Dynamical X-ray Propagation: a Theoretical Approach to the Creation of New Wave Fields

BY F. BALIBAR

Laboratoire de Minéralogie–Cristallographie, associé au CNRS, Université Pierre et Marie Curie (Paris 6) et Paris 7, 4 place Jussieu, 75230 Paris CEDEX 05, France

F. N. CHUKHOVSKII

Institute of Crystallography, Academy of Sciences of the USSR, Moscow, USSR

AND C. MALGRANGE

Laboratoire de Minéralogie–Cristallographie, associé au CNRS, Université Pierre et Marie Curie (Paris 6) et Paris 7, 4 place Jussieu, 75230 Paris CEDEX 05, France

(Received 24 February 1982; accepted 2 December 1982)

Abstract

Although it is commonly invoked, the phenomenon of ‘creation of new wave fields’, which is responsible for some of the features visible on topographic images, has never been really explained in theoretical terms. This is done here in the case of a crystal deformed by a uniform strain gradient. The appropriate Green function is expanded in reciprocal space as a wave packet of non-plane waves, each component corresponding to a single value of the deviation parameter at the entrance surface. It is then shown that each component of this wave packet is made up of four parts, two of which can be identified as ‘normal’ wave fields (i.e. those predicted by the Eikonal theory); the two others are the so-called ‘created wave fields’; it is shown that they correspond to interbranch scattering from one branch of the dispersion surface to the other and give rise to two extra beams. These created wave fields extract a fraction $e^{-2\pi l/v}$ out of the normal energy flow ($l/v$ being inversely proportional to the strain gradient), in full agreement with previous computer experiments.

I. Introduction

Understanding the so-called ‘creation of new wave fields’ in highly distorted parts of a crystal has been one
of the major challenges of the dynamical theory of X-ray propagation, over the past 15 years. This phenomenon was first predicted on a theoretical basis by Penning (1966) in his thesis and was suggested by A. Authier in 1966 at the 15th Denver Conference on X-ray Analysis as an empirical explanation (Authier, 1967) for some of the features of the topographic image of a single dislocation: according to Authier, when travelling in a sufficiently distorted region, a given wave field (i.e. a set of two plane waves, represented by a single point \( P_i \) on the dispersion surface in reciprocal space) would give rise to two wave fields; one of them, the ‘ordinary’ wave field, being the expected continuation of the initial wave field (with a tie-point lying on the same branch of the dispersion surface as \( P_i \)), while the other, the ‘newly created wave field’, would propagate in a quite different, unexpected direction and would correspond to a tie-point lying on the opposite branch of the dispersion surface (this is the reason why this phenomenon is sometimes called ‘interbranch scattering’).

The idea of interbranch scattering already lies implicitly in the lamellar models proposed for the study of the propagation of X-rays in deformed crystals (Authier, 1961; Kato, 1963a). In these models the boundary conditions are applied at the interface between neighbouring slices. Since then, this phenomenological statement has proved to be very useful as an empirical tool for the explanation of the observed images of certain types of defects (Authier, 1977). But no theoretical formulation of it has ever been given.

Clearly this phenomenon which contradicts the usual ray theory occurs when the Eikonal approximation (Kato, 1964; Penning, 1966) becomes invalid. Its theoretical treatment requires that the dynamical theory be expanded beyond the limits of applicability of the Eikonal approximation. This is, at least in principle, achieved by Takagi’s (1969) theory which establishes the partial differential equations (along with the boundary conditions) to which the amplitude of the crystal wave must obey. If one takes into account the actual experimental resolution, this theory is valid for any strength of the deformation.

In contrast to the Eikonal theory, Takagi’s treatment does not provide a direct analytical expression for the crystal wave. This latter is obtained as the convolution product of the amplitude distribution on the entrance surface (which depends on the form of the incident wave in vacuum) by the ‘influence’ or ‘Green’ function which is a function of \( r_\alpha \), \( \chi \) and \( r_\alpha \), \( \chi \) at \( P_0 \). Writing then this sine as a sum of two imaginary exponentials, one retrieves the usual wave fields \( 1 \) and \( 2 \) of the Ewald–Laue theory (Balibar, 1969a), as expected. But the mathematical manipulation involved here [writing \( \sin x \) as \( e^{ix} - e^{-ix})/2i \)] is of the most trivial type, one still lacks physical reasons for doing so. Even in that case, the two wave fields come out of the Green function in a rather artificial manner.

(2) It would seem then, that separating the Green function itself into two parts would make the structure in wave fields appear more naturally. Since \( J_0(\chi) = \frac{1}{2} \{ H_0^0(\chi) + iH_0^1(\chi) \} \) (where \( H_0^0 \) and \( H_0^1 \) are two Hankel functions), the expression for the amplitude at \( P \) is, for any shape of the incident wave, made up of two parts: one which is obtained through convolution of the incident amplitude distribution by \( H_0^0 \) and the other which involves \( H_0^1 \). Having shown that these two parts correspond, respectively, to a weakly absorbed mode, and a strongly absorbed mode, one of us (Balibar, 1968, 1969b, 1970) has proposed a description of the crystal wave in terms of ‘generalized wave fields’. Apart from the fact that it relies on a
mathematical formula \( J_0 = \frac{1}{2}(H_0^1 + H_0^2) \) without any real physical meaning, this model does not provide any understanding of how the structure in \( K \) space of the crystal wave is related to that of the incident wave.

(3) Our last example is the work by Chukhovskii & Petrashen’ (1977) where the procedure used in example (2) is extended to the case of a crystal with a uniform strain gradient. Having explicitly calculated the function which replaces \( J_0 \) in that case, these authors were able to represent it as a sum of two functions (the equivalent of the previous Hankel functions \( H_0^1 \) and \( H_0^2 \)). But this separation, obtained by means of a general mathematical formula, still does not provide any understanding of how the \( K \) structure of the incident wave is transformed in the crystal. Nor does it show any ‘creation of new wave fields’ for sufficiently large values of the strain gradient.

In this paper we show that by a proper expansion of the Green function in reciprocal space (or \( K \) vectors space) the problem of how one wavefield can (for large values of the deformation) give two wave fields (i.e. two points in reciprocal space) can be solved. This treatment, which is performed for the case of a uniform strain gradient, could give some hints on how to deal with a more general type of deformation.

