized parallel to the reflecting planes. The strain of the crystal is directly proportional to $\eta t$.

Fig. 8. The integrated intensities of the transmitted ($T$) and reflected ($R$) beams as a function of $\beta t$ for the same conditions as in fig. 7.
In figs 7 and 8 some numerical results are shown. In fig. 7 the transmitted and reflected intensities are given as a function of $\eta_t$, the deviation from the exact Bragg angle of the incident beam. For the unstrained specimen ($\beta = 0$), $I_T$ and $I_R$ are approximately equal and show symmetry about $\eta_t = 0$. For the deformed crystal ($\beta t \neq 0$) the $I_R$ and $I_T$ curves are symmetrical around $\eta_t = -\frac{1}{2} \beta t$. The maxima are smaller than for the unstrained crystal. Several details discussed above also appear in fig. 7, such as $I_T = I_R$ if $\eta_t = -\beta t$ and the reversal of the ratio $I_R/I_T$ if $\beta$ changes sign. It is noteworthy that in this last case $I_T$ remains equal. In fig. 8 the integrated intensities obtained by numerical integration according to eq. (27) are shown as a function of $\beta t$.

Finally we want to emphasize that very small temperature gradients already have an influence on the anomalous transmission. The parameter $\beta t$ is directly proportional to the temperature difference $\Delta T$ between two points a distance $t$ apart in the direction of the temperature gradient. From fig. 7 it follows that the influence of the temperature gradient on the anomalous transmission may be detected if $\beta t = 1$. Since the coefficient of thermal expansion ($a$) and $\psi_1$ are both of the order of magnitude of $10^{-5}$ to $10^{-6}$, we may conclude (see eq. (29)) that $\Delta T = 1 \degree C$ is sufficient. For a specimen of 1 cm thick this would correspond to a radius of curvature of the reflecting planes of approximately one mile.

5.2. Crystals strained by a bending moment

We now consider the case of a crystal deformed elastically by a bending moment. For convenience, we assume the crystal to be isotropic with Poisson's ratio $\nu$. The geometry is shown in fig. 9. The axis of bending is parallel to the $Y$-axis. The reflecting lattice planes make an angle of $\frac{1}{2} \pi + \varphi$ with the positive $X$-axis. The radius of curvature in the $XZ$-plane is denoted by $R$. The compo-

Fig. 9. The geometry of the crystal studied in sub-section 5.2. In the situation as drawn both $\varphi$ and $R$ are positive. The curvature of the reflecting planes is too small to be visible in the figure.
nents of the displacement vector in the $x$, $y$ and $z$ directions are respectively given by

$$u = \frac{xz}{R}; \quad v = -\frac{vyz}{R}; \quad w = -(x^2 - vy^2 + vz^2)/2R.$$  

From this displacement vector and the given orientation of the reflecting planes we obtain from eq. (24), after some manipulation,

$$d\eta = \frac{\gamma - 1}{\psi_1 R} [1 + (\cos 2\theta + \cos 2\phi)(1 + \nu)/2] \, dz.$$  

As in the previous case $d\eta/dz$ is constant and we may write

$$2\eta = \xi - \frac{\gamma}{\xi} = \xi_t - \gamma/\xi_t + 2\beta z,$$  

where

$$\beta = \frac{\gamma - 1}{\psi_1 R} [1 + (\cos 2\theta + \cos 2\phi)(1 + \nu)/2].$$  

As $\gamma$ is given by eq. (11), we see that, for $\phi = 0$, $\gamma = 1$ and $\beta = 0$, indicating that now the beam propagates through the crystal uninfluenced by the strain. It must be noted that only in this case are the reflecting lattice planes flat, although not parallel. Since eq. (33) is quite similar to eq. (28), derived for the previous case, we may expect a similar behaviour of the X-ray beam inside the crystal as discussed in sub-section 5.1. The path is curved and more energy is absorbed than in the unbent crystal, provided $\phi \neq 0$. In this case also the slowly damped mode is curved in the same direction as the reflecting planes.

