

Statistical Dynamical Theory of Crystal Diffraction. I. General Formulation

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(Received 16 January 1980; accepted 14 March 1980)

Abstract

The statistical dynamical theory is reformulated as an extension of the previous theory [Kato (1976). *Acta Cryst.* A32, 453–457, 458–466] by taking a more general form of the correlation function of the lattice phase factor. A 'static' Debye–Waller factor E and short-range correlation length τ are introduced for characterizing crystalline media. The fundamental equations consist of a set of differential equations for the averaged (coherent) wave fields $\{\langle D_o \rangle, \langle D_g \rangle\}$ and a set of differential equations for the incoherent part of the intensity fields $\{I_o^i, I_g^i\}$. They are connected through the transformation to the incoherent beams from the coherent waves. In non-absorbing crystals, energy conservation holds for the total intensities $\{I_o^c + I_o^i, I_g^c + I_g^i\}$, where $I_o^c = |\langle D_o \rangle|^2$ and $I_g^c = |\langle D_g \rangle|^2$. The theory can be applied to the diffraction phenomena of the crystalline materials of any degree of perfection.

1. Introduction

In a series of papers (Kato, 1976*a,b*, 1979, 1980*a*) which will be referred to as I, II, III and IV, respectively, a statistical theory of dynamical diffraction has been developed, primarily in order to understand the physical meanings of extinction. I dealt with the basic concepts of the present approach. The theory was applied to the case in which 'secondary extinction' was predominant in II and III. Finally, in IV, the integrated intensity was discussed for parallel-sided crystals.

In this paper and the following one, the theory will be reformulated with a wider scope of application. Firstly, the theory is generalized in such a way that it can be applied to the cases in which both 'primary' and 'secondary' extinctions are appreciable. Secondly, not only the extinction problems but also the applications to diffraction topography are concerned. In particular, the intensity distribution of the section and traverse topographs will be worked out in the next paper. When either the size of the defects is considerably smaller than the spatial resolution or the density of visible

defects is very large to such an extent that they are not individually distinguishable, a statistical approach is inevitable.

The essence of the generalization is to take the most general form of the second-order correlation function of the lattice phase factor (*cf.* equation II.1). As a consequence, a simple energy-transfer equation can no longer describe the diffraction phenomena. Instead, under a certain approximation, a mutually connected set of the averaged wave equations and the energy-transfer equations must be adopted. The former describes the coherent component and the latter the incoherent component as well as the mixed components of the intensity fields. They are connected through the transformation from the coherent waves to the incoherent beams. The diffraction phenomena can be described by two parameters, which characterize the crystal perfection on the short- or long-range scale compared with the extinction distance.

2. Integro-differential equations for $\langle D_o \rangle$ and $\langle D_g \rangle$

(a) Fundamental equations

In this section, we shall derive the fundamental equations for the averaged wave functions $\langle D_o \rangle$ and $\langle D_g \rangle$ from the wave equations of Takagi–Taupin type (Kato, 1973). We shall write them in the form

$$\frac{\partial D_o}{\partial s_o} = i\kappa_{-g} \varphi(s_o, s_g) D_g(s_o, s_g), \quad (1a)$$

$$\frac{\partial D_g}{\partial s_g} = i\kappa_g \varphi^*(s_o, s_g) D_o(s_o, s_g), \quad (1b)$$

where φ is the lattice phase factor defined by

$$\varphi = \exp iG(s_o, s_g) \quad (2)$$

and the lattice phase G is defined by equation (I.3). The variables (s_o, s_g) are the oblique coordinates along the directions of the O and G beams, respectively. In the following, we shall often omit the variables or one of them in the expressions of D_o , D_g and φ when the omission is obvious. The reflection strength $\kappa_{\pm g}$ in (1) is defined by equation (I.2).

The formal solutions of (1) for a narrow incident wave can be given in the form of integral equations:

$$D_o(s_o, s_g) = \delta(s_g) + i\kappa_{-g} \int_0^{s_o} \varphi(s_o - \xi, s_g) D_g(s_o - \xi, s_g) d\xi; \quad (3a)$$

$$D_g(s_o, s_g) = i\kappa_g \int_0^{s_g} \varphi^*(s_o, s_g - \eta) D_o(s_o, s_g - \eta) d\eta. \quad (3b)$$

The term $\delta(s_g)$ represents the incident wave of unit strength. Since, however, we are interested in the positive domain of (s_o, s_g) , we omit the term henceforth.