II. Expansion of the Green function as a wave packet (for a constant strain gradient)

Because of its (relative) simplicity, the case of a crystal with a uniform strain gradient has been extensively studied. Kato (1964) and Penning & Polder (1961) who have treated it on the basis of the Eikonal approximation (i.e. small strain gradient), have shown that the energy trajectories for the two wave fields induced by an incident plane wave are portions of hyperbolae, the characteristics of which depend on the values of the deformation and on the departure of the incident wave from Bragg’s angle at the entrance surface. The general treatment, on the basis of Takagi’s equations, has been performed by Chukhovskii (1974), Katagawa & Kato (1974), and Litzman & Janacek (1974) who all have given the exact analytical form of the influence function.

For reasons of simplicity, and after Chukhovskii & Petrashen’ (1977), let us assume a transmission symmetric case and a constant strain gradient such that:

\[
\mathbf{h} \cdot \mathbf{u} = 4B \xi_0 \xi_h
\]

\[
B = \frac{1}{4} \frac{\partial^2}{\partial \xi_0 \partial \xi_h} (\mathbf{h} \cdot \mathbf{u}),
\]

where \( \mathbf{h} = \) reciprocal-lattice vector (= \( 2\pi \) times the usual reciprocal-lattice vector = \( 2n\mathbf{h}_{k}\)) \( \mathbf{u} = \) atomic displacement, and \( \xi_0 \) and \( \xi_h \) are reduced coordinates in the transmitted and reflected directions (see Table 1 and Fig. 1).

The Green function for the reflected \((h)\) wave is (see Chukhovskii & Petrashen’, 1977):

\[
G_h(P_o, P) = G_h[r(P_o), r(P)] = [\Theta(\xi_h) - \Theta(\xi_h)] F([-v, 1; -4iB\xi_0 \xi_h]).
\]

Table 1. Comparison of the system of coordinates and deformation parameter used by different authors (symmetric case)

<table>
<thead>
<tr>
<th>Kato</th>
<th>Penning &amp; Polder</th>
<th>Chukhovskii and this paper</th>
</tr>
</thead>
<tbody>
<tr>
<td>(</td>
<td>h</td>
<td>/2 \sin \theta)</td>
</tr>
<tr>
<td>Coordinate system</td>
<td>(x \rightarrow 0)</td>
<td>(x \rightarrow 0)</td>
</tr>
<tr>
<td>Coordinates along (K_o) and (K_h)</td>
<td>([s_x], [s_y])</td>
<td>([s_x], [s_y])</td>
</tr>
<tr>
<td>Strain gradient</td>
<td>(\beta_k)</td>
<td>(-\beta_k)</td>
</tr>
<tr>
<td>Parameter (</td>
<td>\eta</td>
<td>) at depth (z)</td>
</tr>
</tbody>
</table>
The Green function (2) can be expanded in reciprocal space by means of the Laplace transform, according to the following procedure. This is carried out here only on the term

$$\Theta(\xi_h) F_1(-v, 1; -4iB\xi_0 \xi_h)$$

since the calculation relative to

$$-\Theta(-\xi_0) F_1(-v; 1; -4iB\xi_0 \xi_h)$$

would be quite similar.

As a function of $\xi_h$ ($\xi_0$ being considered as a parameter),

$$\Theta(\xi_h) F_1(-v, 1; -4iB\xi_0 \xi_h)$$

is expanded as (see *Higher Transcendental Functions*, 1953):

$$\Theta(\xi_h) F_1(-v, 1; -4iB\xi_0 \xi_h) = \frac{1}{2\pi i} \int_{p_0}^{p_0+\infty} p^{-v-1}(p + 4iB\xi_0)^v e^{plx} dp,$$  \hspace{1cm} (4)

where $p$ and $\xi_h$ are conjugate variables relative to the Laplace transform.

Expressing in turn $(p + 4iB\xi_0)^v$ in terms of its inverse Laplace transform, one obtains:

$$\Theta(\xi_h) F_1(-v, 1; -4iB\xi_0 \xi_h) = \exp[-2iB(\xi_0 + \xi_h)^2 + 2iB\xi_0^2] \int_0^{\infty} e^{4iB\xi_0^2} \frac{t^{-v-1} (\xi_h - t)^v}{\Gamma(1+v)} e^{-2it\xi_0} dt. \hspace{1cm} (5)$$

A second Laplace transform performed on this convolution product then leads (after some straightforward manipulation) to:

$$\Theta(\xi_h) F_1(-v, 1; -4iB\xi_0 \xi_h) = \frac{1}{2\pi i} e^{-2iv2} \left(-\frac{i}{4B}\right)^{1/2} \exp[iB(\xi_0^2 - \xi_h^2 - 2\xi_0 \xi_h)]$$

$$\times \int_{p_0-\infty}^{p_0+\infty} \exp\left[\frac{p}{2} (\xi_h - \xi_0)\right] D_v\left[\left(-\frac{i}{4B}\right)^{1/2}\right] D_{-v-1}\left[\left(-\frac{i}{4B}\right)^{1/2}\right] \{p - 4iB(\xi_0 + \xi_h)\} dp, \hspace{1cm} (6)$$

where $D_v(z)$ is the parabolic cylinder function of order $v$.

A similar calculation would show that:

$$\Theta(-\xi_0) F_1(-v, 1; -4iB\xi_0 \xi_h) = \frac{1}{2\pi i} e^{-2iv2} \left(-\frac{i}{4B}\right)^{1/2} \exp[iB(\xi_0^2 - \xi_h^2 - 2\xi_0 \xi_h)]$$

$$\times \int_{p_0-\infty}^{p_0+\infty} \exp\left[\frac{p}{2} (\xi_h - \xi_0)\right] D_{-v-1}\left[\left(-\frac{i}{4B}\right)^{1/2}\right] D_v\left[\left(-\frac{i}{4B}\right)^{1/2}\right] \{p - 4iB(\xi_0 + \xi_h)\} dp. \hspace{1cm} (7)$$

Fig. 1. Geometrical parameters in the case of a unit point source located at $P_0$ on the entrance surface. One calculates the wave $G_h(P_0, P)$ induced by such a source at $P(\xi_h, \xi_0)$ in the crystal.

