Acta Cryst. (1977). A33, 311–319

A General Dynamical Theory of the X-ray Laue Diffraction from a Homogeneously Bent Crystal

By F. N. Chukhovskii

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

and P. V. Petrashen'

Physical–Technical Institute, Academy of Sciences of the USSR, Leningrad, USSR

(*Received* 20 *March* 1976; *accepted* 27 *October* 1976)

General properties of the rigorous solution of the problem of the X-ray dynamical Laue diffraction from a bent crystal are discussed. The solution based on the Takagi equations is formulated in the form of the Huygens–Fresnel principle. Special attention is paid to the behaviour of the quasi-classical asymptotic expansion of the exact dynamical wave fields and to the comparison of the results with those obtained by the eikonal theory. The eikonal theory is developed as a result of the application of the stationary-phase method for the evaluation of the Kirchhoff integral in accordance with the Huygens–Fresnel principle. The focusing of X-rays (the intersection of the ray trajectories and the formation of a caustic) is analysed. The generalized eikonal theory when elaborated yields that the integrated diffracted intensity from a bent crystal tends to the correct kinematical value as the strain gradient increases. For practical purposes, a simple numerical method of calculation of the integrated intensity applied in a general case of asymmetric Laue diffraction is proposed.

1. Introduction

The dynamical theory of X-ray diffraction from a bent crystal was first developed by Penning & Polder (1961), Kato (1964), Penning (1966) and Bonse (1964). It deals with the eikonal approximation of the wave optics and makes it possible to explain a number of the experimental data, in particular, the constriction of the *Pendellösung* fringes (Hart, 1966; Kato & Ando, 1966) and the asymmetry of the integral reflecting power with respect to the sign of the lattice bending (Fukushima, Hayakawa & Nimura, 1963; Meieran & Blech, 1965; Schwuttke & Howard, 1968). Further, the solution of the problem obtained affords some ground for the adequate description of X-ray topographs in the case of any continuously distorted crystal (Ando & Kato, 1970; Ando, Patel & Kato, 1973; Fishman & Lutzau, 1973; Kato & Patel, 1973; Patel & Kato, 1973).

At the same time, because of the restrictions imposed by the applicability of the ray-optics concept the eikonal theory reveals two apparent faults: one cannot correctly describe the X-ray propagation through the strongly distorted crystal or near the edges of the Borrman fan.

For this reason, of special interest is the rigorous consideration of the X-ray diffraction problem for a crystal with a uniform strain gradient (Petrashen', 1973; Chukhovskii, 1974*a*, *b*; Katagawa & Kato, 1974; Litzman & Janacek, 1974). The exact analytical solution based on the Takagi equations (Takagi, 1962; 1969) has been shown to be expressed in terms of confluent hypergeometric functions. On the one hand, this complicates the mathematical treatment; on the other hand, the physical analysis of the solution mentioned above is absolutely necessary if one is ever to construct an adequate description of the diffraction phenomenon in a homogeneously bent crystal. Hence, this may properly be the subject of a separate study.

The aim of the present paper is to give a theoretical contribution to the same field: X-ray Laue diffraction from a homogeneously bent crystal. The results, which will be described here, may be regarded as a generalization of our earlier work (Chukhovskii & Petrashen', 1975; Petrashen' & Chukhovskii, 1975). We shall (i) discuss the physical features of the exact dynamical wave fields inside a crystal with a uniform strain gradient in a most general form (§2); (ii) consider the behaviour of the quasi-classical asymptotic expansion of the rigorous solution and compare the results with those of the eikonal theory (§§3, 4). This is useful for establishing the range of applicability of the eikonal theory and to point out how its results should be corrected in order to include the case of any strain gradient.

In §4 we treat the ray optics of the X-ray field in a crystal for both the plane and the spherical incident wave. The ray trajectories appear as a result of the application of the stationary-phase method for the evaluation of the Kirchhoff integral in accordance with the Huygens–Fresnel principle. Generally, ray intersections (singular points, caustic) may occur which can be interpreted as focusing points of the wave field. Near these points the stationary-phase method does not hold, nor does the eikonal theory. It turns out that the effect of the X-ray focusing persists even when the component of the strain gradient along the reflexion vector is equal to zero.

The generalized eikonal theory when elaborated, yields automatically that the integral reflecting power approaches the kinematical value with increasing strain gradient. Thus, the 'divergence' problem of the integrated intensity as a function of strain gradient which arises for a transparent (non-absorbing) crystal in the eikonal theory (Kato, 1964) is completely removed (§5). For the practical calculation of the integrated intensity a simple numerical method is proposed. It is applied in the general case of asymmetric Laue diffraction.

Some additional treatment of the results obtained is carried out in §6.

2. The integral basis of the Huygens–Fresnel principle

The X-ray coherent wave field inside a crystal orientated near the exact Bragg reflexion is described by the dynamical Takagi equations (Takagi, 1962; 1969)

$$i\frac{\partial E_0}{\partial s_0}+\sigma_{-h}\exp\left[-i(\mathbf{hu})\right]E_h=0$$

$$i\frac{\partial E_h}{\partial s_h}+\sigma_h\exp\left[i(\mathbf{hu})\right]E_0=0 \tag{2.1}$$

(with reference to the form of the equations and the notation used see, for example, Petrashen', 1973; Petrashen' & Chukhovskii, 1975).

