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Dynamical Theory of X-ray Diffraction in Crystals with Defects

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Sets of integral equations are obtained that describe the X-ray diffraction in defective crystals. A simple description of defects is suggested both for weakly and strongly distorted regions. In the case of ideal crystals, the solution for the wave fields with arbitrary incident beam distribution is given for crystals of arbitrary thickness. For distorted crystals, the integral equations give the universal method of treatment of both weakly and strongly distorted regions. The problem of image determination from strongly distorted regions is reduced to the solution of a simple one-dimensional integral equation. The first iteration approximation of initial integral equations is shown to give results similar to those of a Fourier analysis method with the defect being treated as a small perturbation.

1. Introduction

In recent years, there have appeared many works on the dynamical theory of X-ray diffraction in distorted crystals or crystals containing faults (Penning & Polder, 1961, 1964; Kato, 1963; 1964*a*, *b*; Taupin, 1967; Takagi, 1962; Schlangenotto, 1967; Dubrovskii, Molodkin, Tikhonova & Tikhonov, 1969; Molodkin, 1969; Slobodetskii, Chukhovskii & Indenbom, 1968; Authier & Simon, 1968). Nevertheless, the problem at large remains far from being solved because of the mathematical difficulties which arise. One solution is connected with the works of Penning & Polder (1961, 1964) and Kato (1963, 1964*a*, *b*) and involves a method close to the WKB approximation (phase integral method) of quantum mechanics. In these works rather interesting results in an analytical form were obtained. However, this method is strongly limited to cases of very weakly distorted crystals.

Another approach, developed by Taupin (1967), uses direct numerical methods to solve the linear differential equations for a wave field in a crystal. These are modifications of Takagi's (1962) equations. Although this approach allows the problem to be solved for many kinds of defects, it deals primarily with the mathematical problems involved without considering physical phenomena, which should simplify the analysis. Moreover, difficulties arise when one describes strongly distorted regions of a crystal. Detailed analysis of Kato's method and equations used by Taupin are given, by Schlangenotto (1967).

The Fourier analysis method is used by Dubrovskii *et al.* (1969) and Molodkin (1969).

The problem of wave field determination in an ideal crystal with arbitrary boundary conditions has also been considered. For the solution of this problem, the integral formulae, which connect wave fields inside a crystal and on the entrance surface, were obtained (Kato, 1961, 1968; Slobodetskii *et al.*, 1968; Authier & Simon, 1968).

In the present paper, a new approach based on the use of integral equations is developed. A simple description of the distorted region in a crystal, including strongly distorted regions (*cf.* § 2), is given. In § 2, the set of differential equations of the Takagi kind, which also describes the strongly distorted region, is derived.

In § 3, the sets of integral equations for the wave fields in crystals containing faults are obtained for both the Laue and the Bragg diffraction cases. First, the problem of the field distribution inside the ideal crystal is solved by using these equations for the Bragg case, when arbitrary boundary conditions are defined. (In works by Kato (1961, 1968), Slobodetskii *et al.* (1968) and Authier & Simon (1968) the analogous problem is solved for the Laue case only.*)

In § 4, the one-dimensional integral equations, which define the image contrast of the strongly distorted region of an arbitrary form, are obtained.

In § 5, the Fourier analysis of the problem, which is based on the method by Afanas'ev, Kagan & Chukhovskii (1968), is carried out. It turns out, however, that since the defect is considered to be a small perturbation, the Fourier analysis method gives the same results as the first iteration approximation of integral equations.

2. Derivation of the initial set of differential equations

To describe the electromagnetic field inside the crystal, we use Maxwell's equations for the electrical field vector $\mathbf{E}(\mathbf{r},\omega)$ (ω is the frequency of the incident wave)

$$\nabla^2\mathbf{E}-\text{grad div}\,\mathbf{E}+\kappa^2\mathbf{E}=-\kappa^2\frac{4\pi i}{\omega}\mathbf{j} \qquad (2\cdot1)$$

* Recently, in the works of Takagi (1969) and Uragami (1969) the integration method of solving the problem was also suggested but in another form than in the present paper. In the work of Uragami, a similar problem has been solved for the thick crystals. We became acquainted with these papers only when the present work was completed.

where $\kappa=\omega/c$ (c is the velocity of light), $\mathbf{j}(\mathbf{r},\omega)$ is the current density induced by the electromagnetic wave, which is, in fact, a linear function of $\mathbf{E}(\mathbf{r},\omega)$.

$$j^i(\mathbf{r},\omega)=\int d\mathbf{r}'\sigma_\omega^{ik}(\mathbf{r},\mathbf{r}')E^k(\mathbf{r}',\omega). \qquad (2\cdot2)$$

The convenience of the equation (2·1) lies in that the calculation of the current density $\mathbf{j}$, which takes into account all possible interactions between the electromagnetic wave and the crystal, can be carried out (Afanas'ev & Kagan, 1968). In the general case, equation (2·2) describes non-local coupling between $\mathbf{j}$ and $\mathbf{E}$. This coupling arises owing to photoelectric absorption, Compton scattering and, moreover, to inelastic scattering by phonons. However, the main contribution to σ_ω^{ik}, connected with Thomson scattering, has a strictly local character, that is

$$\sigma_\omega^{ik}(\mathbf{r},\mathbf{r}')=\sigma(\mathbf{r})\delta^{ik}\delta(\mathbf{r}-\mathbf{r}'). \qquad (2\cdot3)$$

For simplicity, we shall assume local coupling (2·3) for the other effects since the mathematical account of non-localities is complicated, and, in any case, their presence would not greatly affect the final results. According to (2·3), the right-hand side of equation (2·1) takes the form

$$\frac{4\pi i}{\omega}\mathbf{j}(\mathbf{r},\omega)=\chi(\mathbf{r})E(\mathbf{r},\omega) \qquad (2\cdot4)$$

where $\chi(\mathbf{r})=\sigma(\mathbf{r})4\pi i/\omega$ is the crystal polarizability.

Consider a crystal containing faults, which are assumed to be finite regions with distorted regular structure (Fig. 1). In the areas without defects, the polarizability is a periodic function with the period of the crystal lattice. It can therefore be expanded as a Fourier series.

$$\chi^{(\mathrm{id})}(\mathbf{r})=\sum_h\chi_h^{(\mathrm{id})}\exp\{i\mathbf{K}_h\mathbf{r}\} \qquad (2\cdot5)$$

where $\mathbf{K}_h$ is the reciprocal-lattice vector, multiplied by 2π.

We shall divide the region of the defect into two parts; a strongly distorted region A and a weakly distorted region B. Region B is assumed to be such that distortions of the crystal lattice can be described by the deformation vector $\mathbf{u}(\mathbf{r})$ ($\mathbf{r}$ being a point of real crystal) and, moreover, that the relative displacement is small, namely

$$\left|\frac{\partial u^i}{\partial x^k}\right|\ll 1. \qquad (2\cdot6)$$

Condition (2·6) permits the equation for the polarizability to be used (*cf.* Kato, 1963, 1964*a*, *b*)

$$\chi(\mathbf{r})=\chi^{(\mathrm{id})}(\mathbf{r}-\mathbf{u}(\mathbf{r})). \qquad (2\cdot7)$$

We shall assume area A to be distorted so that any diffraction scattering would be practically absent in this region. It may be a region without any periodic structure (*e.g.* the nucleus of dislocation) or a region where the deformation vector changes so quickly that

$$\left|\frac{\partial^2 u^i}{\partial x^k\partial x^m}\right|\kappa l_0^2\gg 1, \qquad (2\cdot8)$$

where $l_0=(|\kappa\chi_0^{(\mathrm{id})}|)^{-1}$ is the diffraction length of the ideal crystal. In fact, condition (2·8) means that there are no areas, with linear dimensions of the order l_0, where the local reciprocal-lattice vector still satisfies the Bragg conditions.