Although the appearance of the present formalism is rather different from that of the previous theory (I–IV), the physical implications of these equations are equivalent to the statement in deriving equation (I.13); namely ‘the wave fields are composed of zig-zag routes starting from the entrance point (0,0) and arriving at the observation point $(N = s_o/a, M = s_g/a)$ ’. This point will be used extensively in the diagrams (Figs. 1–3) to interpret the correlations of the lattice phase and the wave fields.

Taking the average of (1), we have

$$\frac{\partial \langle D_o \rangle}{\partial s_o} = i\kappa_{-g} \langle \varphi D_g \rangle, \quad (4a)$$

$$\frac{\partial \langle D_g \rangle}{\partial s_g} = i\kappa_g \langle \varphi^* D_o \rangle. \quad (4b)$$

Using the notation $\partial\varphi = \varphi - \langle \varphi \rangle$ and (3b), the correlation appearing in (4a) is given by

$$\begin{aligned} \langle \varphi D_g \rangle &= \langle \varphi \rangle \langle D_g \rangle + \langle \partial\varphi D_g \rangle \\ &= \langle \varphi \rangle \langle D_g \rangle \\ &\quad + i\kappa_g \int_0^{s_g} \langle \partial\varphi \varphi^* \rangle D_o(s_o, s_g - \eta) d\eta \\ &\quad + i\kappa_g \int_0^{s_g} \langle \partial\varphi(s_o, s_g) \partial\varphi^*(s_o, s_g - \eta) \\ &\quad \times D_o(s_o, s_g - \eta) \rangle d\eta. \end{aligned} \quad (5a)$$

Here, we shall consider only the intrinsic correlation of second order, namely the correlation between $\partial\varphi$ and $\partial\varphi^*$ at the neighbouring kink points of an optical route. The correlation between $\partial\varphi(s_o, s_g)$ and $D_o(s_o, s_g - \eta)$, therefore, can be neglected. Also, by definition, $\langle \partial\varphi \rangle$ must be zero. Thus,

$$\begin{aligned} \langle \varphi D_g \rangle &= \langle \varphi \rangle \langle D_g \rangle + i\kappa_g \int_0^{s_g} \langle \partial\varphi(s_o, s_g) \partial\varphi^*(s_o, s_g - \eta) \\ &\quad \times \langle D_o(s_o, s_g - \eta) \rangle d\eta. \end{aligned} \quad (5b)$$

Fig. 1 shows the physical implication of each term in this expression.

Here, for convenience, we shall introduce a few notations regarding the correlation between φ and φ^* . The correlation function is defined by

$$\begin{aligned} \langle \varphi(0)\varphi^*(z) \rangle &\equiv f(z) \\ &= \langle \varphi \rangle \langle \varphi^* \rangle + \langle \partial\varphi \partial\varphi^* \rangle, \end{aligned} \quad (6)$$

where z is the distance between the neighbouring kink points. In short, we shall write

$$\langle \varphi \rangle = E \quad (7)$$

$$\langle \partial\varphi \partial\varphi^* \rangle = (1 - E^2)g(z), \quad (8)$$

where $g(z)$ is called the intrinsic correlation function.

E is the average of the lattice phase and it characterizes long-range perfection. In the case of thermally vibrating and otherwise perfect crystals, E is nothing but the Debye–Waller factor. In addition, we shall define the intrinsic correlation length by

$$\tau = \int_0^\infty g(z) dz. \quad (9)$$

This is a parameter which characterizes short-range perfection.

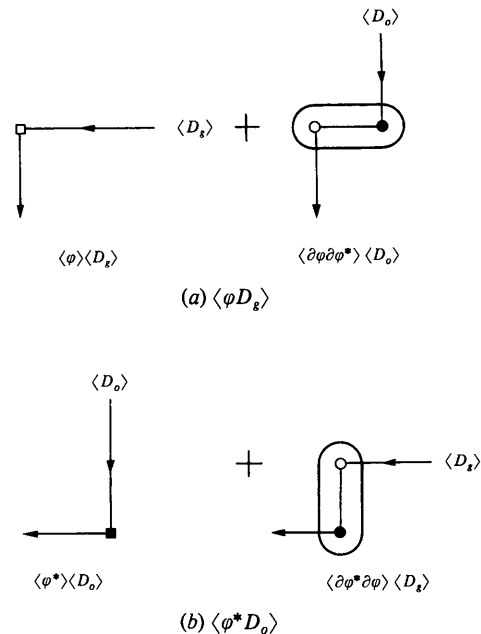


Fig. 1. Diagram showing the correlations of the lattice phase factor and the wave field. The square and circle indicate the average and the intrinsic part of the correlation of the lattice phase factor. The intrinsic part appears only as a pair correlation between the neighbours, which are enclosed by the elliptic circle. The unfilled and filled symbols refer to the lattice phase φ and its complex conjugate, respectively.