In the general case of a crystal with a uniform strain gradient the function (**hu**) has a quadratic coordinate dependence of the type

$$(\mathbf{hu})=2(As_0^2+2Bs_0s_h+Cs_h^2)\,. \tag{2.2}$$

In the expression for the displacement field (2.2) the terms linear in coordinates are omitted for simplicity, account of them reducing only to the renormalization of the Bragg angle θ_B. For some interesting practical cases the coefficients A,B,C are given in Appendix I.

Now, making of use of the substitution

$$E_0=\tilde{E}_0\exp(-2iCs_h^2)\,,\quad E_h=\tilde{E}_h\exp(2iAs_0^2) \tag{2.3}$$

one can easily see that the set of linked equations for the amplitudes $\tilde{E}_0,\tilde{E}_h$ retains the form (2.1) with

$$(\mathbf{h\tilde{u}})=4Bs_0s_h \tag{2.4}$$

instead of the function (2.2).

Then, the set (2.1), taking into account (2.2)–(2.4), is reduced to the following second-order partial differential equations for the amplitude of the transmitted wave and the diffracted wave respectively

$$\frac{\partial^2\tilde{E}_0}{\partial s_0\partial s_h}-i\frac{\partial(\mathbf{h\tilde{u}})}{\partial s_h}\frac{\partial\tilde{E}_0}{\partial s_0}+\sigma^2\tilde{E}_0=0$$

$$\frac{\partial^2\tilde{E}_h}{\partial s_0\partial s_h}+i\frac{\partial(\mathbf{h\tilde{u}})}{\partial s_0}\frac{\partial\tilde{E}_h}{\partial s_h}+\sigma^2\tilde{E}_h=0 \tag{2.5}$$

($\sigma^2=\sigma_h\sigma_{\bar{h}}\equiv 1+2ik$, k being the normalized dynamical absorption coefficient, $k<0$).

According to the Riemann method (Petrashen', 1973) the solutions of equations (2.5), satisfying the known boundary conditions on the contour RQ in the scattering plane, take the form:

$$\tilde{E}_0(P)=\tilde{E}_0(R)+\int_{RQ}\left(\frac{\partial R_0}{\partial s_h}+4iBs_0R_0\right)\tilde{E}_0\mathrm{d}s_h+\int_{RQ}R_0\frac{\partial\tilde{E}_0}{\partial s_0}\mathrm{d}s_0$$

$$\tilde{E}_h(P)=\tilde{E}_h(Q)+\int_{RQ}\left(\frac{\partial R_h}{\partial s_0}-4iBs_hR_h\right)\tilde{E}_h\mathrm{d}s_0+\int_{RQ}R_h\frac{\partial\tilde{E}_h}{\partial s_h}\mathrm{d}s_h \tag{2.6}$$

where the Riemann functions R_0 and R_h are found from the homogeneous conjugate equations:

$$\frac{\partial^2R_0}{\partial s_0\partial s_h}+4iB\frac{\partial}{\partial s_0}(s_0R_0)+\sigma^2R_0=0$$

$$\frac{\partial^2R_h}{\partial s_0\partial s_h}-4iB\frac{\partial}{\partial s_h}(s_hR_h)+\sigma^2R_h=0\,, \tag{2.7}$$

and from the characteristics should obey the conditions:

$$R_0(s_h=s_{hP})=1\,,\quad R_0(s_0=s_{0P})=\exp\left[-4iB(s_h-s_{hP})s_{0P}\right] \tag{2.8a}$$

$$R_h(s_0=s_{0P})=1\,,\quad R_h(s_h=s_{hP})=\exp\left[4iB(s_0-s_{0P})s_{hP}\right]\,. \tag{2.8b}$$

Notice that as (2.8) follows from (2.7) the functions R_0 and R_h become equal to each other, provided that $s_0\rightleftarrows s_h$ and $B\to -B$ occur simultaneously. Thus, to solve the problem one has to find either one of the functions R_0 or R_h. The Riemann functions under consideration were obtained in the previous papers (Petrashen', 1973; Chukhovskii, 1974*a*, *b*), therefore, we write directly the results for the functions R_0 and R_h

$$R_0=\exp\left[4iB(s_{hP}-s_h)s_0\right]\times{}_1F_1\left[i\frac{\sigma^2}{4B},1;4iB(s_{0P}-s_0)(s_{hP}-s_h)\right]$$

$$R_h=\exp\left[-4iB(s_{0P}-s_0)s_h\right]\times{}_1F_1\left[-i\frac{\sigma^2}{4B},1;-4iB(s_{hP}-s_h)(s_{0P}-s_0)\right] \tag{2.9}$$

where ${}_1F_1$ is the confluent hypergeometric function.

(2.6) and (2.9) define a general solution of the problem under consideration, *i.e.* the X-ray dynamical propagation through a crystal with a uniform strain gradient.

Hereafter we shall use the 'special' dimensionless system (Fig. 1):

$$z=(s_0+s_h)\,,\quad x=s_0-s_h \tag{2.10}$$

in which the characteristic rays (the edges of the Borrmann fan) are given by the equation $x=\pm z$ for any asymmetry of the diffraction geometry. This permits us to describe mathematically the asymmetric Laue diffraction in the same way as the symmetric (Petrashen' & Chukhovskii, 1975) and simplifies the physical analysis of the results obtained.