The absence of the diffraction scattering in region A permits us to describe this region as homogeneous, with an average polarizability

$$\overline{\chi(\mathbf{r})}=\chi_0=\frac{1}{v}\int_v\chi(\mathbf{r})d\mathbf{r} \qquad (2\cdot9)$$

which defines the usual X-ray refraction and absorption. The integration in (2·9) is carried out over a volume whose linear dimensions are much greater than the interatomic distance a. If in region A the density is close to that of the ideal crystal (which is the case for most conditions), then

$$\chi_0=\chi_0^{(\mathrm{id})}. \qquad (2\cdot10)$$

We note that region A can be extended considerably to part of region B. Indeed, the Bragg scattering is practically absent in the areas where

$$\left|\frac{\partial u^i}{\partial x^k}\right|\gg|\chi_0^{(\mathrm{id})}| \qquad (2\cdot11)$$

and since $|\chi_0^{(\mathrm{id})}|\sim 10^{-5}$ to 10^{-6}, regions exist where both inequalities (2·6) and (2·11) occur.

Thus, equations (2·7), (2·9) and (2·10) provide a relatively simple description of the polarization properties of a crystal in all regions of the defect.

We shall seek the solution of the equation (2·1) in the form

$$\mathbf{E}(\mathbf{r})=\exp\{i\boldsymbol{\kappa}\mathbf{r}\}\sum_h\mathbf{E}_h(\mathbf{r})\exp\{i\mathbf{K}_h\mathbf{r}\}. \qquad (2\cdot12)$$

Here $\mathbf{K}$ is the incident-wave-vector, and the sum is to be taken over all reciprocal-lattice vectors of the ideal crystal. The absence of the diffraction scattering in region A, and the satisfaction of inequality (2·6) in area B result in the amplitudes $\mathbf{E}_h(\mathbf{r})$ being slowly varying functions with the characteristic length of the order l_0. Therefore, if we neglect, as usual, the second derivatives of $\mathbf{E}_h(\mathbf{r})$ and take into account that the electromagnetic

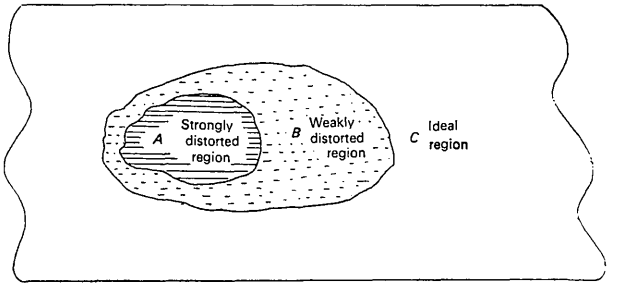

Fig. 1. Crystal containing faults.

wave inside the crystal remains practically transverse, we obtain from (2·1)

$$\sum_{h'} \exp\{i\mathbf{K}_{h'}\mathbf{r}\}\left(\alpha_{h'} - \frac{2i}{\kappa}\frac{\partial}{\partial s_{h'}}\right)\mathbf{E}_{h'}(\mathbf{r}) = \chi(r)\sum_{h'}\exp\{i\mathbf{K}_{h'}\mathbf{r}\}\,\mathbf{E}_{h'}(\mathbf{r}), \quad (2\cdot13)$$

where

$$\alpha_h = \frac{\kappa_h^2-\kappa^2}{\kappa^2}, \qquad \boldsymbol{\kappa}_h = \boldsymbol{\kappa}+\mathbf{K}_h,$$
$$\frac{\partial}{\partial s_h} = (\mathbf{s}_h\nabla), \qquad \mathbf{s}_h = \frac{\boldsymbol{\kappa}_h}{|\boldsymbol{\kappa}_h|}. \quad (2\cdot14)$$

Now we multiply the equation (2·13) by $\exp(-i\mathbf{K}_h\mathbf{r})$, and integrate over the volume V with linear dimensions l, where

$$a \ll l \ll l_0. \quad (2\cdot15)$$

Since the amplitudes, $\mathbf{E}_h(\mathbf{r})$, change only slightly in the length l, they can be omitted from the integration. Thus

$$\frac{1}{V}\int_V \exp\{i(\mathbf{K}_h-\mathbf{K}_{h'})\mathbf{r}\}d\mathbf{r} \simeq \delta_{hh'}. \quad (2\cdot16)$$

Then we have

$$\left(\alpha_h - \frac{2i}{\kappa}\frac{\partial}{\partial s_h}\right)\mathbf{E}_h(\mathbf{r}) = \sum_{h'}\chi_{hh'}(\mathbf{r})\mathbf{E}_{h'}(\mathbf{r}) \quad (2\cdot17)$$

where

$$\chi_{hh'}(\mathbf{r}) = \frac{1}{V}\int_V \chi(\mathbf{r})\exp\{i(\mathbf{K}_{h'}-\mathbf{K}_h)\mathbf{r}\}d\mathbf{r}. \quad (2\cdot18)$$

In the ideal crystal region, according to (2·5) and (2·16)

$$\chi^c_{hh'}(\mathbf{r}) = \chi^{(\mathrm{id})}_{h-h'}. \quad (2\cdot19)$$

In region A, taking into account (2·9), (2·10) and (2·16), we obtain

$$\chi^A_{hh'}(\mathbf{r}) = \chi_0^{(\mathrm{id})}\delta^{hh'}. \quad (2\cdot20)$$

In area B, according to (2·7), we have

$$\chi^B_{hh'}(\mathbf{r}) = \sum_{h''}\chi^{(\mathrm{id})}_{h''}\frac{1}{V}\int_V \exp\{-i\mathbf{K}_{h''}\mathbf{u}(\mathbf{r})\} \times \exp\{i(\mathbf{K}_{h''}+\mathbf{K}_{h'}-\mathbf{K}_h)\mathbf{r}\}d\mathbf{r}.$$

In the sum over h'', inequality (2·6) allows us to neglect all terms except those with $\mathbf{K}_{h''} = \mathbf{K}_h - \mathbf{K}_{h'}$.

Therefore

$$\chi^B_{hh'}(\mathbf{r}) = \chi^{(\mathrm{id})}_{h-h'}\frac{1}{V}\int_V \exp\{-i(\mathbf{K}_h-\mathbf{K}_{h'})\mathbf{u}(\mathbf{r})\}d\mathbf{r}. \quad (2\cdot21)$$

If $\mathbf{u}(\mathbf{r})$ change slowly over a distance of order l, then (2·21) turns into the formula

$$\chi^B_{hh'}(\mathbf{r}) = \chi^{(\mathrm{id})}_{h-h'}\exp\{-i(\mathbf{K}_h-\mathbf{K}_{h'})\mathbf{u}(\mathbf{r})\}. \quad (2\cdot22)$$

In the case of a rapid change of $\mathbf{u}(\mathbf{r})$ in the volume V (for example, when inequality (2·11) is satisfied), the only integral in (2·21) which would not, in practice, be equal to zero would be that for which $\mathbf{K}_h = \mathbf{K}_{h'}$. Making this substitution, we again obtain equation (2·20). Thus, we see once more that area A can be extended to area B. Further, we shall assume that region A includes the nucleus of the defect as well as the distorted areas where

$$2\pi\left|\frac{\partial u^i}{\partial x^k}\right|\frac{l}{a} \geq 1.$$

Here l is defined by inequalities (2·15). (It may be noticed that l can always be chosen almost equal to l_0, because the diffraction scattering is small in both cases.) We shall treat the remainder of the distorted region as region B, and use equation (2·22).