With the use of (5*b*), (7) and (8), (4*a*) can be rewritten as

$$\frac{\partial \langle D_o \rangle}{\partial s_o} = i\kappa_{-g} E \langle D_g \rangle - \kappa^2(1 - E^2) \times \int_0^{s_g} g(\eta) \langle D_o(s_o, s_g - \eta) \rangle d\eta, \quad (10a)$$

where

$$\kappa^2 = \kappa_g \kappa_{-g} \quad (11)$$

Similarly, (4*b*) can be written as

$$\frac{\partial \langle D_g \rangle}{\partial s_g} = i\kappa_g E \langle D_o \rangle - \kappa^2(1 - E^2) \times \int_0^{s_o} g(\xi) \langle D_g(s_o - \xi, s_g) \rangle d\xi. \quad (10b)$$

Equations (10) are the fundamental equations for $\langle D_o \rangle$ and $\langle D_g \rangle$. Sometimes, $\langle D_o \rangle$ and $\langle D_g \rangle$ are called coherent waves.

When the spatial variations of $\langle D_o \rangle$ and $\langle D_g \rangle$ are negligible within a range of τ , (10*a,b*) can be simplified in the forms of the differential equations,

$$\frac{\partial \langle D_o \rangle}{\partial s_o} = i\kappa_{-g} E \langle D_g \rangle - \kappa^2(1 - E^2)\tau \langle D_o \rangle, \quad (12a)$$

$$\frac{\partial \langle D_g \rangle}{\partial s_g} = i\kappa_g E \langle D_o \rangle - \kappa^2(1 - E^2)\tau \langle D_g \rangle. \quad (12b)$$

Here it is assumed that the position of interest is sufficiently far (more than τ by an order of magnitude) from the edges of the intensity triangle so that the integral limits (s_o, s_g) in (10) are regarded as infinite.

(*b*) Energy conservation

The fundamental equations (10) or (12) do not obey the conservation of energy even in non-absorbing crystals where $\kappa_{-g} = \kappa_g^*$. For example, in the case of (12),

$$\frac{\partial}{\partial s_o} |\langle D_o \rangle|^2 + \frac{\partial}{\partial s_g} |\langle D_g \rangle|^2 = -2 \operatorname{Re}(\kappa^2)(1 - E^2)\tau(|\langle D_o \rangle|^2 + |\langle D_g \rangle|^2). \quad (13)$$

More energy of the coherent waves dissipates with decreasing long-range perfection specified by E than with increasing short-range perfection specified by τ . As will be seen in the next section, the energy is transferred to the incoherent component of the intensity fields. This is the case where relatively large mosaic blocks (τ large) aggregate with large misorientation (E small). The local distortion (for example thermal vibration) does not break the coherence of the waves

provided that the crystal is perfect as a whole [τ small, $E \simeq 1$].

3. The equations for $\frac{\partial}{\partial s_o} \langle I_o \rangle$ and $\frac{\partial}{\partial s_g} \langle I_g \rangle$

(*a*) Fundamental equations

By similar procedures to those used in the previous section, the spatial variations of $\langle I_o \rangle$ and $\langle I_g \rangle$ are first considered based on the wave equations (1). It is obvious that

$$\begin{aligned} \frac{\partial \langle I_o \rangle}{\partial s_o} &= \langle D_o^* \frac{\partial}{\partial s_o} D_o \rangle + \langle D_o \frac{\partial}{\partial s_o} D_o^* \rangle \\ &= i\kappa_{-g} \langle D_o^*(\varphi D_g) \rangle + \text{c.c.}, \end{aligned} \quad (14)$$

where c.c. stands for complex conjugate. As illustrated in Fig. 2, it is assumed that the intrinsic part of the phase factor $\partial\varphi$ at a kink point can correlate only with that at the nearest kink point along an optical route of either D_g or D_o^* . Therefore, the correlation concerned here has the form

$$\begin{aligned} \langle D_o^*(\varphi D_g) \rangle &= \langle \varphi \rangle \langle D_o^* D_g \rangle + i\kappa_{-g} \int_0^{s_g} \langle \partial\varphi(s_g) \partial\varphi^*(s_g - \eta) \rangle \\ &\quad \times \langle D_o^*(s_g) D_o(s_g - \eta) \rangle d\eta \\ &\quad + (i\kappa_{-g})^* \int_0^{s_o} \langle \partial\varphi^*(s_o - \xi) \partial\varphi(s_o) \rangle \\ &\quad \times \langle D_g^*(s_o - \xi) D_g(s_o) \rangle d\xi. \end{aligned} \quad (15)$$