Finally, by use of (2.6), (2.9) with (2.10) the proper expressions for the dynamical wave field can be written in the form:

$$\begin{aligned}\mathscr{E}_0(P) = &\int_{RQ} \mathscr{G}_{00}(\mathbf{r}_P,\mathbf{r})\mathscr{E}_0(\mathbf{r})\,(\mathrm{d}x-\mathrm{d}z)\\ &+\int_{RQ} \mathscr{G}_{0h}(\mathbf{r}_P,\mathbf{r})\mathscr{E}_h(\mathbf{r})\,(\mathrm{d}x+\mathrm{d}z),\\ \mathscr{E}_h(P) = &\int_{RQ} \mathscr{G}_{h0}(\mathbf{r}_P,\mathbf{r})\mathscr{E}_0(\mathbf{r})\,(\mathrm{d}x-\mathrm{d}z)\\ &+\int_{RQ} \mathscr{G}_{hh}(\mathbf{r}_P,\mathbf{r})\mathscr{E}_h(\mathbf{r})\,(\mathrm{d}x+\mathrm{d}z).\end{aligned} \quad (2.11)$$

Here $\mathscr{E}_{0,h}(P)$ are the total amplitudes of the transmitted and diffracted waves, respectively, at the observation point (x_P,z_P); $\mathscr{E}_{0,h}(\mathbf{r})$ are these at any point (x,z) on the contour RQ; the integration is carried out along the segment of the contour restricted by the characteristics $|x_P-x|=z_P-z$, which are drawn from the observation point (x_P,z_P), *i.e.* between the points R and Q. Note that for validity of (2.11) the contour RQ should not be crossed twice by any characteristic. The influence functions $\mathscr{G}_{mn}$ are determined as follows

$$\mathscr{G}_{mn}=\exp\,[i\boldsymbol{\eta}(\mathbf{r}_P-\mathbf{r})]G_{mn}$$

$$\begin{aligned}G_{00}(\mathbf{r}_P,\mathbf{r})=\exp\,(i\Phi_0)\Big[&\delta(x-x_P+z_P-z-0)\\ &-\frac{\sigma^2}{4}(z_P-z+x_P-x)\\ &\times\exp\left(-i\frac{B\varrho^2}{2}\right){}_1F_1\left(1+i\frac{\sigma^2}{4B},2;iB\varrho^2\right)\Big],\end{aligned}$$

$$\begin{aligned}G_{h0}(\mathbf{r}_P,\mathbf{r}) &=\frac{i\sigma_h}{2}\exp\left[i\Phi_0-i(\mathbf{hu})_P-i\frac{B\varrho^2}{2}\right]\\ &\quad\times{}_1F_1\left(1+i\frac{\sigma^2}{4B},\ 1;iB\varrho^2\right)\\ G_{hh}(\mathbf{r}_P,\mathbf{r}) &=\exp\,(-i\Phi_h)[\delta(x-x_P+z-z_P+0)\\ &\quad-\frac{\sigma^2}{4}(z_P-z-x_P+x)\\ &\quad\times\exp\left(i\frac{B\varrho^2}{2}\right){}_1F_1\left(1-i\frac{\sigma^2}{4B},2;-iB\varrho^2\right)\Big],\\ G_{0h}(\mathbf{r}_P,\mathbf{r}) &=\frac{i\sigma_{-h}}{2}\exp\left[i(\mathbf{hu})_P-i\Phi_h+\frac{iB\varrho^2}{2}\right]\\ &\quad\times{}_1F_1\left(1-i\frac{\sigma^2}{4B},1;-iB\varrho^2\right)\end{aligned} \quad (2.12)$$

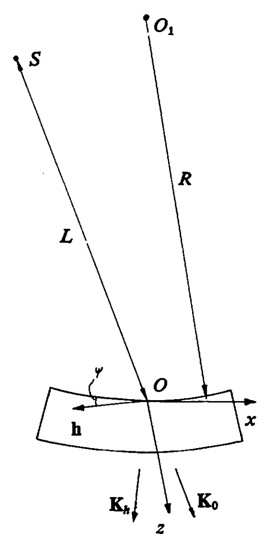

Fig. 1. The diffraction geometry and the coordinate systems used.

where $\varrho^2=(z_P-z)^2-(x_P-x)^2$; the functions $\Phi_{0,h}$ have quadratic coordinate dependence of the form:

$$\begin{aligned}\Phi_0(\mathbf{r}_P,\mathbf{r}) &=\frac{C}{2}\,[(z_P-x_P)^2-(z-x)^2]\\ &\quad+\frac{B}{2}\,[(z_P+x)^2-(x_P+z)^2]\\ \Phi_h(\mathbf{r}_P,\mathbf{r}) &=\frac{A}{2}\,[(z_P+x_P)^2-(z+x)^2]\\ &\quad+\frac{B}{2}\,[(z_P-x)^2-(x_P-z)^2].\end{aligned} \quad (2.13)$$

The components of the vector $\boldsymbol{\eta}$ are connected with the deviation from the true Bragg condition in the coordinate origin $\alpha=-2\sin 2\theta_B\Delta\theta_B$ and the Fourier zero-component of the crystal polarizability χ_0 by the relation

$$\eta_{x,z}=\frac{\chi_0(1\mp b)\pm\alpha b}{2\mathscr{C}\sqrt{[|b|\,\mathrm{Re}\,(\chi_{-h}\chi_h)]}}. \quad (2.14)$$

In (2.12) the symbols 0 provide that the singular points of the δ functions are included in the integration region.