A current point $P_0$ on the entrance surface and of the point $P$ on the exit surface where the amplitude of the $h$ wave is to be calculated (Fig. 1). $\Theta$ is the usual step function.

$$\xi_h = s_h(P) - s_h(P_0);$$
$$\xi_0 = s_0(P) - s_0(P_0);$$
$$v = \frac{i}{4B};$$

$1F_1$ is the confluent hypergeometric function.
so that finally the Green function (2) is:

\[ G_n(\xi_0, \xi_h) = \int_{p_0-i\infty}^{p_0+i\infty} P_n(p) \, dp, \]

where

\[ P_n(p) = \frac{1}{2\pi} e^{-i\pi v^{1/2} p^{1/2}} \exp\left[iB(\xi_0^2 - \xi_h^2 - 2\xi_0 \xi_h)\right] \]
\[ \times \exp\left[ \frac{p}{2} (\xi_h - \xi_0) \right] \left[ D_p(-iY_0) D_{-p-1}(-Y) - D_{-p-1}(-Y_0) D_p(-iY) \right]. \]

The parameters \( Y_0 \) and \( Y \) introduced in (9) are such that

\[ \left( \frac{i}{4B} \right)^{1/2} p = \nu^{1/2} p = -iY_0 \]

and

\[ \left( \frac{i}{4B} \right)^{1/2} [p - 4iB(\xi_0 + \xi_h)] = \nu^{1/2} \left( p - \frac{4iB\pi}{A} \right) = -iY \]

so that

\[ Y = Y_0 + 4\nu^{1/2} B \frac{\pi}{A} \frac{z}{z_0}. \]

This should be compared to the well known formula relating the value of the deviation parameter \( \eta \) at a depth \( z \) to its value \( \eta_0 \) at the entrance surface:

\[ \eta = \eta_0 + 2B\pi \frac{z}{z_0}. \]

Let us recall that, in a symmetrical case, \( \eta = \Delta\theta \sin 2\theta/(C\sqrt{\chi_h\chi_k}) \), where \( \Delta\theta \) is the departure from Bragg angle, \( \chi_h \) and \( \chi_k \) are the \( h \) and \( k \) Fourier coefficients of the electrical susceptibility and \( C \) is the polarization factor. Comparing (10), (12) and (13) leads to

\[ p = -i\nu^{-1/2} Y_0 = -2i\eta_0 \]

so that

\[ Y(z) = 2\nu^{1/2} \eta(z). \]

Equation (14) shows that the variable of integration in (8) is directly proportional to the deviation parameter \( \eta_0 \) at the entrance surface. The interpretation of \( P_n(p) \) then becomes clear: if one expands the spherical wave (which on the vacuum side of the entrance surface represents a unit point source at \( P_0 \)) as a sum of plane waves (each being characterized by a single value of \( p \) or, alternatively, \( \eta_0 \), then \( P_n(p) \) is the wave induced in the crystal at a point \( P(\xi_0, \xi_h) \) by the component \( p \) of this expansion. In other words: each of the vacuum plane-wave components is transformed, through the crystal, in \( P_n(p) \). Integrating \( P_n(p) \) over all values of \( p \) then gives the field at \( P \) due to a unit point source at \( P_0(0,0) \); in other words, the Green function \( G_n(\xi_0, \xi_h) \).

III. Analytic expression of each component \( P_n(p) \) as a function of the deviation parameter

Since we are interested here in the phenomenon of 'creation' of 'new' wave fields, the analytic form of \( P_n(p) \) will be calculated assuming a situation for which this phenomenon is expected. According to an argument first stated by Penning & Polder (1961), this 'creation' is most likely to occur at a depth \( z = z_0 \) such that \( \eta(z_0) = 0 \), since the curvature of the ray trajectory is then at its maximum. This conjecture has been amply verified by a computer experiment performed on the basis of Takagi's equations (Balibar, Epelboin & Malgrange, 1975). In this same computer experiment, the value of \( |B| \) for which 'creation' becomes noticeable has been estimated: \( 4|B| \) must be of the order of 3 so that 10% of the total intensity be diverted in the 'created' wave fields. This result is in agreement with the criterion previously given by Balibar (1970) on a theoretical basis: creation of new wave fields is expected for \( 4|B| \gg 1 \). We shall, therefore, from now on, assume:

1. \( |B| \gg 1 \) and, for instance, \( B > 0 \). (A positive value of \( B \) corresponds to the geometry of Fig. 2.)
2. The plane \( z = z_0 \) [such that \( \eta(z_0) = 0 \)] lies inside the crystal (see Fig. 2). For a positive value of \( B \), this imposes a large and negative value for \( \eta_0 = \eta(0) \). A priori, we expect that for \( z < z_0 \), the crystal wave will be of the 'normal' type (i.e. only two wave fields) while for \( z > z_0 \) it will exhibit two extra terms.

The assumed conditions and their implications regarding the various parameters involved are
summarized below:

(1) \( B \) large and \( >0 \) \( \Rightarrow \ |v| = \frac{i}{4B} \ll 1 \Rightarrow v = |v| e^{i\pi/2}; \)

(16)

(2) \( \eta_0 = \eta(0) \) large and \( <0 \) \( \Rightarrow Y_0 = |Y_0| e^{3i\pi/4}; \)

(17)

(3) \( \eta(z) = \eta(0) + 2\pi \frac{B}{A} \) large and \( >0 \) \( (z > z_0) \)

\( \Rightarrow Y = |Y| e^{i\pi/4}. \)  

(18)

Under these conditions \( P_h(p) \) at a given point \((\xi_0, \xi_h)\) is (see Table 2):

\[ P_h(p) = \exp\left[iB(\xi_h^2 - \xi_0^2 - 2\xi_0 \xi_h)\right] \left| \frac{Y}{Y_0} \right|^\nu \frac{1}{|Y|} \exp\left[\frac{i}{2}(Y^2 - Y_0^2)\right] \]

\[ \times e^{i\pi/4} e^{-3i\pi/4} \left( 1 + e^{2i\pi/4} \right) \left( 1 - e^{-2i\pi/4} \right) \]

\[ \times \exp\left[-\frac{i}{2}(Y^2 + Y_0^2)\right]. \quad (19) \]

As conjectured, \( P_h(p) \) is a sum of four terms, \( A, B, C, D; \)

\[ A = \frac{1}{2\pi} \exp\left[iB(\xi_h^2 - \xi_0^2 - 2\xi_0 \xi_h)\right] \]

\[ \times e^{3i\pi/4} \left( 1 + e^{2i\pi/4} \right) \left( 1 - e^{-2i\pi/4} \right) \]

\[ \times \exp\left[-\frac{i}{2}(Y^2 + Y_0^2)\right]. \quad (20a) \]

**Table 2. Asymptotic expansion of the parabolic cylinder functions \( D_\nu \) for large values of the argument \( u \)**

<table>
<thead>
<tr>
<th>Parabolic cylinder functions ( D_\nu )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( D_\nu(u) = u^\nu e^{\nu\pi/4} - \left( \frac{2\pi}{\Gamma(-\nu)} \right)^{1/2} u^{-\nu-1} e^{i\nu\pi/4} e_\nu(u) )</td>
</tr>
</tbody>
</table>

where \( e_\nu(u) \) depends on the argument \( \nu \) of \( u \).