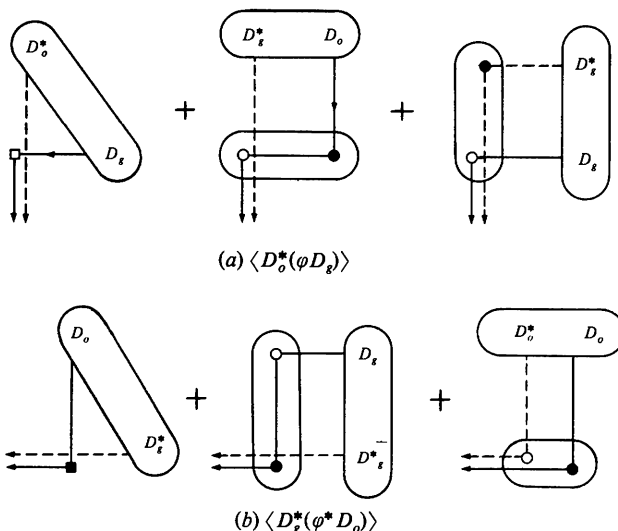


Fig. 2. The diagram showing the correlations of the phase factor and two wave fields. The meanings of the squares and circles are the same as in Fig. 1. The elliptic closing line indicates correlation.

Using (7) and (8), therefore, one can write

$$\begin{aligned} \frac{\partial \langle I_o \rangle}{\partial s_o} &= i\kappa_{-g} E \langle D_o^* D_g \rangle - \kappa^2 (1 - E^2) \\ &\quad \times \int_0^{s_g} g(\eta) \langle D_o^*(s_g) D_o(s_g - \eta) \rangle d\eta \\ &\quad + |\kappa_{-g}|^2 (1 - E^2) \int_0^{s_o} g(\xi) \\ &\quad \times \langle D_g^*(s_o - \xi) D_g(s_o) \rangle d\xi + \text{c.c.} \end{aligned} \quad (16a)$$

Similarly, one obtains

$$\begin{aligned} \frac{\partial \langle I_g \rangle}{\partial s_g} &= i\kappa_g E \langle D_g^* D_o \rangle - \kappa^2 (1 - E^2) \int_0^{s_o} g(\xi) \\ &\quad \times \langle D_g^*(s_o) D_g(s_o - \xi) \rangle d\xi \\ &\quad + |\kappa_g|^2 (1 - E^2) \int_0^{s_g} g(\eta) \\ &\quad \times \langle D_o^*(s_g - \eta) D_o(s_g) \rangle d\eta + \text{c.c.} \end{aligned} \quad (16b)$$

If one can neglect the variation of D_o and D_g in the range of τ and use the approximation mentioned below, (12) and (16) reduce to

$$\begin{aligned} \frac{\partial \langle I_o \rangle}{\partial s_o} &= i\kappa_{-g} E \langle D_o^* D_g \rangle - \kappa^2 (1 - E^2) \tau \langle I_o \rangle \\ &\quad + |\kappa_{-g}|^2 (1 - E^2) \tau \langle I_g \rangle + \text{c.c.} \end{aligned} \quad (17a)$$

$$\begin{aligned} \frac{\partial \langle I_g \rangle}{\partial s_g} &= i\kappa_g E \langle D_g^* D_o \rangle - \kappa^2 (1 - E^2) \tau \langle I_g \rangle \\ &\quad + |\kappa_g|^2 (1 - E^2) \tau \langle I_o \rangle + \text{c.c.} \end{aligned} \quad (17b)$$

For non-absorbing crystals ($\kappa^2 = |\kappa_g|^2 = |\kappa_{-g}|^2$; $\kappa_g^* = -\kappa_{-g}$), (16) and (17) satisfy the conservation of energy

$$\frac{\partial \langle I_o \rangle}{\partial s_o} + \frac{\partial \langle I_g \rangle}{\partial s_g} = 0. \quad (18)$$

(b) The coherent and incoherent parts of the intensity fields

As in the case of lattice phase [cf. (6)], the second-order correlation of any quantities can be divided into two parts; the product of the averages and the intrinsic correlation between them. Applying this rule to the intensity fields, one can write them as follows.