General formulae (2.11) combined with (2.12) represent the Huygens–Fresnel principle in Kirchhoff's integral form for the X-ray dynamical wave fields, since they express the wave amplitudes at any point (x_P,z_P) through their values on the boundary contour RQ. The influence functions $\mathscr{G}_{mn}(\mathbf{r}_P,\mathbf{r})$ have the physical meaning of the wave observed at the point $\mathbf{r}_P$ and initiated by a point source of unit strength, located at the point $\mathbf{r}$. From (2.12) it follows that the influence functions, with accuracy of the phase factor, are invariant with respect to translations $\mathbf{r}\to\mathbf{r}+\mathbf{a}$, $\mathbf{r}_P\to\mathbf{r}_P+\mathbf{a}$. Physically, this is connected with the invariance of the intensity distribution of the point source inside a crystal, in this particular case with respect to translations which are the superposition of two subsequent rotations of equal and opposite directed angles around the centre of curvature either of the crystal or of its net planes and the location point of the source (Chukhovskii & Petrashen', 1975; Petrashen' & Chukhovskii, 1975). At each of these rotations the intensity distribution is invariant because of the cylindrical symmetry. It should be mentioned that the influence functions, as is easy to prove, coincide with the corresponding functions for a perfect crystal when the displacement field (2.2) vanishes. If only (2.3) does so, *i.e.* $B=0$, the influence functions differ from those for a perfect crystal by the phase factor only. The latter case is realized for symmetric Laue diffraction of X-rays from a bent crystal.

In the case of Laue diffraction geometry, the amplitudes $\mathscr{E}_{0h}$ are given on the entrance surface of a crystal, $z=0$,

$$\mathscr{E}_0(x,0)=\mathscr{E}(x), \quad \mathscr{E}_h(x,0)=0 \tag{2.15}$$

and from (2.11) one obtains

$$\mathscr{E}_0(r_P)=\int_{x_P-z_P}^{x_P+z_P} dx\mathscr{G}_{00}(x_P,x,z_P,0)\mathscr{E}(x)$$

$$\mathscr{E}_h(r_P)=\int_{x_P-z_P}^{x_P+z_P} dx\mathscr{G}_{h0}(x_P,x,z_P,0)\mathscr{E}(x). \tag{2.16}$$

Generally, the influence functions are determined by an expression of the form [see (2.12)]

$$\exp\left(-\frac{iB\varrho^2}{2}\right){}_1F_1\left(1+i\frac{\sigma^2}{4B}, \nu; iB\varrho^2\right)$$

($\nu=1,2$ for the diffracted and transmitted waves, respectively).

Making use of the Kummer transformation for the confluent hypergeometric function (Slater, 1960; *Higher Transcendental Functions*, 1953) one finds

$$\exp\left(-\frac{iB\varrho^2}{2}\right){}_1F_1\left(1+i\frac{\sigma^2}{4B}, \nu; iB\varrho^2\right)$$
$$=\exp\left(-i\varepsilon\frac{|B|\varrho^2}{2}\right){}_1F_1\left(\frac{\nu}{2}+\varepsilon\frac{\tilde{\sigma}^2}{4|B|}, \nu; i\varepsilon|B|\varrho^2\right) \tag{2.17}$$

where

$$\tilde{\sigma}^2=1+2i\tilde{k}\equiv 1+2i(k+\varepsilon|B|(\nu-2)), \quad \varepsilon=\operatorname{sign}B \tag{2.18}$$

and either $\varepsilon=1$ or $\varepsilon=-1$ may be chosen.

The right-hand side of (2.17) depends on the strain sign ε through the parameter $\tilde{\sigma}^2$ only. The transition from the dynamical coefficient k to $\tilde{k}$ can be interpreted as the renormalization of the dynamical absorption (Chukhovskii, 1974*a*). This renormalization takes place for the diffracted wave, $\nu=1$, and therefore not for the transmitted wave. Hence, the intensity distribution of the transmitted wave from a point source is not sensitive to the sign of the strain gradient. Concerning the diffracted wave, the situation essentially depends on whether a crystal is transparent or absorbing. In the first case, $|k|z_P\ll 1$, in accordance with (2.17) change of the sign of B is equivalent to the transition to the complex conjugate expressions for the influence functions, which causes no change in either the diffracted intensity distribution or the integral reflecting power. However, in the second case, $|k|z_P\gg 1$, because of the renormalization of the dynamical absorption, depending on the sign of B, the intensity of the diffracted wave varies with the sign of B (the alternation of the strain-gradient sign may be caused by the change of the deformation sign or be due to the inversion of the reflexion vector). As a result, the Friedel law for the integral reflecting power does not hold.

All the features of the X-ray diffraction discussed here were first described within the frame of the eikonal theory by Ando & Kato (1970). The treatment above shows that they persist in the rigorous theory also.

According to the physical concept of the propagation of the Bloch waves in the bulk crystal, each of the influence functions can be represented as a sum of two terms:

$$\exp\left(-\frac{i|B|\varrho^2}{2}\right){}_1F_1\left(\frac{\nu}{2}+i\kappa, \nu; i|B|\varrho^2\right)=\exp(-\pi\kappa)\Gamma(\nu)$$
$$\times\left[\frac{\exp\left(-\frac{i|B|\varrho^2}{2}-i\pi\frac{\nu}{2}\right)}{\Gamma\left(\frac{\nu}{2}+i\kappa\right)}\psi\left(\frac{\nu}{2}-i\kappa, \nu; -i|B|\varrho^2\right)\right.$$
$$\left.+\frac{\exp\left(\frac{i|B|\varrho^2}{2}+i\pi\frac{\nu}{2}\right)}{\Gamma\left(\frac{\nu}{2}-i\kappa\right)}\psi\left(\frac{\nu}{2}+i\kappa, \nu; i|B|\varrho^2\right)\right] \tag{2.19}$$

where $\psi(a,c;x)$ is the second solution of the Kummer equation (*Higher Transcendental Functions*, 1953), $\kappa=\tilde{\sigma}^2/4|B|$.