Further, we restrict ourselves to the case in which only one Bragg reflexion with a corresponding vector $\mathbf{K}_1$ of the reciprocal lattice exists (two-beam approximation). Then, passing to the set of equations for the scalar amplitudes, we obtain

$$g_{10}E_0 + \left(g_{00}-\alpha+\frac{2i}{\kappa}\frac{\partial}{\partial s_1}\right)E_1 = g_{10}\psi_+E_0$$
$$\left(g_{00}+\frac{2i}{\kappa}\frac{\partial}{\partial s_0}\right)E_0 + g_{01}E_1 = g_{01}\psi_-E_1 \quad (2\cdot23)$$

where the following notations have been introduced

$$\psi_\pm(\mathbf{r}) = \begin{cases} 1 & \text{in } A, \\ 1-\exp\{\mp i\mathbf{K}_1\mathbf{u}(\mathbf{r})\} & \text{in } B, \\ 0 & \text{in } C, \end{cases} \quad (2\cdot24)$$

$$g_{hh''} = \chi^{(\mathrm{id})}_{h-h'}\eta_h\eta_{h'}, \quad h,h' = 0,1,$$

$\boldsymbol{\eta}_h$ are the polarization vectors.

Equations (2·23) must be defined by boundary conditions. In the Laue case, these conditions are determined on the entrance surface of the crystal and take the form

$$E_0(\mathbf{r}) = E_0^{(\mathrm{in})}(\mathbf{r}), \quad E_1(\mathbf{r}) = 0. \quad (2\cdot25)$$

In the Bragg case, we have $E_0(\mathbf{r}) = E_0^{(\mathrm{in})}(\mathbf{r})$ on the entrance surface, and $E_1(\mathbf{r}) = 0$ on the exit one. Here $E_0^{(\mathrm{in})}(\mathbf{r})$ is the amplitude of the incident wave.

Finally, we note that, in regions B and C, replacing $E_h(\mathbf{r})$ by $\exp\{-i\mathbf{K}_h\mathbf{u}(\mathbf{r})\}E_h(\mathbf{r})$ gives the set of equations which have been obtained by Taupin (1967) and Schlangenotto (1967). The set of equations (2·23) is more convenient, because it also describes the strongly distorted region of a crystal.

3. Integral forms of the set of equations (2·23)

(A) *The Laue case*

We first consider the common property of equations (2·23). It is convenient to introduce oblique coordinates along the vectors $\mathbf{s}_0$ and $\mathbf{s}_1$, such that

$$\mathbf{r} = s_0\mathbf{s}_0 + s_1\mathbf{s}_1. \quad (3\cdot1)$$

We then make the replacement

$$E_h=\tilde{E}_h \exp\left(i\kappa\frac{g_{00}}{2}s_0+i\kappa\frac{(g_{00}-\alpha)}{2}s_1\right). \quad (3\cdot2)$$

The set of equations for amplitudes $\tilde{\mathbf{E}}_h$ has the simple form

$$\begin{aligned} i\frac{\partial\tilde{E}_0}{\partial s_0}+c_0\tilde{E}_1&=c_0\psi_-\tilde{E}_1\\ i\frac{\partial\tilde{E}_1}{\partial s_1}+c_1\tilde{E}_0&=c_1\psi_+\tilde{E}_0 \end{aligned} \quad (3\cdot3)$$

where

$$c_0=\frac{\kappa g_{01}}{2}, \qquad c_1=\frac{\kappa g_{10}}{2}.$$

From (3·3), we also have

$$\hat{L}\tilde{E}_{0,1}=F_{0,1} \quad (3\cdot4)$$

where

$$F_{0,1}=c^2\tilde{E}_{0,1}(\psi_++\psi_--\psi_+\psi_-)-ic_{1,0}\tilde{E}_{1,0}\frac{\partial\psi_{-,+}}{\partial s_{1,0}}. \quad (3\cdot5)$$

$c^2=c_0c_1$ and $\hat{L}$ is the differential operator

$$\hat{L}=\frac{\partial^2}{\partial s_0\partial s_1}+c^2. \quad (3\cdot6)$$

The equations (3·4) are hyperbolic and their characteristics are the sets of straight-line curves parallel to the vectors $\mathbf{s}_0, \mathbf{s}_1$. The fields inside the region G (Fig. 2) are strictly determined by amplitudes E_0 and E_1 on segment $A^{(0)}A^{(1)}$. Moreover, by using the Riemann method, integral equations can be obtained, which connect the fields at the point P and the fields inside the region G, (*cf.* Courant, 1962).

We introduce the function R which is the solution of the equation

$$\hat{L}R=0 \quad (3\cdot7)$$

with boundary conditions

$$\left.\frac{\partial R}{\partial s_0}\right|_{s_1=s_{1p}}=0, \qquad \left.\frac{\partial R}{\partial s_1}\right|_{s_0=s_{0p}}=0, \qquad \left.R\right|_{\substack{s_0=s_{0p}\\ s_1=s_{1p}}}=1. \quad (3\cdot8)$$

The solution to the problem is

$$R=J_0\left(2c\sqrt{(s_{0p}-s_0)(s_{1p}-s_1)}\right) \quad (3\cdot9)$$

where $J_0(z)$ is a Bessel function of zero order, and s_{0p}, s_{1p} are the coordinates of point P. Using equations (3·4) and (3·7), we obtain directly

$$\iint_G ds_0ds_1[R\hat{L}\tilde{E}_1-\tilde{E}_1\hat{L}R]=\iint_G ds_0ds_1RF_1. \quad (3\cdot10)$$

Using Green's theorem, the left-hand side of equation (3·10) can be turned into the integral over the boundary of the region G. According to (3·8) and (3·3), we have

$$\iint_G ds_0ds_1[R\hat{L}\tilde{E}_1-\tilde{E}_1\hat{L}R]=\tilde{E}_1(P)-\tilde{E}_1(A^{(1)})+ic_1\int_{A^{(0)}A^{(1)}}ds_1R\tilde{E}_0(1-\psi_+)+\int_{A^{(0)}A^{(1)}}ds_0\frac{\partial R}{\partial s_0}\tilde{E}_1. \quad (3\cdot11)$$

The final result is given by

$$\tilde{E}_1(P)=\tilde{E}_1(A^{(1)})-\int_{A^{(0)}A^{(1)}}ds_0\frac{\partial R}{\partial s_0}\tilde{E}_1-ic_1\int_{A^{(0)}A^{(1)}}ds_1R\tilde{E}_0(1-\psi_+)+\iint_G ds_0ds_1RF_1. \quad (3\cdot12)$$

The equation for $\tilde{E}_0(P)$ can be obtained from (3·12) by replacing the indices 0 by 1, + by − and *vice versa*.

In the Laue case, when the boundary conditions on $E_0(\mathbf{r})$ and $E_1(\mathbf{r})$ are defined on the same (entrance) surface of a crystal, we obtain the set of integral equations for the fields which automatically takes into account the boundary conditions (2·25).

$$\tilde{E}_0(P)=\tilde{E}_0^{(\mathrm{in})}(A^{(0)})-\int_{A^{(1)}A^{(0)}}ds^1\frac{\partial R}{\partial s_1}\tilde{E}_0^{(\mathrm{in})}+\iint_G ds_0ds_1RF_0 \quad (3\cdot13a)$$

$$\tilde{E}_1(P)=ic_1\int_{A^{(1)}A^{(0)}}ds_1R\tilde{E}_0^{(\mathrm{in})}(1-\psi_+)+\iint_G ds_0ds_1RF_1. \quad (3\cdot13b)$$

If the crystal does not contain defects, *i.e.* $\psi_+=\psi_-=0$, equations (3·13) give the direct connexion between the field in an arbitrary point of a crystal and the fields on the entrance surface

$$\begin{aligned} \tilde{E}_0^{(\mathrm{id})}(P)&=\tilde{E}_0^{(\mathrm{in})}(A^{(0)})+\int_{A^{(0)}A^{(1)}}ds_1\frac{\partial R}{\partial s_1}\tilde{E}_0^{(\mathrm{in})}\\ \tilde{E}_1^{(\mathrm{id})}(P)&=ic_1\int_{A^{(1)}A^{(0)}}ds_1R\tilde{E}_0^{(\mathrm{in})}. \end{aligned} \quad (3\cdot14)$$

This problem had been solved earlier by Slobodetskii *et al.* (1968) and Authier & Simon (1968).