$$\langle I_o \rangle = I_o^c + I_o^i = \langle D_o^* \rangle \langle D_o \rangle + \langle \partial D_o^* \partial D_o \rangle, \quad (19a)$$

$$\langle I_g \rangle = I_g^c + I_g^i = \langle D_g^* \rangle \langle D_g \rangle + \langle \partial D_g^* \partial D_g \rangle, \quad (19b)$$

$$\langle D_o^* D_g \rangle = \langle D_o^* \rangle \langle D_g \rangle + \langle \partial D_o^* \partial D_g \rangle. \quad (19c)$$

Since the wave fields are inhomogeneous even after a statistical average is taken, I_o^c , I_o^i , etc. must be regarded as position dependent. Traditionally, the first and

second terms of each of (19) are called 'coherent' and 'incoherent' intensities, respectively.

In this section, for simplicity, we shall continue the formulation mainly with the approximate equations (12) and (17). Analogous treatments can be made with the fundamental equations (10) and (16).

From (12), one can construct the equations for I_o^c and I_g^c as follows.

$$\frac{\partial I_o^c}{\partial s_o} = i\kappa_{-g} E \langle D_o^* \rangle \langle D_g \rangle - \kappa^2 (1 - E^2) \tau I_o^c + \text{c.c.}, \quad (20a)$$

$$\frac{\partial I_g^c}{\partial s_g} = i\kappa_g E \langle D_g^* \rangle \langle D_o \rangle - \kappa^2 (1 - E^2) \tau I_g^c + \text{c.c.} \quad (20b)$$

Subtracting these from (17), we have

$$\begin{aligned} \frac{\partial I_o^i}{\partial s_o} &= i\kappa_{-g} E \langle \partial D_o^* \partial D_g \rangle + |\kappa_{-g}|^2 (1 - E^2) \tau I_o^i \\ &\quad - \kappa^2 (1 - E^2) \tau I_o^i + |\kappa_{-g}|^2 (1 - E^2) \tau I_g^i + \text{c.c.}, \end{aligned} \quad (21a)$$

$$\begin{aligned} \frac{\partial I_g^i}{\partial s_g} &= i\kappa_g E \langle \partial D_g^* \partial D_o \rangle + |\kappa_g|^2 (1 - E^2) \tau I_g^i \\ &\quad - \kappa^2 (1 - E^2) \tau I_g^i + |\kappa_g|^2 (1 - E^2) \tau I_o^i + \text{c.c.} \end{aligned} \quad (21b)$$

The first term on the right of (21a) plus its complex conjugate can be written in the form

$$\begin{aligned} &i\kappa_{-g} E \langle \partial D_o^* \partial D_g \rangle + \text{c.c.} \\ &= -\kappa^2 E^2 \int_0^{s_g} \langle \partial D_o^*(s_g) \partial D_o(s_g - \eta) \rangle d\eta \\ &\quad + |\kappa_{-g}|^2 E^2 \int_0^{s_o} \langle \partial D_g^*(s_o - \xi) \partial D_g(s_o) \rangle d\xi + \text{c.c.} \\ &= -2 \text{Re}(\kappa^2) E^2 \Gamma I_o^i + 2|\kappa_{-g}|^2 E^2 \Gamma I_g^i, \end{aligned} \quad (22a)$$

Similarly, the first term and its c.c. of (21b) can be written as

$$\begin{aligned} &i\kappa_g E \langle \partial D_g^* \partial D_o \rangle + \text{c.c.} \\ &= -2 \text{Re}(\kappa^2) E^2 \Gamma I_g^i + 2|\kappa_g|^2 E^2 \Gamma I_o^i, \end{aligned} \quad (22b)$$

where Γ is the correlation length of the wave fields, ∂D_o^* and ∂D_o (or ∂D_g^* and ∂D_g). Here, the correlation lengths for O and G waves are intuitively assumed to be identical, since they are to be treated equivalently within the crystal. The exact form of Γ is unknown and may depend on the crystal perfection. We shall leave the problem for a while and discuss it in § 5(c).

The assumption of using (22) is equivalent to taking the effective correlation length of the lattice phase in the form

$$\tau_e = (1 - E^2)\tau + E^2 \Gamma. \quad (23)$$

4. The procedures for finding the intensity fields

In this section, we shall summarize the procedures to obtain the total intensities with a few supplementary arguments. For making the theory complete, the terms of the normal absorption are explicitly included in the differential equations. The justification of this revision is explained in § 2 of I.