- \( -\frac{3\pi}{4} < \nu < -\frac{3\pi}{4} \) \( e_\nu(u) = 0 \)
- \( -\frac{\pi}{4} < \nu < -\frac{\pi}{4} \) \( e_\nu(u) = e^{i\nu} \)
- \( -\frac{5\pi}{4} < \nu < -\frac{5\pi}{4} \) \( e_\nu(u) = e^{-i\nu} \)

Correlatively, \( G_h(P_0, P) \) is a sum of four integrals.

Note that this conclusion holds only under the conditions [see (17)-(18)] that \( Y \) and \( Y_0 \) be of opposite signs. It can be easily shown that if \( Y \) and \( Y_0 \) were of the same sign, i.e. if the conditions \( \eta(z) = 0 \) were not fulfilled inside the crystal, then \( P_h(p) \) in (19) would reduce to only two terms – as expected.

**IV. Physical interpretation – ‘creation’ of new waves**

At this stage one would like to follow Kato’s procedure and obtain the physical interpretation of the four terms involved in (20) by means of the stationary-phase method (Kato, 1961).

Let us call \( \phi_A, \phi_B, \phi_C \) and \( \phi_D \) the phases in (20a), (20b), (20c) and (20d), respectively. They can be written, using (10) and (11), as:

\[ \phi_A = -2iB\xi_0^2 - 4iB\xi_0 \xi_h + p\xi_h \]

\[ \phi_B = 2iB\xi_0^2 - p\xi_0 \]

\[ \phi_C = 2iB\xi_0^2 - p\xi_0 - \frac{ip^2}{8B} \]

\[ \phi_D = -2iB\xi_0^2 - 4iB\xi_0 \xi_h + p\xi_h + \frac{i}{8B} p^2. \quad (21) \]

Unfortunately, it turns out that integration by the stationary-phase method can be performed only on \( \phi_C \) and \( \phi_D \) since the phases \( \phi_A \) and \( \phi_B \) cannot be made stationary owing to their linearity in \( p \). We shall therefore use the stationary-phase method for \( C \) and \( D \) only and another method for \( A \) and \( B \).

**A. The normal part of \( G_h(P_0, P) \)**

The phases \( \phi_C \) and \( \phi_D \) are stationary for

\[ p_{[1]}^* = 4iB\xi_0 \] and \[ p_{[2]}^* = 4iB\xi_h, \]

respectively.
The corresponding values of \( \eta_0 \) are:

\[
\eta_{0[1]}^{*} = -2B\xi_0 \quad \text{and} \quad \eta_{0[2]}^{*} = -2B\xi_h. \tag{23}
\]

Comparison with (A.1.3) and (A.1.4) in Appendix 1 shows that these values of \( \eta_0 \) are precisely those which would characterize the two hyperbolic trajectories which, according to the Eikonal theory, link \( P_0(0,0) \) to \( P(\xi_0, \xi_h) \) in the limit \( B \gg 1 \) and \( |\eta_0| \) and \( |\eta_p| \) are.

In other words: in the case \( B \gg 1 \), the 'normal' part of \( G_h(P_0, P) \) is zero everywhere except along the trajectories (see Fig. 10) along which energy is normally transferred in the case \( B \ll 1 \). This is, of course, the reason why we call this part of \( G_h(P_0, P) \) the 'normal' one.

B. The 'non-normal' part of \( G_h(P_0, P) \)

We call 'non-normal' what is left once the 'normal' part has been taken into account:

\[
\begin{align*}
\int_{p_0 - \infty}^{p_s + \infty} & \exp\left[iB(\xi_0^2 - \xi^2 - 2\xi_0\xi)\right] e^{p/2(4\xi_0 - k)} \\
& \times \frac{\nu/2}{2\pi} \left(\frac{Y_0}{Y}\right)^{\nu/2} \frac{1}{Y} \exp\left[\frac{1}{4}(Y_0^2 - Y^2)\right] dp \quad (24a)
\end{align*}
\]

and

\[
\begin{align*}
\int_{p_0 - \infty}^{p_s + \infty} & \exp\left[iB(\xi_0^2 - \xi^2 - 2\xi_0\xi)\right] e^{p/2(4\xi_0 - k)} e^{2i\pi\nu} \\
& \times \frac{\nu/2}{2\pi} \left(\frac{Y}{Y_0}\right)^{\nu/2} \frac{1}{Y_0} \exp\left[\frac{1}{4}(Y^2 - Y_0^2)\right] dp \quad (24b)
\end{align*}
\]

or, alternatively (upon replacement of \( Y_0 \) and \( Y \) by their expression as functions of \( p \)):

\[
\begin{align*}
\frac{1}{2\pi} & \exp\left(-2B\xi_h^2 - 4iB\xi_0 \xi_h\right) \\
& \times \int_{p_0 - \infty}^{p_s + \infty} p^{\nu}[p - 4iB(\xi_0 + \xi_h)]^{-\nu - 1} e^{p/k} dp \quad (25a)
\end{align*}
\]

and

\[
\begin{align*}
\frac{1}{2\pi} & \exp\left(2iB\xi_h^2\right) e^{2i\pi\nu} \\
& \times \int_{p_0 - \infty}^{p_s + \infty} p^{-\nu - 1}[p - 4iB(\xi_0 + \xi_h)]^{\nu} e^{-p/k} dp. \quad (25b)
\end{align*}
\]

As already mentioned, integration by the stationary-phase method is not possible. Nevertheless, (25a) and (25b) can be calculated directly using the properties of the Laplace transform (see Higher Transcendental Functions, 1953), which gives for (25a)

\[
i \exp(2iB\xi_h^2) F_i[-\nu, 1; -4iB(\xi_0 + \xi_h)] \Theta(\xi_h). \tag{26a}
\]

and for (25b)

\[
-i e^{2i\pi\nu} \exp(2iB\xi_h^2) F_i[-\nu, 1; -4iB(\xi_0 + \xi_h)] \Theta(\xi_h). \tag{26b}
\]