Equations (3·13) can be also written in the following form:

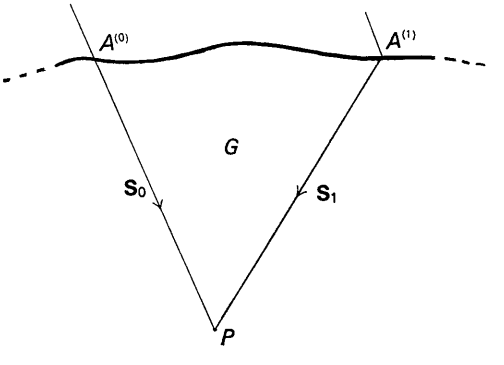

Fig. 2. Fields inside the region G.

$$\tilde{E}_0(P)=\tilde{E}_0^{(id)}(P)-ic_0\int_{A^{(0)}P} ds_0\tilde{E}_1\psi_- + \iint_G ds_0 ds_1\left[c^2R\tilde{E}_0\psi_+ + ic_0\frac{\partial R}{\partial s_1}\tilde{E}_1\psi_-\right] \quad (3\cdot15a)$$

$$\tilde{E}_1(P)=\tilde{E}_1^{(id)}(P)-ic_1\int_{A^{(1)}P} ds_1\tilde{E}_0\psi_+ + \iint_G ds_0 ds_1\left[c^2R\tilde{E}_1\psi_- + ic_1\frac{\partial R}{\partial s_0}\tilde{E}_0\psi_+\right]. \quad (3\cdot15b)$$

The sets of equations we have obtained are in a convenient form for determining an approximate solution by an iteration procedure. In a region of type A, the double integrals in (3·15) can be transformed into the integrals along a contour (*cf.* § 4), and this greatly simplifies the treatment of strongly distorted regions. In region B, it is convenient to use equations (3·13) because here the derivatives $\partial\psi/\partial s$ are small, and moreover

$$\psi_+ + \psi_- - \psi_+\psi_- \equiv 0\,. \quad (3\cdot16)$$

(*B*) *The Bragg case*

If the boundary conditions are defined on different surfaces as in the Bragg problem, then it turns out that the treatment of closed integral equations such as (3·13) is more complex.

Consider a crystal in the form of a plate of thickness t. Let the finite beam of X-rays fall on to the crystal in the direction of the vector $\boldsymbol{\kappa}$ (Fig. 3). We shall find the field of the reflected wave at point P_1 on the entrance surface of a crystal. The field at this point is determined by fields inside the region G which is limited by the line $AP_1A_1^{(1)}$ in the scattering film. Evidently, the amplitude $\tilde{E}_1$ equals zero on the segment AB. Let the function $R_B^{(1)}$ satisfy equation (3·7), but with the boundary conditions

$$\left.\frac{\partial R_B^{(1)}}{\partial s_0}\right|_{AP_1}=0\,,\quad \left.\frac{\partial R_B^{(1)}}{\partial s_1}\right|_{s_0=s_{0p}}=0\,,\quad \left.R_B^{(1)}\right|_{\substack{s_0=s_{0p}\\ s_1=s_{1p}}}=1\,. \quad (3\cdot17)$$

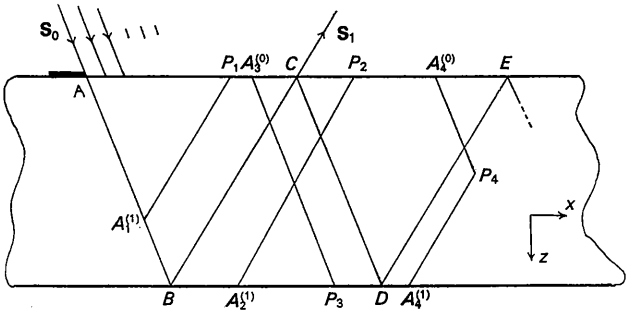

Fig. 3. Schematic diagram representing the scattering of an X-ray beam by the crystal.

The solution of this problem is given by

$$R_B^{(1)}=J_0\left(2c\sqrt{(s_{0p}-s_0)(s_{1p}-s_1)}\right) -\beta\frac{(s_{0p}-s_0)}{(s_{1p}-s_1)}J_2\left(2c\sqrt{(s_{0p}-s_0)(s_{1p}-s_1)}\right) \quad (3\cdot18)$$

where $\beta=\gamma_0/\gamma_1$, $\gamma_{0,1}=(\mathbf{n}\mathbf{s}_{0,1})$ and $\mathbf{n}$ is the vector of the inner normal to the entrance surface. The analogous procedure which has been used for the derivation (3·12) gives the following result

$$\tilde{E}_1(P_1)=ic_1\int_{AP_1} ds_1R_B^{(1)}\tilde{E}_0^{(in)}(1-\psi_+)+\iint_G ds_0ds_1R_B^{(1)}F_1. \quad (3\cdot19)$$

Equation (3·19) is valid for the points P_1 lying on the area AC of the entrance surface. For the points lying to the right of C (*e.g.* P_2) the following integral must be added in the right-hand side of equation (3·19):

$$\Delta\tilde{E}_1(P_2)=-ic_1\int_{BA_2^{(1)}} ds_1R_B^{(1)}\tilde{E}_0(1-\psi_+)\,. \quad (3\cdot20)$$

If the crystal is sufficiently thick, so that $\mu t\gg 1$, where μ is the absorption coefficient, then it can be easily shown that this integral gives an exponentially small contribution, and can be neglected. Thus, in the case of a thick absorbing crystal, equation (3·19) defines the field $\tilde{E}_1$ at all points on the entrance surface.

For an ideal crystal, when $\psi_\pm=0$, according to (3·19) we have

$$\tilde{E}_1(P)=ic_1\int_{AP} ds_1R_B^{(1)}\tilde{E}_0^{(in)}\,. \quad (3\cdot21)$$

Equation (3·21) defines, in the general case, the field of a reflected wave on the entrance surface for an arbitrary distribution of the incident wave field. Introducing the coordinate x along the crystal surface in the scattering plane (A being the zero point) we can rewrite this equation for the amplitude $E_1(x)$ directly [*cf.* (3·2)].

$$E_1(x)=i\frac{c_1\gamma_0}{\sin 2\theta_B}\int_0^x dx^1[J_0(Bx^1)+J_2(Bx^1)] \times\exp\{iAx^1\}E_0^{(in)}(x-x^1) \quad (3\cdot22)$$

where

$$A=\kappa g_{00}\frac{(\gamma_0+|\gamma_1|)}{2\sin 2\theta_B}-\kappa\alpha\frac{\gamma_0}{2\sin 2\theta_B}\,,\quad B=2c\frac{\sqrt{\gamma_0|\gamma_1|}}{\sin 2\theta_B}\,. \quad (3\cdot23)$$

If the field $E_0^{(in)}(x)$ is constant

$$E_0^{(in)}(x)=E_0\,,\quad x>0\,,$$

then, according to (3·22), when $x\to\infty$, we obtain after a number of simple transformations

$$E_1(\infty)=\frac{E_0}{2g_{01}}\left[-\{\alpha\beta+g_{00}(1-\beta)\} +\sqrt{\{\alpha\beta+g_{00}(1-\beta)\}^2+4\beta g_{01}g_{10}}\right]. \quad (3\cdot24)$$

This result agrees exactly with the result of the usual

dynamical theory for the thick absorbing crystals (Zachariasen, 1946).