In the limit of $B\to 0$ (2.19) tends to the suitable relation pointed out by Balibar (1969) for a perfect crystal. On the other hand, the exact relation (2.19) manifests a lack of the interbranch scattering of the waves in the homogeneously bent crystal for any strain gradient.

In the case of a perfect crystal, the first term on the right-hand side of (2.19) corresponds to the weakly absorbing wave mode (α-branch of the dispersion surface), whereas the second term corresponds to the strongly absorbing wave mode (β-branch). So, the first term in (2.19) should be related to the α-branch and the second term to the β-branch. Nevertheless, the behaviour of the wave fields in the case under consideration is more complicated.

By use of any suitable asymptotic representation of $\psi(a,c;x)$ (see, for example, Slater, 1960 and §3) one obtains that the first term in (2.19) becomes much larger than the second term with increase of ϱ for $\tilde{k}<0$ [$\operatorname{Re}(i\kappa)>0$] and *vice versa* for $\tilde{k}>0$. The transmitted part ($\nu=2$) of the α-mode is always weakly absorbing. The diffracted part of the α-mode is weakly (strongly) absorbing for $\tilde{k}<0$ ($\tilde{k}>0$). In the case of

$k=B$, the amplitudes of the diffracted components of both the Bloch waves are equal to each other and only normal absorption takes place. This is a consequence of the renormalization of the dynamical absorption due to a strain gradient.

The practical aspect of the analysis is that for a bent crystal the contrast of the *Pendellösung* fringes depends on the sign of the strain gradient (Hashizume & Kohra, 1972). From this point of view the case of $B<0$ is preferable.

3. The quasi-classical asymptotes of the wave field

The appropriate asymptotic expansions of the influence functions in powers of the eikonal function are obviously effective in physical applications. The investigation of the dynamical wave fields (2.12), (2.16), (2.19) in the central region of the Borrmann fan can be carried out by means of the quasi-classical asymptotic representation of (2.19). The following asymptotic expansion of the confluent hypergeometric function is feasible:

$$\exp\left(-i\frac{|B|\varrho^2}{2}\right){}_1F_1\left(\frac{v}{2}+i\frac{\tilde{\sigma}^2}{4|B|},v;i|B|\varrho^2\right)$$
$$\sim\left[\left(\frac{\varrho}{2}\right)^{1-v}\frac{1-\exp(-\pi/2|B|)}{2\pi\varrho\sqrt{(1+B^2\varrho^2)}}\right]^{1/2}$$
$$\times\{\exp[i\Phi(\varrho)-i\varphi(v,|B|)]+\exp[-i\Phi(\varrho)+i\varphi(v,|B|)]\}$$
$$\times\left\{1+O\left[\frac{1}{\varrho\sqrt{(1+B^2\varrho^2)}}\right]\right\}\ . \quad (3.1)$$

(3.1) may be derived from the more general asymptotic expansion discussed in Appendix II provided that usually the X-ray dynamical absorption coefficient $|k|\ll 1$.

The applicability range of (3.1) is determined by the condition

$$\varrho\sqrt{1+B^2\varrho^2}\gg 1 \quad (3.2)$$

which may be fulfilled for any B, when the crystal thickness $t\gg 1$.

In (3.1) the eikonal function $\Phi(\varrho)$ and the scattering phase $\varphi(v,|B|)$ are

$$\Phi(\varrho)=\varrho/2\sqrt{(1+B^2\varrho^2)}+\frac{1+2i\tilde{k}}{2|B|}\ln[\sqrt{(1+B^2\varrho^2)}+|B|\varrho] \quad (3.3)$$

$$\varphi(v,|B|)=\frac{\pi}{2}(v-1)+\mathrm{Im}\ln\left[\Gamma\left(1+\frac{i}{4|B|}\right)\right]+\frac{1}{4|B|}[\ln(4|B|)+1]\ . \quad (3.4)$$

The succession of terms in the right-hand side of (3.1) is the same as in (2.19), *i.e.* the term corresponding to the α-branch of the dispersion surface is the first one.

The imaginary part of $\Phi(\varrho)$ has the form:

$$\mathrm{Im}\,\Phi(\varrho)=\frac{k}{|B|}\,\mathrm{arsinh}\,(|B|\varrho)+\varepsilon(v-2)\ln[\sqrt{(1+B^2\varrho^2)}+|B|\varrho]\ . \quad (3.5)$$

The real part, $\mathrm{Re}\,\Phi(\varrho)$, in conjunction with the first term in (3.5) is completely equivalent to the Kato eikonal (Kato, 1964). The transition to Kato's formulae is obtained by the relations

$$2Bz=Z\ ,\quad 2Bx=X\ ,\quad \frac{1}{2|B|}=\frac{m_0^2c}{|f|}$$

where Z, X, m_0, c and f are Kato's variables. The second term in (3.5) is included in the amplitude of the diffracted wave in the Kato theory.

The quasi-classical asymptote (3.1) represents by itself the generalized eikonal approach of the theory. The generalization consists in the appearance of the static scattering factor $[1-\exp(-\pi/2|B|)]^{1/2}$ and the scattering phase $\varphi(v,|B|)$ as functions of $|B|$ [see (3.1), (3.4)].