The same \( F_i \) function as in \( G_h(P_0, P) \) appears [see equation (2)] except that the argument \( \zeta_0 \zeta_h \) has to be replaced either by \( (\zeta_0 + \zeta_h) \zeta_h \) in (26a) or \( (\zeta_0 + \zeta_h) \zeta_h \) in (26b). Expression (26a), for instance, is then calculated following the procedure which led from (4) to (8) and (9), \( \zeta_h \) being replaced by \( (\zeta_0 + \zeta_h) \) and \( \zeta_h \) unchanged. One then obtains for the integrand, in the limit \( \nu \to 0 \) and \( |Y_0| \) and \( |Y| \gg 1 \), a sum of four terms analogous to (20a)-(20d). It will be shown in the following section that, among these four terms, (20c) is predominant. Since the phase of this major term varies quadratically with \( p \), it can be integrated using the stationary-phase method. The stationary condition is similar to (22) and (23) except that \( \zeta_0 \) has to be replaced by \( (\zeta_0 + \zeta_h) \); this gives

\[
\begin{align*}
\eta_{0[1]}^{*} = 4iB(\xi_0 + \xi_h) \quad \text{or} \quad \eta_{0[2]}^{*} = -2B(\xi_0 + \xi_h). \tag{27}
\end{align*}
\]

The corresponding optical path (Fig. 3) is a broken line made of two straight segments, similar to that of the normal [1] wave field except that the turning point is now defined by \( P_0S_{1[1]} = (A/\pi \cos \theta)(\zeta_0 + \zeta_h) \) so that \( S_{1[1]} \) coincides with \( A \), the limit of the Borrmann fan on the exit surface. We therefore come to the conclusion that the 'non-normal' part (26a) of \( G_h(P_0, P) \) is zero everywhere except along \( s_0 \). A similar procedure would show that the 'non-normal' part (26b) of \( G_h(P_0, P) \) is zero everywhere except along \( s_h \).
zero everywhere except along \( s_h \). For this second extra wave:
\[
p_{[2]} = 4iB(\xi_0 + \xi_h) \quad \text{or} \quad \eta_{[2]} = -2B(\xi_0 + \xi_h).
\] (28)

V. Energy flow of an incident pseudo plane wave. Interbranch scattering

Let us now consider an incident pseudo plane wave, i.e. a plane wave of finite lateral expansion (see Appendix 1). Let \( \eta_0 \) be its characteristic deviation parameter at the entrance surface. \( G_s(\rho, P) \) has been expressed in (8) as an integral over \( \rho \) or alternatively over \( \eta_0 \) as \( \rho = -2i\eta_0 \); therefore the integrand in (8), \( P_s(\rho) = P_s(-2i\eta_0) \), can be considered as representing the wave which is induced in the crystal by the considered pseudo plane wave. This conjecture is confirmed by the fact that the phases of the normal parts of \( P_s(\rho) \) are identical to the Eikonal calculated in Appendix 1 [compare \( \varphi_c \) and \( \varphi_p \) in (21) with (A.1.12)].

Let us now study in more detail the four terms \( A, B, C \) and \( D \) involved in \( P_s(\rho) = A + B + C + D \) [equation (20)].

A. Energy trajectories

In the previous section we have shown how the energy of a unit point source (i.e. an incident spherical wave) is distributed inside the crystal. These results are pictured on the left side of Fig. 4 where 4(c) corresponds to \( |B| \ll 1 \) and 4(e) to \( |B| \gg 1 \). The main difference between 4(e) and 4(c) is that in the case \( |B| \gg 1 \) new energy flow trajectories appear on the edges of the Borrmann fan and only there (§ IV). From this, one can infer the energy flow inside the crystal for an incident pseudo plane wave in the case \( |B| \gg 1 \) (Fig. 4f) from the case \( |B| \ll 1 \) (Fig. 4d). The conclusion is that an incident pseudo plane wave induces four wave fields inside the crystal; two of these are 'normal', and the other two are the so-called 'recreated wave fields'.

B. Intensity splitting

The intensities of these four wave fields are obtained by squaring the amplitudes \( A, B, C \) and \( D \) in (20).

In the limit \(|\nu| \to 0\) this gives:
\[
I_A \approx 1 \times e^{-2\pi|v|} \times \frac{1}{4\eta^2}
\]
\[
I_B \approx \frac{1}{4\eta_0^2} \times e^{-2\pi|v|} \times 1
\]
\[
I_C \approx 1 \times (1 - e^{-2\pi|v|}) \times 1
\]
\[
I_D \approx \frac{1}{4\eta_0^2} \times (1 - e^{-2\pi|v|}) \times \frac{1}{4\eta^2}.
\] (29)

The intensities have been written in this peculiar form on purpose, in order to evidence three successive splittings of the intensity during propagation:

(a) Remembering (see Appendix 2) that at the entrance surface the incident beam (of intensity normalized to 1) corresponding to a pseudo plane wave of deviation parameter \( \eta_0 \) is split into two wave fields, of respective intensities \( 1/4\eta_0^2 \) and \( 1 - (1/4\eta_0^2) \approx 1 \) (as \( |\eta_0| \) is large), we can interpret the first factor in each of the four intensities (29) as representing the splitting of the incident intensity between the two wave fields at the entrance surface. \( I_A \) and \( I_C \) thus pertain to the same wave field (wave field \( [1] \) if \( B > 0 \)) while \( I_B \) and \( I_D \) should be associated with the other.

(b) These wave fields propagate normally (i.e. according to hyperbolic trajectories which in the case \( |B| \gg 1 \) reduce to broken lines) up to a region at a depth \( z_0 \) such that \( \eta(z_0) \approx 0 \), where, as already shown creation of new wave fields occurs. The second factor in the intensities (29) indicates how the intensity of a given wave field is then shared between the normal and the created wave fields. For instance, the wave field which propagates with an intensity \( 1/4\eta_0^2 \) in the region \( z < z_0 \) (see \( I_B \) and \( I_D \)) is split in the region \( z \gtrsim z_0 \) into two parts of relative intensities \( e^{-2\pi|v|} \) (extra wave field) and \( (1 - e^{-2\pi|v|}) \) (normal wave field).

(c) The third factor in each term of (29) represents the splitting of the intensity at the exit surface for each of the four wave fields which propagate in the region

Fig. 4. Wave propagation in a crystal, assuming: left: an incident spherical wave (a,c,e); right: an incident pseudo plane wave (b,d,f). (a),(b) A perfect crystal \( B = 0 \). (c),(d) A slightly distorted crystal \( |B| \neq 0 \) and \( |B| \ll 1 \). (e),(f) A highly distorted crystal \( |B| \gg 1 \).

z > z_0. \( \eta \), the deviation parameter at the exit surface, is the same for all four wave fields which means that equation (13) holds for new wave fields as well. This discussion is summarized in Fig. 5.

C. Interbranch scattering

The question now is: 'Do the extra wave fields correspond to interbranch scattering?' (interbranch meaning a 'jump' of the tie-point from one branch to the other in the process of the creation of a new wave field at \( z \approx z_0 \)).