In addition to equation (3·19) one can obtain, by a fully analogous method, the equation which determines the amplitude $\tilde{E}_0$ on an exit surface:

$$\tilde{E}_0(P_3)=\tilde{E}_0^{(in)}(A_3^{(0)})-\int_{AA_3^{(0)}} ds_1 \frac{\partial R_B^{(0)}}{\partial s_1}\tilde{E}_0^{(in)} - ic_0\int_{AA_3^{(0)}} ds_0 R_B^{(0)}\tilde{E}_1(1-\psi_-)+\iint_G ds_0 ds_1 R_B^{(0)}F_0 . \quad (3\cdot25)$$

Here

$$R_B^{(0)}=J_0\left(2c\sqrt{(s_{0p}-s_0)\,(s_{1p}-s_1)}\right) - \frac{1}{\beta}\frac{(s_{1p}-s_1)}{(s_{0p}-s_0)} J_2\left(2c\sqrt{(s_{0p}-s_0)\,(s_{1p}-s_1)}\right) . \quad (3\cdot26)$$

Moreover, we have the general equations (3·11) for the inner points P_4 of a crystal where, in a given case, a contour $A^{(0)}A^{(1)}$ is $A_4^{(0)}ABA_4^{(1)}$. Since $\tilde{E}_1=0$ on the line $ABA_4^{(1)}$ the integral along $A_4^{(0)}\cdots A_4^{(1)}$ is reduced to the integrals along the lines $AA_4^{(0)}$ and $BA_4^{(1)}$, then

$$\tilde{E}_0(P_4)=\tilde{E}_0^{(in)}(A_4^{(0)})-\int_{AA_4^{(0)}} ds_1 \frac{\partial R}{\partial s_1}\tilde{E}_0^{(in)} - ic_0\int_{AA_4^{(0)}} ds_0 R\tilde{E}_1(1-\psi_-)+\int_{BA_4^{(1)}} ds_1 \frac{\partial R}{\partial s_1}\tilde{E}_0 + \iint_G ds_0 ds_1 R F_0 , \quad (3\cdot27a)$$

$$\tilde{E}_1(P_4)=ic_1\int_{AA_4^{(0)}} ds_1 R\tilde{E}_0^{(in)}(1-\psi_+) + \int_{AA_4^{(0)}} ds_0 \frac{\partial R}{\partial s_0}\tilde{E}_1 - ic_1\int_{BA_4^{(1)}} ds_1 R\tilde{E}_0(1-\psi_+) + \iint_G ds_0 ds_1 R F_1 . \quad (3\cdot27b)$$

The sets of integral equations (3·19), (3·25), (3·27) permit the use of the iteration procedure to determine amplitudes $\tilde{E}_0$ and $\tilde{E}_1$ in a distorted crystal. In the case of the thick absorbing crystal ($\mu t\gg 1$) the integral along the line $BA_4^{(1)}$ in (3·20) and (3·27) gives the exponentially small contribution and may be neglected. Therefore, it is not necessary to use equation (3·25).

In the case of the ideal crystal ($\psi_\pm=0$) we have, according to (3·25),

$$E_0(x,t)=\exp\left\{i\kappa\frac{g_{00}}{2}\frac{t}{\gamma^0}\right\} \times\left\{E_0^{(in)}(x_0)-c\frac{\sqrt{|\gamma_0|\gamma_1|}}{\sin 2\theta_B}\int_0^{x_0} dx' \frac{2l}{z} \times J_1(Bz)\exp\{iAx'\}E_0^{(in)}(x_0-x')-i\frac{c_0|\gamma_1|}{\sin 2\theta_B} \times\int_0^{x_0} dx'\left[J_0(Bz)+\frac{x'}{x'+2l}J_2(Bz)\right] \times\exp\{iAx'\}E_1(x_0-x',0)\right\} \quad (3\cdot28)$$

where

$$z=\sqrt{x'(x'+2l)}\,,\quad 2l=t\frac{\sin 2\theta_B}{\gamma_0|\gamma_1|}\,,\quad x_0=x-t\sqrt{1-\gamma_0^2}/\gamma_0 .$$

Here we use the true amplitude (3·2) again. The equation (3·28) contains the field E_1 defined by equation (3·22). Knowing the field E_0 on the segment BD, we obtain easily the field E_1 on the segment CE which now is defined by sum of equations (3·20) and (3·22). The equation (3·20), we rewrite in the detailed form

$$\Delta E_1(x)=-i\frac{c_1\gamma_0}{\sin 2\theta_B}\exp\left\{i\kappa\frac{(g_{00}-\alpha)}{2}\frac{t}{|\gamma_1|}\right\} \times\int_0^{x-2l} dx'\left[J_0(Bz)+\frac{x'}{x'+2l}J_2(Bz)\right] \times\exp\{iAx'\}E_0(x_1-x',t)\,, \quad (3\cdot29)$$

where $x_1=x-t\sqrt{1-\gamma_1^2}/|\gamma_1|$. Since the field $E_1(x)$ on the segment CE is known, the field $E_0(x,t)$ can be defined in the points to the right of D and so on.

The procedure outlined above permits the reflected wave field to be determined over the entire surface of a crystal, but this is rather cumbersome. Nevertheless, the formula for $E_1(x)$ may be obtained in a more compact form. By substituting into equation (3·29) for E_0 [from equation (3·28)] and for the field E_1 on the line AC [from equation (3·22)], the expression for $\Delta E_1(x)$ on the line CE breaks up into the sum of single, double and triple integrals. The double and triple integrals can be transformed into a single integral, so that the final expression for the field $\Delta E_1(x)$ has the form:

$$\Delta E_1(x)=ic_1\frac{\gamma_0}{\sin 2\theta_B}\int_0^x dx' G_1(x',2l)E_0^{(in)}(x-x'), \quad (3\cdot30)$$

where

$$G_n(x,2l)=\theta(x-2ln)\,(-1)^n\exp\{iAx\}\{\xi^{n-1}J_{2n-2}(B\eta) +2\xi^n J_{2n}(B\eta)+\xi^{n+1}J_{2n+2}(B\eta)\}\,, \quad (3\cdot31)$$

$$\xi=\frac{x-2ln}{x+2ln}\,,\qquad \eta=\sqrt{x^2-(2ln)^2}\,,$$

$$\theta(x)=\begin{cases}0 & x<0\\ 1 & x>0\,.\end{cases} \quad (3\cdot32)$$

For the general case one can obtain the following expression for the field $E_1(x)$ at an arbitrary point in the surface:

$$E_1(x)=ic_1\frac{\gamma_0}{\sin 2\theta_B}\int_0^x dx' G(x')E_0^{(in)}(x-x')\,, \quad (3\cdot33)$$

where

$$G(x)=G_0(x)+\sum_{n=1}^{n_{max}} G_n(x,2l)\,. \quad (3\cdot34)$$

Here n_{max} is the integer part of $x/2l$; $G_0(x)$ is deter-

mined from equation (3·22)

$$G_0(x)=\exp\{iAx\}\{J_0(Bx)+J_2(Bx)\} \qquad (3\cdot35)$$

and represents Green's function approximated for an infinitely thick absorbing crystal. $G_n(x,2l)$ is given by equations (3·31) and (3·32) and describes the n-fold reflexion by the lower surface of the crystal.