For small $|B|\ll 1$ one has

$$1-\exp\left(-\frac{\pi}{2|B|}\right)\simeq 1\ ,\quad \varphi(v,|B|)\simeq\frac{\pi}{2}(v-1)+\frac{\pi}{4}\ ,$$

and (3.1), (3.3)–(3.5) reduce to the results of the Kato theory. In the case of large $|B|\gg 1$ one has

$$1-\exp\left(-\frac{\pi}{2|B|}\right)\simeq\frac{\pi}{2|B|}\ ,\quad \varphi(v,|B|)\simeq\frac{\pi}{2}(v-1)\ ,$$

i.e. the wave amplitudes of (3.1) are $(\pi/2|B|)^{1/2}$ times smaller than those in the eikonal theory. As is known in the eikonal theory (Kato, 1964), the integrated diffracted intensity from a transparent bent crystal increases in proportion to $|B|$, when $|B|$ tends to infinity. In the present study the static scattering factor appears to remove this unphysical result and leads to the above correct kinematical limit of the intensity (see §5 for details). Concerning the dependence of the scattering phase $\varphi(v,|B|)$ on $|B|$, it is hardly observable because of the large difference in the amplitudes in (3.1) for $|B|\gg 1$.

4. The ray trajectories

In order to complete the comparison of the present study with the eikonal theory let us consider the ray trajectories of the wave-field propagation. They can be obtained as a result of the asymptotic evaluation of the integrals (2.16) by the stationary-phase method. Taking into account (2.12), (2.13) and (3.1), in the case of a plane incident wave, the stationary points can be found from

$$\frac{\partial}{\partial x}[\mathrm{Re}\,\Phi_\pm(x_P,x,z_P,0)]=0 \quad (4.1)$$

where

$$\mathrm{Re}\,\Phi_\pm(\mathbf{r}_P,\mathbf{r})=\boldsymbol{\eta}(\mathbf{r}_P-\mathbf{r})+\Phi_0(\mathbf{r}_P,\mathbf{r})\pm[\Phi(\varrho)-\varphi]\ .$$

Here the $\pm$ signs correspond to two wave modes.

Notice that the imaginary part of the eikonal, Im $\Phi_\pm$, is smaller than the real part for any B when (3.2) holds. For this reason, the effect of absorption on the position of the stationary points is negligible and the method above in the form of (4.1) is applicable for any strain gradient.

Each of the equations (4.1) may be interpreted as a trajectory equation with its origins at two points on the entrance surface and at the running observation point (x_P, z_P). After some transformations one finds

$$[2B(x_P-x)\mp\xi(x)]^2-[2Bz_P-\eta(x)]^2=1 \quad (4.2)$$

where

$$\eta(x)=\mathrm{Re}\,\eta_x+(C-B)x\,,\quad \xi(x)=\sqrt{[1+\eta^2(x)]}\,. \quad (4.3)$$

The trajectories (4.2) are similar to those obtained with the eikonal theory (Penning & Polder, 1961; Kato, 1964). The new circumstance is the dependence of the parameters $\eta(x)$ and $\xi(x)$ on the coordinate x. This is because of the phase factor in (2.12) and describes the linear alternation of the deviation from the Bragg condition along the entrance surface. Thus, the plane incident wave generates two 'fans' of trajectories. One 'fan' is always divergent, whereas the other is convergent. From this point of view the formation of caustics may be possible, *i.e.* the formation of the ray intersection points where the ray optics fails in general. These points can be determined by the compatible solution of two equations, one of which is (4.1) and the other:

$$\frac{\partial^2}{\partial x^2}[\mathrm{Re}\,\Phi_\pm(x_P,x,z_P,0)]=0. \quad (4.4)$$

Excluding the coordinate x from (4.1) and (4.4), one obtains the equation of the caustic, which consists of two sheets corresponding to the two branches of the dispersion surface [or two signs in (4.1)]. Each point of any sheet of the caustic is a focusing point for either one or the other wave mode. The lower sheet represents the real focusing points corresponding to the convergent 'fan' of trajectories; the upper sheet corresponds to the divergent 'fan', its focusing points being imaginary. In the particular case of the symmetrical Laue diffraction, when $B=0$, the caustic is given by

$$Cz_P=\pm[(Cx_P+\mathrm{Re}\,\eta_x)^{2/3}+1]^{3/2}. \quad (4.5)$$

From (4.5) it follows that the critical thickness of a crystal, from which the caustic is formed, is

$$z_{\min}=|C|^{-1}(Cx_P+\mathrm{Re}\,\eta_x=0)\,. \quad (4.6)$$

It may be seen that the point defined by (4.6) lies on the central trajectory $x_P=$constant and this point is a singular point of the caustic, since the derivative $\mathrm{d}z_P/\mathrm{d}x_P$ is indefinite. As an example, the caustic and several central trajectories are plotted in Fig. 2.