This question can be answered by consideration of the phases involved in (20). Except for a factor \( B(\xi_0^2 - \xi_h^2 - 2\xi_0\xi_h - \eta(\xi_h - \xi_0)) \) these phases are:

\[
\begin{align*}
\varphi_A &= \frac{1}{4|B|} (\eta_0^2 - \eta^2) \\
\varphi_B &= \frac{1}{4|B|} (\eta^2 - \eta_0^2) \\
\varphi_C &= \frac{1}{4|B|} (\eta_0^2 + \eta^2) \\
\varphi_D &= \frac{1}{4|B|} (-\eta_0^2 - \eta^2).
\end{align*}
\]

As can be seen from (A.1.12) in Appendix 1, a + sign in front of \( \eta^2 \) (respectively \( \eta_0^2 \)) corresponds to a wave field of type [1] while a - sign is characteristic of a type [2] wave field.

Therefore, the tie-points of 'normal wave fields' [C and D in (20)] stay on the same branch of the dispersion surface (see in Fig. 6 the black arrows going from \( M \) to \( R \) for wave field [1], for example, which corresponds to the C term). The 'extra wave fields' [A and B in (20)] exhibit a mixed dependence \((\eta_0^2/4|B|) - (\eta^2/4|B|)\) or \((-\eta_0^2/4|B|) + (\eta^2/4|B|)\). The \( A \) term corresponds to a tie-point on branch [1] (+ \( \eta_0^2/4|B| \)), which upon arrival at region \( z \approx z_0 \), jumps to branch [2] \((-\eta_0^2/4|B|)\) — see black arrows from \( M \) to \( N \) followed by white arrows from \( P \) to \( Q \) after the jump from \( N \) to \( P \). This term is responsible for the interbranch scattering from branch [1] to branch [2]. Similarly the \( B \) term takes into account interbranch scattering from branch [2] to branch [1].

This argument can be stated more precisely by comparing the phase \( \varphi_A \) (or \( \varphi_B \)) with the Eikonal along the corresponding trajectory of mixed [1] and [2] type.

Let us consider, as in Fig. 7, a wave field of type [1] which, after the turning point \( S_{1[1]} \) where \( \eta = 0 \), splits into a normal wave field (trajectory \( S_{1[1]} P \)) and a newly

Fig. 5. Propagation of a pseudo plane wave inside a crystal distorted by a constant strain gradient \(|B| \gg 1 \) (here: \( B > 0 \)). \( \eta_p \), the value of the deviation parameter at the entrance surface, is large and negative. \( \eta \) then varies monotonically with the depth \( z \) inside the crystal. At \( z = z_0 \), \( \eta \) reaches the value \( \eta = 0 \), the curvature of the wave field is the maximum and new wave fields are 'created'; each new wave field takes a fraction \( e^{-2\eta_0'} \) of the intensity of the wave from which it is 'created'. The splitting of the intensity among the two wave fields at the entrance surface, and among the refracted and reflected wave at the exit surface, is in agreement with the results of the ordinary dynamical theory (as long as one considers that the variations of \( \eta \) follows the same laws as in a slightly distorted crystal).

Fig. 6. Interbranch scattering (only one wave field, here [1], has been pictured for clarity). At a depth \( z \approx z_0 \) the wave field which from \( z = 0 \) to \( z_0 \) propagates as a type [1] wave field (black arrows from \( M \) to \( R \)), splits into two waves, one of type [1] (black arrows from \( N \) to \( R \)) and one of type [2] (white arrows from \( P \) to \( Q \)).

Fig. 7. Schematic drawing showing the ray paths corresponding to interbranch scattering. A normal wave field (here of type [1]) follows \( P_0 S_{1[1]} \) and then splits into two wave fields: a normal one propagating along \( S_{1[1]} P \) and a new one (here of type [2]) propagating along \( S_{1[1]} P' \).
created wave field (trajectory $S_{1}[P']$). The phase change along $P_0 S_{1}[P']$ is, from (20),

$$\phi = B(\eta_0^2 - \eta^2 - 2\eta_0 \eta \xi_0) + \frac{\eta_0^2 - \eta^2}{4|B|},$$

(31)

where $\xi_0$ and $\xi_h$ are the coordinates of $P'$, i.e.

$$\xi_0' = \xi_0 + \xi_h$$

$$\xi_0 = 0$$

(32)

if $\xi_0$ and $\xi_h$ are the coordinates of $P$. $B$ is assumed to be positive.

Let us check that (31), along with (32), is identical to the Eikonal which would correspond to a wave field of type [1] from $P_0$ to $S_{1}$ and then a wave field of type [2] from $S_{1}$ to $P'$. The Eikonal $\phi_1$ along $P_0 S_{1}$ and $\phi_2$ along $S_{1} P'$ can be calculated from (A.1.12) which gives the phase $\phi_1$ along a wave field $j$ propagating from $P_0(0,0)$ to $P(\xi_0, \xi_h)$. Then

$$\phi_1 = B\xi_0^2 + \eta_0 \xi_0' + \frac{\eta_0^2}{4B},$$

(33)

as $\eta = 0$, $\xi_0(S_{1}) = \xi_0$, $\xi_h(S_{1}) = 0$. $\phi_2$ along $S_{1} P'$ is equal to the phase along a wave field 2 going from $P_0$ to $F$:

$$\phi_2 = B\xi_h^2 - \frac{\eta^2}{4B}$$

(34)

as $\eta_0 = 0$, $\xi_0(F) = \xi_h$, $\xi_h(F) = 0$. Adding (33) and (34) gives (31) once $\xi_0'$ and $\xi_h'$ have been replaced by their values (32) and (A.1.3) used.

D. The scattering factor; comparison with previous computer experiments

As has been stated in $\S$ V B, when creation occurs, the new wave field takes a fraction $e^{-2\pi|\nu|}$ out of the initial intensity, leaving a fraction $(1 - e^{-2\pi|\nu|})$ in the beam which keeps going normally. We call this factor $e^{-2\pi|\nu|}$ the scattering factor since the phenomenon here is quite analogous to a scattering process.

This quantity is of importance and it can be related to computer experiments performed by Balibar, Epelboin & Malgrange (1975). They have calculated (by numerical integration of Takagi's equations) the transmitted and reflected intensities by a crystal distorted with a constant strain gradient, assuming a pseudo plane wave and no absorption. The results showed that new wave fields appear for values of $B \gg 1$ and in the region $z \approx z_0$ where $\eta(z_0) = 0$.