Fig. 4 shows the reflected wave intensity, which is proportional to $|G(x)|^2$, for a δ-functional source. It is seen from the Figure that, in this case, intensity peaks appear near the points $x=2ln$. If the incident radiation has a finite spread $d\gtrsim l_0$ and is collimated over a range of angles, then an integration over this spread in equation (3·33) results in a practically complete cancelling of the field $E_1(x)$ because of strong oscillations of the $G_n(x,2l)$ function in these regions.

However, if the incident beam is not collimated and one measures the integral intensity, then these additional peaks will be well displayed. Indeed, in the case of an uncollimated beam the incident fields $E_0(x)$ are incoherent at every point in the crystal. In this case, the integral intensity is given by

$$I_1(x)=|c_1|^2\frac{2\pi\gamma_0}{\kappa\sin^2 2\theta_B}\int_0^x \mathrm{d}x'|G(x')|^2|E_0^{(\mathrm{in})}(x-x')|^2 . \qquad (3\cdot36)$$

In Fig. 4 the integral intensity is plotted for an incident plane wave passing through a slit of width d. As can be seen from the plot, the peaks have an apparent magnitude but lack the fine structure, characteristic of a δ-functional source.

4. Strongly distorted region

Consider, as an example, the case in which only the strongly distorted region exists in a crystal, *i.e.* a region of type A where diffraction scattering is absent. This case, as it will be seen below, is more simple for analysis, than a general case and can give a comprehension of a general picture of the image contrast formation.

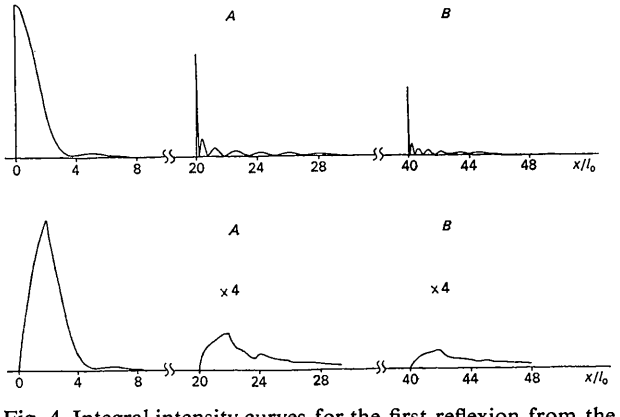

Fig. 4. Integral intensity curves for the first reflexion from the lower surface of the crystal. The upper curves are for a δ-functional source and the lower curves for a slit of width $d=2l_0$. The parameters of the calculation correspond to the following experimental conditions: Si crystal, Mo $K\alpha$ radiation, (220) reflexion, $|\beta|=1$, $2l=20\,l_0$ (curves A) and $2l=40\,l_0$ (curves B), $l_0=1/|c|=12\mu$. The decrease of maximum intensity on the upper curves is due to absorption.

For the sake of simplicity we shall continue the analysis for the Laue case. Let region A (Fig. 5) be the section of a distorted area of a crystal by a scattering plane. Alterations in the fields caused by this defect will occur on the segment $A^{(1)}A^{(0)}$ only. In the case given, it is convenient to use the integral equations (3·15), because $\psi_\pm=1$ inside region A. Considering this fact and using equations (2·23) and (3·3), we transform the double integrals of (3·15) into integrals along a contour. Then the integral equations (3·15) will have the form.

$$\tilde{E}_0(P)=\tilde{E}_0^{(\mathrm{id})}(P)+ic_0\int_{\Gamma_A}\mathrm{d}s_0 R\tilde{E}_1+\int_{\Gamma_A}\mathrm{d}s_1\frac{\partial R}{\partial s_1}\tilde{E}_0 \qquad (4\cdot1a)$$

$$\tilde{E}_1(P)=\tilde{E}_1^{(\mathrm{id})}(P)-ic_1\int_{\Gamma_A}\mathrm{d}s_1 R\tilde{E}_0-\int_{\Gamma_A}\mathrm{d}s_0\frac{\partial R}{\partial s_0}\tilde{E}_1 \qquad (4\cdot1b)$$

where $\tilde{E}_{0,1}^{(\mathrm{id})}$ are the ideal crystal fields, and Γ_A is that part of the boundary of region A which lies inside the region G. For points P, when the region A lies fully inside the region G the contour Γ_A is simply the boundary of the region A. For points of type P_1, the contour is $P_1''B^{(1)}C^{(1)}D^{(1)}P_1'P_1''$.

Now we introduce the quantities

$$e_{0,1}(P)=\tilde{E}_{0,1}(P)-\tilde{E}_{0,1}^{(\mathrm{id})}(P) \qquad (4\cdot2)$$

which define directly the wave-field distortion, caused by the defects. The equations (4·1) now are

$$e_0(P)=ic_0\int_{\Gamma'_A}\mathrm{d}s_0 Re_1+\int_{\Gamma'_A}\mathrm{d}s_1\frac{\partial R}{\partial s_1}e_0 \qquad (4\cdot3a)$$

$$e_1(P)=-ic_1\int_{\Gamma'_A}\mathrm{d}s_1 Re_0-\int_{\Gamma'_A}\mathrm{d}s_0\frac{\partial R}{\partial s_0}e_1 . \qquad (4\cdot3b)$$

In obtaining (4·3) we used the following obvious equality

$$ic_{0,1}\int_\gamma \mathrm{d}s_{0,1}R\tilde{E}_{1,0}^{(\mathrm{id})}+\int_\gamma \mathrm{d}s_{1,0}\frac{\partial R}{\partial s_{1,0}}\tilde{E}_{0,1}^{(\mathrm{id})}=0 \qquad (4\cdot4)$$

where γ is an arbitrary closed contour in the scattering plane. Since the fields $\tilde{E}_{0,1}$ are equivalent to ideal fields, namely $e_{0,1}=0$, on the contour $B^{(1)}B^{(0)}$ the integration in (4·3) is carried out only along the line $B^{(1)}C^{(1)}D^{(1)}\ldots B^{(0)}$.

According to (4·3), the problem of determining the fields in a crystal is reduced to the problem of finding the fields $e_{0,1}$ along the contour Γ'_A. For the solution of this problem, we note, first of all, that inside region A the field $\tilde{E}_0$ is constant along the lines, parallel to the vector $\mathbf{s}_0$ and the field $\tilde{E}_1$ is constant along the lines, parallel to $\mathbf{s}_1$. This can be seen directly from the equations (3·3). Using this fact, we deduce that the fields

e_0 and e_1 along the lines $D^{(1)}D^{(0)}B^{(0)}$ and $B^{(1)}D^{(1)}D^{(0)}$ respectively are defined by simple transition, that is

$$e_0(P_2')=\tilde{E}_0^{(id)}(P_2'')-\tilde{E}_0^{(id)}(P_2') \text{ on } D^{(1)}D^{(0)}B^{(0)}$$
$$e_1(P_1')=\tilde{E}_1^{(id)}(P_1'')-\tilde{E}_1^{(id)}(P_1') \text{ on } B^{(1)}D^{(1)}D^{(0)} . \quad (4\cdot5)$$

To determine the fields $e_{0,1}$ along the remainder of the contour, we use equation (4·3). The equation for the field e_0 along the line $B^{(1)}C^{(1)}$ is

$$e_0(l)=ic_0\int_0^l dl' \frac{ds_0'}{dl'} Re_1+\int_0^l dl' \frac{ds_1'}{dl'} \frac{\partial R}{\partial s_1'} e_0 \quad (4\cdot6)$$

where l is a coordinate of a point along the line $B^{(1)}C^{(1)}$. The first integral term in (4·6) contains known functions, since e_1 is defined exactly along this contour. Thus, we have a Volterra's inhomogeneous integral equation for the determination of the field $e_0(l)$ along the line $B^{(1)}C^{(1)}$. The field e_0 along the line $C^{(1)}D^{(1)}$ is defined by transition from the line $B^{(1)}C^{(1)}$. To define the field e_1 along the contour $B^{(0)}C^{(0)}$, we have the analogous equation.