The above treatment was carried out for the case of a plane incident wave, but the results may be readily expanded to include the case of a spherical wave. With respect to a plane wave with the same direction of incidence (specified by Re η_x) at the origin of the coordinates, the spherical wave introduces a phase of the form $Px^2/2$ which should be added to Re $\Phi_\pm$ in (4.1) and (4.4). This leads to the substitution $C\to C-P$ in all the above formulae. For a point source, located at a distance L from the origin of the coordinates on the entrance surface, the coefficient P is given by

$$P=\frac{\sin^2 2\theta_B}{2\pi\gamma_h^2}\,\frac{\Lambda^2}{\lambda L}\,. \quad (4.7)$$

With the reasonable values $\Lambda\sim 10$ μm, $\lambda\sim 1$ Å, $L\sim 1$ m, P is estimated to be about unity. Hence, in order to obtain the focusing of the spherical incident wave by a thick crystal, $t\sim 100$, the coefficients C and P should have the same order of magnitude, $C\sim P$, *i.e.* $L\sim R$, where R is the radius of the crystal curvature. On the other hand, when $P\gg 1$, $P\gg|C|$, $|B|$, the wave field picture can be calculated with the approximation of infinite P. In the latter case the singular points of the caustic coincide with each other and with the origin of coordinates, while the caustic itself degenerates into the characteristic rays $x_P-x=\pm z_P$ (the edges of the Borrmann fan). Now (4.2) takes different forms for $x=0$ and $x\neq 0$. If $x\neq 0$, there are the characteristic rays $|x_P-x|=z_P$ only and no diffracted intensity may be associated with them. In the case of $x=0$ the trajectory equation has the previous form (Kato, 1964):

$$[2Bx_P\mp(1+\mathrm{Re}^2\,\eta_x)^{1/2}]^2-(2Bz_P-\mathrm{Re}\,\eta_x)^2=1\,. \quad (4.8)$$

However, now the angular derivation parameter Re η_x is uncertain and all the trajectories exist simultaneously.

5. The integrated intensity of the diffracted wave

Let us consider briefly the integral reflecting power from a thick bent crystal. By use of the asymptotic expansion (3.1), for the non-oscillating part of the integrated intensity we obtain

$$\mathscr{R}_h^i(M_0,M_b,M,D,|B|)=\exp(-M_0)\,\frac{1-\exp(-\pi/2|B|)}{\pi}\times$$

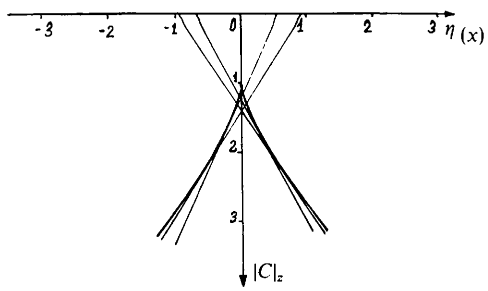

Fig. 2. The caustic and ray trajectories in the case of symmetrical Laue diffraction.

$$\times \int_{-1}^{1} \frac{d\xi}{\sqrt{(1-\xi^2)}} \frac{\cosh (M_b\xi) \cosh [(M/D+2) \ln \{\sqrt{[1+D^2(1-\xi^2)]}+D\sqrt{(1-\xi^2)}\}]}{\sqrt{[1+D^2(1-\xi^2)]}} \quad (5.1)$$

where

$$\xi=\frac{x}{t}, \quad M_0=\frac{\operatorname{Im} \chi_0(1+b)t}{\mathscr{C}\sqrt{[|b| \operatorname{Re}(\chi_{-h}\chi_h)]}}, \quad M_b=\frac{1-b}{1+b}M_0,$$

$$D=Bt, \quad M=2|k|t.$$

Here the parameter $M_0(M)$ describes the normal (anomalous) absorption, M_b the asymmetry of the absorption and D the effective deformation.

The intensity (5.1) is normalized to unity for a perfect transparent crystal, $\mathscr{R}_h^i(0,0,0,0,0)=1$. Generally, integral reflecting power from a perfect absorbing crystal is

$$\mathscr{R}_h^i(M_0,M_b,M,0,0)=\exp(-M_0)I_0[\sqrt{(M_b^2+M^2)}] \quad (5.2)$$

[$I_0(x)$ is the Bessel function of zero order].

The relative error of the intensity (5.1) due to the use of (3.1) instead of the exact formula (2.12) can be shown to decrease with increase of $|B|$ and t as $[t(1+B^2)]^{-1} \ll 1$.

Of special interest is the behaviour of the integrated intensity $\mathscr{R}_h^i$ in the limit $|B| \to \infty$. As $|B|$ increases, formula (5.1) tends to

$$2t \exp(-M_0)\frac{\sinh(M_b)}{M_b} \quad (5.3)$$

in the case of the extremely deformed crystal, *i.e.* $\mathscr{R}_h^i$ is proportional to the crystal thickness. This is nothing but the exact kinematical limit of the integral reflecting power.

For intermediate values of $|B|$ the integral (5.1) cannot be evaluated in an explicit form. Ando & Kato (1970) tabulated the relative intensity

$$E(M,D)=\frac{\mathscr{R}_h^i(M_0,0,M,D)}{\mathscr{R}_h^i(M,0,M,0)}$$

for the symmetrical Laue diffraction and $0 \le M \le 25$, $-5 \le D \le 5$. In a general case, the number of parameters characterizing the integral reflecting power increases from two (M,D) to four $(M,D,M_b,|B|)$, which makes the tabulation difficult.

For practical purposes we suggest an approximate numerical method of the calculation of (5.1) based on the Gauss–Chebyshev integration formula:

$$\int_{-1}^{1} \frac{\eta(\xi)d\xi}{\sqrt{(1-\xi^2)}} \simeq \frac{\pi}{2}\sum_{k=1}^{n}\eta(\xi_k) \quad (5.4)$$

where ξ_k are the roots of the Chebyshev polynomial of nth order:

$$\xi_k=\cos\left(\frac{2k-1}{2n}\pi\right).$$

As an example, Fig. 3 shows the intensity (5.1) *versus* the effective deformation D for several crystals of different thickness $Z=2Bt$. The dashed line corresponds to the results of the eikonal theory without taking into account the static scattering factor $[1-\exp(-\pi/2|B|)]^{1/2}$. The intensity 'saturation' associated with the transition to the kinematical limit is easily noticeable. Owing to its symmetry, the values of the function under the integrand in (5.1) were taken in four points only for $n=7$ provided that the accuracy of the computation is of the order of 0·5%.