(a) The total intensities

$$\langle I_o \rangle = I_o^c + I_o^i, \quad \langle I_g \rangle = I_g^c + I_g^i. \quad (24a,b)$$

(b) The coherent part of the intensities

$$I_o^c = |\langle D_o \rangle|^2, \quad I_g^c = |\langle D_g \rangle|^2. \quad (25a,b)$$

The averaged wave fields $\langle D_o \rangle$ and $\langle D_g \rangle$ are given by the averaged wave equations [cf. (12)],

$$\frac{\partial \langle D_o \rangle}{\partial s_o} = -\frac{1}{2}\mu_e \langle D_o \rangle + i\kappa_{-g} E \langle D_g \rangle, \quad (26a)$$

$$\frac{\partial \langle D_g \rangle}{\partial s_g} = -\frac{1}{2}\mu_e \langle D_g \rangle + i\kappa_g E \langle D_o \rangle, \quad (26b)$$

where

$$\mu_e = \mu_o + 2 \operatorname{Re}(\kappa^2)(1 - E^2)\tau \quad (27)$$

is the effective absorption coefficient of the coherent wave fields.

(c) The incoherent part of the intensities

The intensity fields (I_o^i, I_g^i) can be obtained by the following equations [cf. (21), (22) and (23)].

$$\frac{\partial I_o^i}{\partial s_o} = -\tilde{\mu}_e I_o^i + \tilde{\sigma}_{-g} I_g^i + \sigma_{-g}(1 - E^2)I_o^c, \quad (28a)$$

$$\frac{\partial I_g^i}{\partial s_g} = -\tilde{\mu}_e I_g^i + \tilde{\sigma}_g I_o^i + \sigma_g(1 - E^2)I_o^c + [|\kappa_g|^2(1 - E^2)|A|^2 \exp -\tilde{\mu}_e \tilde{s}_o], \quad (28b)$$

where

$$\tilde{\mu}_e = \mu_o + 2 \operatorname{Re}(\kappa^2)\tau_e = \mu_e + 2 \operatorname{Re}(\kappa^2)E^2 \Gamma \quad (29)$$

is the effective absorption coefficient of the incoherent intensity fields. The coupling constants are given by

$$\tilde{\sigma}_g = 2|\kappa_g|^2 \tau_e, \quad \tilde{\sigma}_{-g} = 2|\kappa_{-g}|^2 \tau_e, \quad (30a,b)$$

$$\sigma_g = 2|\kappa_g|^2 \tau, \quad \sigma_{-g} = 2|\kappa_{-g}|^2 \tau; \quad (30c,d)$$

the term $[\quad]$ will be explained in the next section.

(d) The boundary conditions

In the case of a narrow incident wave $D_e = A\delta(s_g)$, the wave propagating through the crystal without

Bragg reflection must be

$$D_o(s_o, s_g) = A \delta(s_g) \exp -\frac{1}{2}\mu_o s_o \quad (31)$$

because the original wave equations include only photoelectric absorption. Then, the Bragg-reflected wave along the O direction ($s_g = \varepsilon$; a positive infinitesimal) is given by integrating (1b) with (31), in the form

$$D_g(s_o, \varepsilon) = i\kappa_g \varphi(s_o, \varepsilon)A \exp -\frac{1}{2}\mu_o s_o. \quad (32a)$$

Therefore, one can obtain

$$\langle D_g(s_o, \varepsilon) \rangle = i\kappa_g EA \exp -\frac{1}{2}\mu_o s_o, \quad (32b)$$

$$I_g^i(s_o, \varepsilon) = |\kappa_g|^2 |A|^2 (1 - E^2) \exp -\mu_o s_o. \quad (32c)$$

These conditions, however, cannot be applied directly to the problems of solving (26) and (28) because the equations are valid only for the region $s_g \gtrsim \tau$ as discussed above. To be exact, one has to know how the wave field $\langle D_g(s_o, \tau) \rangle$ and the intensity field $I_g^i(s_o, \tau)$ are built up from the purely wave-optical arguments. Since the task is not easy, we shall assume that (26) and (28) can be extended to $s_g \gtrsim \varepsilon$. This assumption, however, may not be serious because the ambiguity in s_g is merely τ in order of magnitude and τ is usually smaller than a spatially resolvable distance ρ . If $\tau \gtrsim \rho$, the homogeneity of the medium is no longer valid. Such cases are beyond the scope of the present theory.