Thus, the problem has been reduced to the solution of a relatively simple one-dimension integral equation. Specific examples will be considered in the next work.

5. Fourier analysis

In this section, we examine another approach to the general problem. This is the transformation from the set of differential equations (2·22) to a set of algebraic ones for the Fourier components of amplitudes $E_0(\mathbf{r})$, $E_1(\mathbf{r})$.

We shall assume the distortion of a crystal to be sufficiently weak for the alteration in the wave field to be small.

$$E_{0,1}(\mathbf{r})=E_{0,1}^{(id)}(\mathbf{r})+E_{0,1}'(\mathbf{r}) , \quad |E_{0,1}'|\ll|E_{0,1}^{(id)}| . \quad (5\cdot1)$$

Further, we shall restrict ourselves to the Laue case. Let a plane wave fall on to a crystal at an angle close to the Bragg angle. Then the fields inside a ideal crystal are known (*cf.* Zachariasen, 1946).

$$E_{0,1}^{(id)}(z)=\sum_\delta E_{0,1}^{(\delta)} \exp\left\{i\kappa\varepsilon_0^{(\delta)}\frac{z}{\gamma_0}\right\} \quad (5\cdot2)$$

where $z=(\mathbf{nr})$, $\delta=1,2$

$$E_0^{(1,2)}=\frac{2\varepsilon_0^{(2,1)}-g_{00}}{2(\varepsilon_0^{(2,1)}-\varepsilon_0^{(1,2)})} , \quad E_1^{(1,2)}=\frac{\beta g_{10}}{2(\varepsilon_0^{(1,2)}-\varepsilon_0^{(2,1)})} \quad (5\cdot3)$$

$$\varepsilon_0^{(1,2)}=\tfrac{1}{2}g_{00}+\tfrac{1}{4}\left[-(\alpha\beta+g_{00}(1-\beta)) \pm\sqrt{(\alpha\beta+g_{00}(1-\beta))^2+4\beta g_{01}g_{10}}\right] ; \quad (5\cdot4)$$

the sign of the radical is defined so that

$$\varepsilon_0^{(1)''}\geq\varepsilon_0^{(2)''} \quad (\varepsilon=\varepsilon'+i\varepsilon'') . \quad (5\cdot5)$$

Now we expand the fields $E_{0,1}'$ in the following Fourier series

$$E_{0,1}'(\mathbf{r})=\sum_{\mathbf{q}\neq0}\exp\{i\mathbf{qr}\}\sum_\delta E_{0,1\mathbf{q}}^{(\delta)}\exp\{i\kappa\varepsilon_0^{(\delta)}\frac{z}{\gamma_0}\}. \quad (5\cdot6)$$

Making the substitution $E_{0,1}=E_{0,1}^{(id)}$ in the right-hand side of equations (2·23), we obtain for the Fourier components $E_{0,1\mathbf{q}}^{(\delta)}$

$$(-2\varepsilon_{0\mathbf{q}}^{(\delta)}+g_{00})E_{0\mathbf{q}}^{(\delta)}+g_{01}E_{1\mathbf{q}}^{(\delta)}=g_{01}\psi_-(\mathbf{q})E_1^{(\delta)} \quad (5\cdot7)$$
$$g_{10}E_{0\mathbf{q}}^{(\delta)}+(-2\varepsilon_{1\mathbf{q}}^{(\delta)}+g_{00})E_{1\mathbf{q}}^{(\delta)}=g_{10}\psi_+(\mathbf{q})E_0^{(\delta)}$$

where

$$\varepsilon_{0,1\mathbf{q}}^{(\delta)}=\varepsilon_{0,1}^{(\delta)}+\frac{(\mathbf{qs}_{0,1})}{\kappa} , \quad \varepsilon_1^{(\delta)}=\frac{\alpha}{2}+\frac{\varepsilon_0^{(\delta)}}{\beta} . \quad (5\cdot8)$$

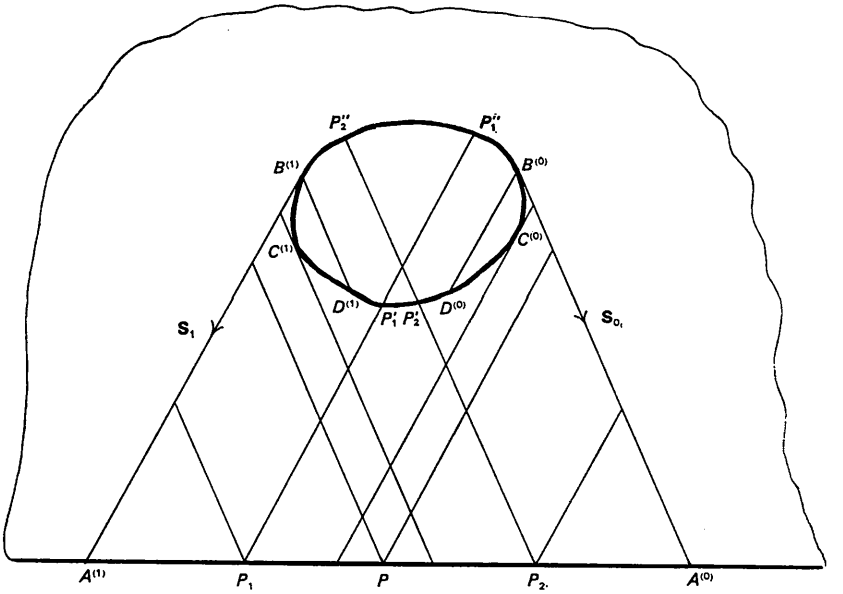

Fig. 5. Section of a distorted area of a crystal by a scattering plane.

The system of type (5·7) has already been obtained (Afanas'ev, Kagan & Chukhovskii, 1968), where the method for its solution was also given. Here, two conditions are essential. The first one is that the set of equations (5·7) must be defined by boundary conditions for the waves scattered by faults, and a second is that it is necessary to account for the solution of corresponding homogeneous sets of equations [*cf.* Afanas'ev *et al.* (1968) for details]. Considering these two conditions, the final expression, for example, for $E'_0(\mathbf{r})$ is given by

$$E'_0(\mathbf{r})=\sum_{\mathbf{q}\neq 0}\exp\{i\mathbf{q}\mathbf{r}\}\sum_{\delta\delta'}\frac{(-1)^{\delta'}\beta g_{01}g_{10}}{2(\tilde{\varepsilon}_0^{(2)}-\tilde{\varepsilon}_0^{(1)})}\times\left(E_0^{(\delta)}\psi_+(\mathbf{q})+\frac{2\tilde{\varepsilon}_1^{(\delta')}-g_{00}}{g_{10}}E_1^{(\delta)}\psi_-(\mathbf{q})\right)\times\frac{\left(\exp\left\{i\kappa\varepsilon_0^{(\delta)}\frac{z}{\gamma_0}\right\}-\exp\left\{i\kappa(\tilde{\varepsilon}_0^{(\delta')}-\sigma)\frac{z}{\gamma_0}\right\}\right)}{2(\varepsilon_{0q}^{(\delta)}-\tilde{\varepsilon}_0^{(\delta')})}\quad(5\cdot9)$$

where

$$\sigma=\frac{(\mathbf{q}\mathbf{s}_0)}{\kappa},\qquad \tilde{\varepsilon}_0^{(\delta)}=\varepsilon_0^{(\delta)}(\tilde{\alpha}),$$

$$\tilde{\alpha}=\alpha-\frac{2}{\kappa\beta}[\mathbf{q}(\mathbf{s}_0-\beta\mathbf{s}_1)],\quad \tilde{\varepsilon}_1^{(\delta)}=\frac{\tilde{\alpha}}{2}+\frac{\tilde{\varepsilon}_0^{(\delta)}}{\beta}.\quad(5\cdot10)$$