The intensity $I_N$ of the new wave field, as compared to that of the incident intensity $I_o$, was empirically shown, from the numerical results obtained, to be of the type:

$$\frac{I_N}{I_o} = \exp \left( - \frac{\alpha}{B} \right)$$

(35)

where $\alpha$ was a constant.

The present work, apart from the fact that it provides a theoretical explanation of these 'experimental' results, allows one to give a theoretical value for $\alpha$: identifying $\exp(-\alpha/B)$ with $\exp(-2\pi|\nu|)$ gives $\alpha = \pi/2$.

Introducing the parameter $\beta = 2\pi B/\lambda$ which, in the above-mentioned computer experiment, served as a measure of the strain gradient, gives the theoretical result:

$$\frac{I_N}{I_o} = e^{-\pi^2/\beta^2}.$$  

(36)

Comparison of the slope of the curve $\log(I_N/I_o)$ as a function of $1/\beta$ in Balibar, Epelboin & Malgrange (1975) ($0.29 \mu m^{-1}$) and of the numerical value of $\pi^2/\lambda$ ($0.28 \mu m^{-1}$ in that case) shows that theory and 'computer experiments' are in very good agreement.

Conclusion

Penning, who was a pioneer (his thesis goes back to 1966) in the investigation of X-ray propagation in a crystal with a uniform strain gradient, has already mentioned the possibility of interbranch scattering for large values of $|B|$ and even made a conjecture as to the analytical form of the extra wave-field intensity in the frame of the Eikonal theory. The present work differs from his in the fact that the existence of such an extra field has been demonstrated, i.e. is extracted from Maxwell's equations themselves, by an analysis of the appropriate Green function.

Following this procedure, it has been shown that the 'normal' propagation of a given wave field is perturbed whenever the curvature of its trajectory becomes too strong: a new wave field then appears, precisely in the region of maximum curvature. Our treatment allows an exact calculation of the fraction $e^{-2\pi|\nu|}$ of the original intensity which is transferred to the new wave field. This fraction depends only on the value of the deformation gradient. From which it follows that the reflecting power of a crystal with a uniform strain gradient should differ from that of a perfect crystal by a simple multiplicative factor $e^{-2\pi|\nu|}$.

Still, the present analysis is restricted to the case of a uniform strain gradient, a rather academic situation. The next step should now be to perform the same work assuming a real defect (twin boundary or, even better, a dislocation). This is mathematically more involved. In this respect, the analogy which can be drawn between the present situation and that of scattering by a...
potential barrier in quantum mechanics should serve as
a starting point for a 'quasi-classical' treatment of the
wave-field scattering by a dislocation. This will be, we
hope, the object of a further publication.

APPENDIX 1

Here we recall and develop some of the results of the
Eikonal theory in view of a further comparison with
our own results.

The Eikonal theory deals with the case of a pseudo
plane wave, i.e. a wave characterized by a given single
value \( \eta_0 \) of its deviation parameter but of finite lateral
extension. These two characteristics are, in principle,
contradictory, since a finite lateral width should result
in a finite dispersion \( \Delta \eta \) in \( \eta \); in spite of this, the
concept of a pseudo plane wave is relevant if \( \Delta \eta \ll 1 \)
and it corresponds to the experimental situation of a
collimated plane wave.

Trajectories

Penning & Polder (1961), and Kato (1963b, 1964)
have shown that the energy of such a pseudo plane
wave flows, in the crystal, along two hyperbolic
trajectories (Fig. 8), the parametric equations of which are:

\[
x = \frac{A}{\pi} \tan \theta (\xi_h - \xi_0)
\]

\[
z = \frac{A}{\pi} (\xi_h + \xi_0) = \frac{A}{2\pi B} (\eta - \eta_0)
\]

In (A.1.2) and in the following results the upper sign
(lower sign) corresponds to wave field [1] (wave field
[2]). Now, if one considers a source point \( P_0 \) and a
point \( P \) inside the crystal (Fig. 9), there exist two
possible energy trajectories from \( P_0 \) to \( P \). They corre-
spond to two different values of \( \eta_{0[1]} \) and \( \eta_{0[2]} \)
associated with wave fields [1] and [2] respectively. For large
values of \( B, |\eta_0| \) and

\[
|\eta| = |\eta_0 + (2\pi B z/A)|,
\]

the corresponding hyperbolae reduce to two broken lines (Fig. 10). In this case, \( \eta_{0[1]} \) and \( \eta_{0[2]} \) reduce to:

\[
\eta_{0[1]} = -2B \xi_0
\]

\[
\eta_{0[2]} = -2B \xi_h.
\]

Phase change along a trajectory

The general formula for the phase change along a
trajectory \( P_0 \rightarrow P \) is given by Kato (1964, 1974):

\[
\Delta \phi_f(P_0 \rightarrow P) = \frac{\pi z}{\lambda} P_0 \frac{\lambda}{\lambda} (\xi_h + \xi_0) + (T - N_h) \chi.
\]

Fig. 8. Optical paths corresponding to an incident pseudo plane
wave with a given deviation parameter \( \eta_0 \) in the case \( |B| \neq 0 \) but
\( < 1 \).

Fig. 9. The incident wave is spherical. \( |B| \neq 0 \) but \( < 1 \). Given two
points \( P_0 \) and \( P \), energy is transferred from \( P_0 \) to \( P \) along any of
the two hyperbolic optical paths shown here. These paths
 correspond to two different values \( \eta_{0[1]} \) and \( \eta_{0[2]} \) of the parameter
\( \eta_0 \).

Fig. 10. Incident spherical wave \( |B| \neq 0 \) and \( > 1 \). The optical paths
through which energy is transferred from \( P_0 \) to \( P \) reduce to two
broken lines \( P_0 S_{0[1]} P \) and \( P_0 S_{0[2]} P \). \( P_0 S_{0[1]} = (A/\pi \cos \theta) \xi_p \),
\( P_0 S_{0[2]} = (A/\pi \cos \theta) \xi_h \).
\( \mathbf{K}_h \) is a constant wavevector linking the reciprocal-lattice point \( H \) to the Laue point \( L_a \). The first two terms are purely geometrical factors which do not depend on the deviation parameter or on the strain gradient. We shall drop them hereafter and consider only \( (T - N_{h,l,j}) \):

\[
T_{l,j} = \pm \frac{\pi}{A} \int_{P_0}^{P} \frac{dz}{\sqrt{1 + \eta^2}} = \pm \frac{1}{2B} \text{Arg} \text{sh} \eta |_{\eta_0} (A.1.6)
\]

where

\[
\eta = \eta_0 + \frac{2\pi Bz}{A}. \quad (A.1.7)
\]

\[
N_{h,l,j} = \frac{1}{2} \hbar \cdot (\mathbf{u}_p - \mathbf{u}_{P_0}) - \frac{1}{2} \int_{P_0}^{P} \frac{1}{\tan \theta} \frac{\partial}{\partial z} (h \cdot u) dx 
+ \tan \theta \frac{\partial}{\partial x} (h \cdot u) dx \quad (A.1.8)
\]

with

\[
\hbar \cdot u = 4B \varepsilon_0 \xi_h = \frac{B \pi^2}{A^2} \left( z^2 - \frac{x^2}{\tan^2 \theta} \right). \quad (A.1.8)
\]

\( (A.1.8) \) has to be integrated along the trajectory \( P_0 P \).