In the regions where (26) and (28) can be used, we already know that the effective absorption coefficient is either μ_e or $\tilde{\mu}_e$ instead of μ_o in the respective cases. Therefore, we shall modify conditions (32) in the following way:

equations (26)

$$\langle D_g(s_o, \varepsilon) \rangle = i\kappa_g EA \exp -\frac{1}{2}\mu_e s_o; \quad (33a)$$

equations (28)

$$I_g^i(s_o, \varepsilon) = |\kappa_g|^2 (1 - E^2) |A|^2 \exp -\tilde{\mu}_e s_o. \quad (33b)$$

We also need the boundary conditions along the line $s_o = \varepsilon$. Again, we shall assume that (26) and (28) can be used for $s_o \geq \varepsilon$. Since no O wave arrives along the line $s_o = \varepsilon$, it is safe to assume the boundary conditions:

$$\text{equations (26)} \quad \langle D_o(\varepsilon, s_g) \rangle = 0, \quad (34a)$$

$$\text{equations (28)} \quad I_o^i(\varepsilon, s_g) = 0. \quad (34b)$$

So far, we have discussed the case of a narrow incident wave. Often, however, we have to treat a wide homogeneous beam for a crystal of finite shape. It should be noted here that a plane-wave solution of (26) cannot be used in (25) because the homogeneous beam is not the plane wave. The coherent intensities (I_o^c, I_g^c) are given by a spatial integration of the absolute square of the solution of (26) for a narrow incident wave over the entrance surface of the O beam.

With these intensity fields (I_o^c, I_g^c) as the body source, the intensity fields (I_o^i, I_g^i) are obtained from (28). As fully discussed in IV, the incident beam penetrating

through the crystal without creating the Bragg-reflected beam must be eliminated from I_o^i . Then, the incoherent part of the G beam (33b), which is created from the incident beam, is an additional body source to the intensity I_g^i . For this reason, the term $\llbracket \quad \rrbracket$ has to be added to the right side of (28b). Here, s_o is replaced by \bar{s}_o , which is the distance between the point of interest (s_o, s_o) in the crystal and the corresponding entrance point. In general, \bar{s}_o is a function of (s_o, s_g) . With this viewpoint, the boundary conditions must be

$$I_o^i = 0 \quad \text{on the entrance surface of the } O \text{ beam,} \quad (35a)$$

$$I_g^i = 0 \quad \text{on the entrance surface of the } G \text{ beam} \quad (35b)$$

because no incoherent beam arrives on the entrance surface. The incoherent beams are created always inside the crystal.

The concrete solution will be given in the following paper (Kato, 1980b).

5. Discussion and conclusions

(a) The coherent and incoherent components of the intensity fields

As stated in (19), the ensemble average of the intensity can be divided into two components; coherent and incoherent. This dividing is exact or a matter of definition of 'coherent' and 'incoherent' components. The coherent component is the intensity of the averaged wave field, $\langle D_o \rangle$ or $\langle D_g \rangle$. Under the condition $\tau \ll \lambda$, $\langle D_o \rangle$ and $\langle D_g \rangle$ obey a set of wave equations (12), which are different from the original wave equations (1) in two aspects: (i) the averaged structure factor $[E\kappa_g]$ is used instead of the original one $[\kappa_g]$; (ii) a term is added for describing the energy dissipation from the coherent channel.

In the case of thermally vibrating crystals, Parthasarathy (1960) proposed a wave equation in which the structure factor is replaced by the averaged one. The equation is valid only when the Einstein model of thermal vibration can be assumed ($\tau = 0$). In distorted crystals, certainly, this simplification cannot be acceptable.

Owing to the dissipation term, the apparent absorption coefficient must be corrected not only for the effects of thermal vibration but also for the effects of invisible small defects which are very likely included in most crystals. If the accurate intensity fields inside the crystal are of interest (e.g. Wada & Kato, 1976), careful considerations are required on the absorption coefficient.

The incoherent component is defined by $\langle \partial D^* \partial D \rangle$ as shown in (19). The deviation of the wave from the average, $\partial D(s_o, s_g)$, depends on the 'history' that the

wave has encountered in the region $s'_o < s_o$ and $s'_g < s_g$. It is, therefore, a functional of the lattice distortion $u(s_o, s_g)$. The incoherent intensities $\langle \partial D^* \partial D \rangle$, however, can be regarded as a function depending on the position and the statistical parameters of the lattice distortion, E and τ . They obey a set of differential equations (28) under the approximations stated in deriving them.

Energy conservation (18) is valid for the total energy in non-absorbing crystals at any stage of approximation. The same amount as the energy dissipated from the coherent channel is transferred to the incoherent channel as a form of body source.