Though the expression (5·9) is complex in form, the final result can be written more simply. Turning again to the description of the distortion in coordinate space, we obtain for the field $E'_0(\mathbf{r})$, according to (5·9),

$$E'_0(\mathbf{r})=\int d\mathbf{r}'[\mathscr{D}_{00}(\mathbf{r},\mathbf{r}')\psi_+(\mathbf{r}')+\mathscr{D}_{01}(\mathbf{r},\mathbf{r}')\psi_-(\mathbf{r}')]\quad(5\cdot11)$$

where

$$\mathscr{D}_{00}(\mathbf{r},\mathbf{r}')=\frac{1}{(2\pi)^3}\int d\mathbf{q}\exp\{i\mathbf{q}(\mathbf{r}-\mathbf{r}')\}\sum_{\delta\delta'}\frac{(-1)^{\delta'}\beta g_{01}g_{10}}{2(\tilde{\varepsilon}_0^{(2)}-\tilde{\varepsilon}_0^{(1)})}\times E_0^{(\delta)}\frac{\left(\exp\left\{i\kappa\varepsilon_0^{(\delta)}\frac{z}{\gamma^0}\right\}-\exp\left\{i\kappa(\tilde{\varepsilon}_0^{(\delta')}-\sigma)\frac{z}{\gamma_0}\right\}\right)}{2(\varepsilon_{0q}^{(\delta)}-\tilde{\varepsilon}_0^{(\delta')})}\quad(5\cdot12)$$

and we have the analogous expression for $\mathscr{D}_{01}(\mathbf{r},\mathbf{r}')$. The integration over q_y in (5·12) gives $\delta(y-y')$, where y is a coordinate in the direction normal to the scattering plane. The integration over q_z can be carried out by using the residue theorem. As a result of these calculations, we have

$$\mathscr{D}_{00}(\mathbf{r},\mathbf{r}')=i\frac{\kappa}{2\gamma_0}\delta(y-y')\theta(z')\theta(z-z')\times I(x-x',z-z')\sum_{\delta}E_0^{(\delta)}\exp\left\{i\kappa\varepsilon_0^{(\delta)}\frac{z'}{\gamma_0}\right\}\quad(5\cdot13)$$

where

$$I(x,z)=\int_{-\infty}^{\infty}\frac{dq_x}{2\pi}\exp\{iq_xx\}\sum_{\delta'}\frac{(-1)^{\delta'}\beta g_{01}g_{10}}{2(\tilde{\varepsilon}_0^{(2)}-\tilde{\varepsilon}_0^{(1)})}\times\exp\left\{-is_{0x}q_x\frac{z}{\gamma_0}+i\kappa\tilde{\varepsilon}_0^{(\delta')}\frac{z}{\gamma_0}\right\}.\quad(5\cdot14)$$

Upon integrating equation (5·14) we obtain

$$\mathscr{D}_{00}(r,r')=c^2\left|\frac{\partial(s'_0,s'_1)}{\partial(x',z')}\right|\delta(y-y')\theta(z')\theta(z-z')\times\exp\left(i\kappa\frac{g_{00}}{2}(s_0-s'_0)+i\kappa\frac{(g_{00}-\alpha)}{2}(s_1-s'_1)\right)\times A_{00}E_0^{(id)}(z')\quad(5\cdot15)$$

where

$$A_{00}=J_0(2c\sqrt{(s_0-s'_0)(s_1-s'_1)})\times\frac{\operatorname{sign}(s_0-s'_0)+\operatorname{sign}(s_1-s'_1)}{2}.\quad(5\cdot16)$$

For the function $\mathscr{D}_{01}$, the analogous analysis gives an expression in the form of equation (5·15) with the following changes

$$A_{00}\to A_{01}=-\frac{i}{c_1}\frac{\partial A_{00}}{\partial s_1},\quad E_0^{(id)}\to E_1^{(id)}.\quad(5\cdot17)$$

Thus we arrive at the expression for the field E_0 after a rather complicated calculation (in the above, only a scheme of derivation of the formulae (5·12) and (5·16) has been outlined), while the same result can be obtained in a straightforward way from the integral equations (3·15) as the first order approximation over ψ. The analogous analysis in the Bragg case leads us finally to integral equations the form of (3·19). Therefore Fourier analysis is not expedient for definition of the field caused by static defects, because the integral equations (3·13), (3·19), (3·25) and (3·27) give a much more simple method for the solution of the problem.

It should be noted, however, that in the problem of defining diffuse scattering, caused by crystal-lattice vibrations, Fourier analysis is probably the only useful method. The physical difference between this and the static distortion problem is that the scattering of phonons is essentially an incoherent process. Therefore, one can only determine wave intensities, but not the amplitudes and the integral equations for amplitudes, of the forms (3·13), (3·19) and (3·25), cannot in principle exist.

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Ray Tracing with X-rays in Deformed Crystals

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The propagation of X-rays in an elastically deformed crystal has been studied using a ray-optical experimental arrangement. A single incident ray was selected from a Borrmann transmitted beam and was then diffracted through a thin crystal which was elastically strained by a temperature gradient. From the position and intensity of the rays at the exit surface it has been shown that for symmetric transmission, the plane wave boundary condition is maintained in any arbitrary but homogeneous strain field and that the migration of the tie points in good agreement with the theory.

Introduction

An extension of the dynamical theory of X-ray diffraction to include diffraction in slightly strained crystals was first given by Penning & Polder (1961). This theory was modelled on the propagation of light beams through inhomogeneous media and was founded on certain *ad hoc* assumptions. The wave optical foundation to the Penning & Polder theory was provided by Kato (1963, 1964*a*, *b*) who showed that Penning & Polder's basic equation could be derived by applying Fermat's principle to the path of a modified Bloch wave through the deformed crystal. Independently, the basic assumptions of the theory and their range of applicability were investigated by Kambe (1965, 1968). Penning & Polder's theory was later developed by Bonse (1964*a*) to allow for the complex nature of the vectors characterizing the wave-fields.

Another approach to the problem has been to consider directly the modification of the dynamical wavefields by the lattice distortion. With this method Takagi (1962, 1969), Taupin (1964) and Schlangenotto (1967) have used very general formalisms and have obtained differential equations which can be solved numerically for particular experimental cases. Taupin has been primarily concerned with the image forms of line defects whereas the Takagi theory has been used to explain some experiments on elastically-strained crystals (Malgrange, 1968) where it was shown to give the same results as the ray theories over the range of deformation studied.

Experimental verification of some aspects of these theories has been obtained by various workers. A decrease in the diffracted intensity from a thick anomalously transmitting crystal has been observed when the crystal is subjected to a bending moment (Hunter, 1959; Cole & Brock, 1959; Okkerse & Penning, 1963) or to a temperature gradient (Borrmann & Hildebrandt, 1959; Okkerse & Penning, 1963; Malgrange, 1968). This decrease has, in the experiments, been quantitatively explained by Penning & Polder's theory. An experiment of a different nature has demonstrated more dramatically the modification of the crystal wavefield vectors. Hart (1966) measured the displacement of the Pendellösung fringes in a crystal strained by a temperature gradient. The fringe displacement was correctly predicted by calculating the phase advance along the ray paths from the ray theory and by Kato's eikonal theory. This is not surprising since the existence of the eikonal implies ray optics.

In order to obtain direct evidence of the energy propagation changes in a strained crystal, it is desirable

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