The expressions for $I_T$ and $I_R$ are somewhat different in this case, since $\gamma \neq 1$. One obtains by integrating eq. (25) and applying the proper boundary conditions (eqs (13) and (14)):

$$I_T = I_0 - \frac{\gamma}{\xi_t^2 + \gamma} \frac{\gamma}{\xi_0^2 + \gamma} \exp \left\{ -\mu_0 \left[ 1 + \frac{\gamma - 1}{2\beta t} (\xi_0 - \xi_t) + \frac{\gamma}{\beta t} \ln \frac{\xi_0}{\xi_t} \right] \cos (\theta - \phi) \right\},$$

$$I_R = \left( \frac{\xi_0^2}{\gamma} \right) I_T.$$  

(35)

The contribution of the heavily damped mode has been neglected. The relation between $\xi_0$ and $\xi_t$ follows from eq. (33):

$$\xi_0 - \gamma/\xi_0 = \xi_t - \gamma/\xi_t + 2\beta t.$$  

The signs of $\xi_0$ and $\xi_t$ must be the same since the mode remains on one branch during passage through the crystal.

In the bending experiment done by Hunter and Okkerse) the reflecting planes of the crystal are almost perpendicular to the front and back faces of the sample, but not exactly so. A representative value for $\phi$ of 0.5° gives values for $\gamma$ of 1·007 or 0·993 ($\theta = 22.5^\circ$). Equations (35) are not very sensitive for such small variations in $\gamma$, so that we may put $\gamma = 1$ in those cases where $\phi$ is
small, except of course in the value of $\beta$. The dependence of $I_T$ and $I_R$ on $\beta t$ has been discussed in the previous section. With eq. (34) one can show that for $\phi = 0.5^\circ$ and $\psi_1 = 10^{-8}$, the parameter $\beta t$ reaches the value of unity when the bending is such that the maximum strain ($= t/2R$) in the crystal is equal to $3 \cdot 10^{-4}$.

6. Comparison with experimental results

Although some results on the anomalous transmission of X-rays in deformed perfect crystals have been reported, a comparison between these results and the theory outlined above can be given in most cases in a qualitative way only. The lack of detailed experimental information precludes a quantitative comparison. The only exception is the study by Hildebrandt\(^{10}\) of the transmission of X-rays through calcite deformed by a temperature gradient. The theory is in agreement with his results relating to a curved path of the X-ray beam, the curvature being in the same direction as the curvature of the reflecting planes. The radius of curvature of the beam was calculated by Hildebrandt from the direction of energy flow at the exit face of the sample (determined from $I_T/I_R$) and assuming further that the path is part of a circle. If we calculate the radius of curvature defined in this way, we find

$$R(\text{refl. planes})/R(\text{beam}) = 2 \tan^2 \theta/\psi_1.$$  

Introducing the values as used by Hildebrandt, $\theta = 6.7^\circ$, $\psi_1 = 1.95.10^{-8}$, we find the same ratio as he found: $1.4.10^4$. To compare the values of $I_T$ and $I_R$ as measured by Hildebrandt we calculated for his experimental conditions ($t = 3.2$ cm, $\mu ot = 70$, $\gamma = 1.07$, $\epsilon = 0.9$) the integrated transmitted ($T$) and reflected ($R$) intensities of the deformed crystal in respect to $T_\circ$, the integrated transmitted intensity in the undeformed crystal. The anisotropy in the

![Fig. 10. Similar plot as fig. 8, but now for the case of a calcite crystal deformed by a temperature gradient. The following parameters have been used: $\theta = 6.7^\circ$, $\mu ot = 70$, $\epsilon = 0.9$, $\gamma = 1.07$.](image-url)
thermal expansion \((a// = 25.14.10^{-6}, a_\perp = -5.58.10^{-6})\) was taken into account. The results are shown in fig. 10. The ratio \(T/R\) as calculated agrees well with the experimental values found by Hildebrandt, except for the fact that the latter values are all 10% larger than the calculated ones, even in the undeformed crystal. The decrease in \(T\) and \(R\) due to the temperature difference across the sample is observed to be much steeper than the calculated decrease. For a temperature difference of 0.5 °C the measured intensities dropped to approximately 5% of the integrated intensity of the unstrained crystal, whereas the theory gives a drop of less than a factor of 2. We can give no explanation of this discrepancy.

Eindhoven, April 1961

REFERENCES

6) B. Okkerse, private communication.