(b) The relation between the present and the previous theory

The present theory is formulated in the form of integro-differential equations [(10) and (16)]. They are also approximated in the forms of differential equations [(12) and (17)]. The previous approach (I–II) was more or less algebraic; namely enumerating possible routes which have the same amplitude and summing the amplitudes multiplied by the number of the routes. It is instructive to compare the two approaches.

The quantities discussed here, in fact, can be written down in terms of the notations used in the previous papers [cf. equations (I.13–16)]. For example,

$$\langle D_g \rangle = \sum_R B_R \langle \exp iQ \rangle, \quad (36a)$$

$$\langle \partial D_g^* \partial D_g \rangle = \sum_R \sum_{R'} B_R B_{R'}^* \{ \langle \exp i(Q_R - Q_{R'}) \rangle \} - |\langle D_g \rangle|^2. \quad (36b)$$

The present theory is concerned with the extended cases described by (6) for the second-order correlation. When $E = 0$, $\langle \exp iQ_R \rangle$ can be omitted if the route R includes at least one isolated kink point. Here, all routes are taken into account by associating the average reflection strength $[i\kappa_{\pm g} E]$ with every isolated kink point.

Similarly, all pairs of routes R and R' are taken into account in calculating $\langle \exp i(Q_R - Q_{R'}) \rangle$ in the present theory. A typical diagram illustrating the correlation of the routes R and R' is shown in Fig. 3. If both R and R' have no coupling node of isolated kinks such as A, B , the intensity is calculated through $\langle D_g \rangle$. For this reason, the intensity $|\langle D_g \rangle|^2$ has to be subtracted from the right side of (36b).

In the other extreme case that no isolated kink such as a, b, a', b' is included in R and R' , the intensity had to be calculated according to the previous approach discussed in II and III. If we do so, the correlation length τ_2 (II) or a reduced correlation length $R\tau_2$ (III) is expected in the place of τ in the present theory.

Incidentally, according to the definition (II.2), τ is to be read as τ_1 . The present theory using the differential equations leaves out the non-local correlation between R and R' so that only τ appears in the expressions of $\langle \partial D_g^* \partial D_g \rangle$. It is not difficult to revise this deficiency but we shall postpone the problem to the next paper, because it is easier to understand the arguments after obtaining the concrete solution of the differential equations.

(c) *The correlation length of the incoherent part of the wave fields; Γ in (23)*

It is not easy to work out the expression for Γ directly from its definition [cf. (22)]. However, by inspecting each term of the energy-transfer equations (21), we can see the physical meanings of the first terms of (21a,b); from which we shall derive a reasonable expression for Γ .

The second terms of (21) are the increment of the incoherent beam due to the coherent source [I_0^c, I_g^c]. Up to the first node A or B in Fig. 3 each of the routes R and R' is regarded as an optical route describing the coherent waves and the conjugate waves respectively.

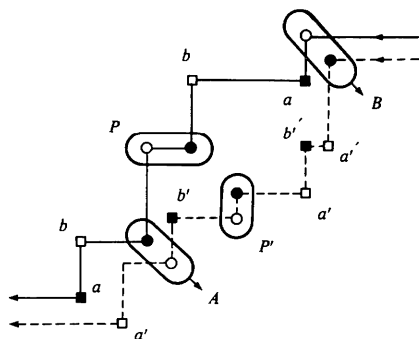


Fig. 3. The typical case of the correlation between the two wavelets associated with the routes R and R' .

If one or both of the routes R and R' includes the node, then the pair of routes will describe the incoherent beam. The incoherent beam changes in intensity for two reasons. The decrease of the intensity is caused by the intrinsic correlation of the kinks forming a kink pair P and P' along R and R' , respectively. This process is represented by the third terms of (21). Also, the increase of the intensity is expected due to the intrinsic correlation of the kinks forming a coupling node A or B . The fourth terms of (21) are responsible for this process.

The rest of the reflection processes illustrated in Fig. 3 is the one due to the isolated kinks a, b, a' and b' associated with $E\kappa_{\pm g}$. This implies that the reflection processes concerned must be the energy transfer in a hypothetical perfect crystal with reflection strength $E\kappa_{\pm g}$ in amplitude.

In perfect crystals, although the correlation length of the lattice phase is large, the intensity of the O and G beams dies out effectively at a distance greater than $(E|\kappa|)^{-1}$. Therefore, one can assume the correlation length Γ as

$$\Gamma = A/E, \quad (37)$$

where A is the extinction distance ($|\kappa|^{-1}$). The numerical factor of unity in the order of magnitude is unknown but the functional form must be correct. For obtaining the concrete solution of the intensity field, we shall use (37) in the following paper.

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