After some straightforward manipulations one obtains

\[
N_{h,l,j} = 2B \xi_0 \xi_h + B(\xi_0^2 - \xi_h^2) \pm \frac{1}{4B} \left[ 2|\eta_{0,l,j}| |1 + \eta^2 | - \eta \sqrt{1 + \eta^2} \right] \text{Arg} \text{sh} \eta |_{\eta_0} (A.1.9)
\]

In the limit \(|\eta_{0,l,j}| \gg 1\)

and

\[
|\eta_{p,l,j}| = \left| \frac{\eta_{0,l,j} + \frac{2\pi Bz}{A}}{A} \right| \gg 1,
\]

one obtains (using \(A.1.2\)):

\[
[T - N_{h,l,j}] = -2B \xi_0 \xi_h + B(\xi_0^2 - \xi_h^2) - \eta_{0,l,j}(\xi_h - \xi_0) \pm \frac{1}{4B} (\eta_{p,l,j} |\eta_{p,l,j}| - |\eta_{0,l,j}| |\eta_{0,l,j}|).
\]

(A.1.10)

Under the conditions:

\( B > 0 \) \( (B < 0) \)

and

\( \eta_{0,l,j} < 0 \) \( (>0) \); \( \eta_{p,l,j} > 0 \) \( (<0) \);

\[
\frac{1}{4B} (\eta_{p,l,j} |\eta_{p,l,j}| - \eta_{0,l,j} |\eta_{0,l,j}|) = \frac{1}{4|B|} (\eta_0^2 + \eta_0^2)
= \frac{1}{2}(|Y|^2 + |Y_0|^2), \quad (A.1.11)
\]

since \( Y = 2\nu^{1/2} \eta = 2(i/4B)^{1/2} \eta \) [see (3) and (15) in the main text] and

\[
[T - N_{h,l,j}] = -2B \xi_0 \xi_h + B(\xi_0^2 - \xi_h^2) - \eta_{0,l,j}(\xi_h - \xi_0) 
\pm \left( \frac{|Y|^2}{4} + \frac{|Y_0|^2}{4} \right). \quad (A.1.12)
\]

This formula holds also if either \( \eta_0 \) or \( \eta \) is equal to zero since the \text{Arg} \text{sh} \eta terms which have been neglected here compared to the terms in \( \eta^2 \) are then equal to zero.

**APPENDIX 2**

Let us consider an incident plane wave of intensity \( I_0 \) with a departure from Bragg angle equal to \( \Delta \theta \) and a corresponding \( \eta \) parameter of value \( \eta_0 \).

In order to simplify we assume that the reflecting planes are normal to the crystal surfaces of the crystal (symmetric Laue case). Consequently

\[
\eta_0 = \frac{\Delta \theta \sin 2\theta}{C \sqrt{\kappa_h \kappa_h}}
\]

According to the usual Ewald–Laue theory, this plane wave generates in the crystal two wave fields of intensity \( I_j \) \( (j = 1,2) \) near the entrance surface:

\[
I_j = \frac{1}{1 + \varepsilon_{0,j}}, \quad (A.2.1)
\]

where

\[
\varepsilon_{0,j} = D_{h,j}/D_{0,j} = -\eta_0 \mp \sqrt{1 + \eta_0^2} \quad (A.2.2)
\]

(upper sign: wave field 1; lower sign: wave field 2).

For a large and negative value of \( \eta_0 \) (as is assumed in this paper)

\[
\varepsilon_{10} \simeq -\frac{1}{2|\eta_0|} \text{ and } \varepsilon_{20} \simeq 2|\eta_0| \quad (A.2.3)
\]

Fig. 11. Splitting of the intensity between wave field 1 and wave field 2 at the entrance surface in the crystal. The wave field which is drawn here in full line is the one into which goes most of the intensity, assuming a large value of \( |\eta_0| \), i.e. wave field 1 if \( \eta_0 < 0 \) or wave field 2 if \( \eta_0 > 0 \).
so that
\[ I_1 \approx 1 - \frac{1}{4\eta_0^2} \approx 1 \]  \hspace{1cm} \text{(A.2.4)}
\[ I_2 \approx \frac{1}{4\eta_0^2}. \]

For large values of \( |\eta_0| \), most of the intensity goes into the wave field which propagates close to \( s_0 \); wave field 1 for \( \eta_0 < 0 \) and wave field 2 for \( \eta_0 > 0 \) (Fig. 11).

In a case of zero absorption, the intensity is conserved along each wave field. At the exit surface each wave field splits into two waves: the reflected wave (intensity \( I_{R1} \)) and the refracted wave (intensity \( I_R \)) such that
\[ I_{R1} = \frac{\xi_j e^{2\xi_j e}}{1 + \xi_j e^2} I_j; \quad I_R = \frac{1}{1 + \xi_j e^2} I_j, \]  \hspace{1cm} \text{(A.2.5)}
where \( \xi_j e \) is the value of \( \xi \) at the exit surface (\( \xi_j e = \xi e \pm \sqrt{1 + \eta_0^2} \)), \( \eta_0 \) being the value of the deviation parameter at the exit surface (Fig. 12). If \( \eta_0 \) is large and positive
\[ I_{R1} \approx I_1 \left(1 - \frac{1}{4\eta_0^2}\right) \approx I_1 \]  \hspace{1cm} \text{(A.2.6)}
\[ I_R \approx -\frac{1}{4\eta_0^2} I_2. \]

If \( \eta_0 \) is large and negative
\[ I_{R1} \approx \frac{1}{4\eta_0^2} I_1 \]
\[ I_R \approx \left(1 - \frac{1}{4\eta_0^2}\right) I_2 \approx I_2. \]  \hspace{1cm} \text{(A.2.7)}

References