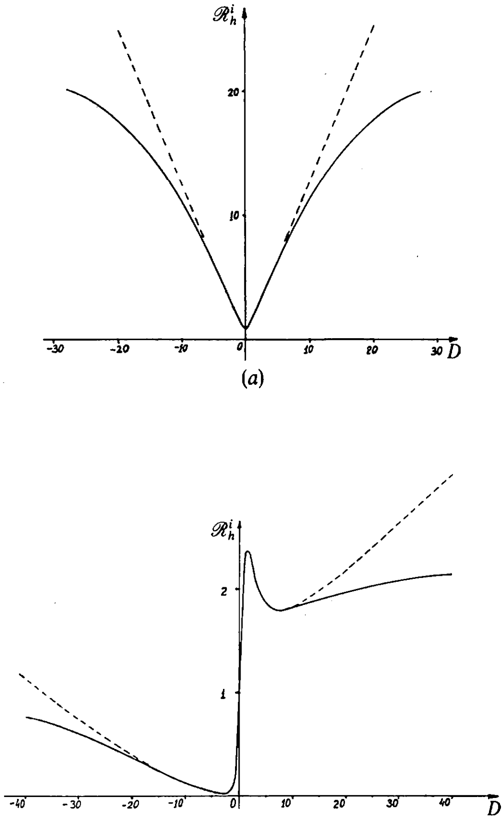

Fig. 3. The integrated diffracted intensity $\mathscr{R}_h^i$ as a function of the effective deformation. (*a*) $M=0$, $Z=15$; (*b*) $M=5$, $Z=30$ (see text).

6. Conclusion

The most significant conclusions to be drawn from the present study are: (1) the extension of the applicability of the ray-optics theory for any strain gradient is feasible. As a consequence, the static scattering factor $[1-\exp(-\pi/2|B|)]^{1/2}$ and the scattering phase $\varphi(|B|)$ in the amplitudes of the dynamical wave fields appear. The static scattering factor yields automatically the kinematical limit of integrated diffracted intensity with increasing strain gradient. (2) The renormalization of the dynamical absorption due to a strain gradient.

Generally, this complicates the division of the dynamical wave fields into strongly and weakly absorbing ones, but images their actual behaviour.

The fact of principal importance is that the basic concept of ray optics – the ray trajectories – is adequate even in the case of large strain gradients. As deformation increases, the trajectories tend to 'kinematical' trajectories. Simultaneously, the applicability range of the generalized eikonal theory is enlarged, so that the trajectories are never meaningless. There is reason for a future attempt to modify the eikonal theory in such a way that the correct asymptotic solution of the Takagi dynamical equations could be obtained for any distortion.

In the general case of an incident wave of finite spatial and angular width some difficulties are encountered because of the intersection of the ray trajectories. In particular, close to the caustic, the stationary-phase method (hence, the ray optics itself) leads to an infinite value of the intensity and is inapplicable. This is of special interest for several practical purposes, such as multiple-crystal topography. The problem pointed out here is treated by Petrashen' & Chukhovskii (1976).

APPENDIX I

From (2.2) it follows that the coefficients A, B, C are determined by the relations:

$$A=\hat{D}_+^2(\mathbf{hu}), \quad B=\hat{D}_+\hat{D}_-(\mathbf{hu}), \quad C=\hat{D}_-^2(\mathbf{hu}),$$

$$\hat{D}_\pm=\tfrac{1}{2}\left(\frac{\partial}{\partial z}\pm\frac{\partial}{\partial x}\right). \quad (AI.1)$$

The differential operators in (AI.1) can be written in terms of Cartesian coordinates as follows:

$$\hat{D}_+^2=\left(\frac{\Lambda}{2\pi}\right)^2\left(\frac{\partial^2}{\partial z^2}+\tan^2\varphi_0\frac{\partial^2}{\partial x^2}+2\tan\varphi_0\frac{\partial^2}{\partial z\partial x}\right),$$

$$\hat{D}_+\hat{D}_-=\left(\frac{\Lambda}{2\pi}\right)^2\left(\frac{\partial^2}{\partial z^2}+\tan\varphi_0\tan\varphi_h\frac{\partial^2}{\partial x^2}+\frac{\sin(2\psi)}{\gamma_0\gamma_h}\frac{\partial^2}{\partial z\partial x}\right),$$

$$\hat{D}_-^2=\left(\frac{\Lambda}{2\pi}\right)^2\left(\frac{\partial^2}{\partial z^2}+\tan^2\varphi_h\frac{\partial^2}{\partial x^2}-2\tan\varphi_h\frac{\partial^2}{\partial x\partial z}\right). \quad (AI.2)$$

In the case of a homogeneously bent crystal, elaborated by Penning & Polder (1961), one obtains the following formulae for A, B and C.

(a) The strain gradient is directed along the z axis. The crystal is bent by a mechanical device.

$$A=-\frac{\Lambda^2}{dR}\,\frac{2\gamma_0\sin\theta_B+\sin\psi[1+\gamma_0^2(1+\nu)]}{2\pi\gamma_0^2},$$

$$B=-\frac{\Lambda^2}{dR}\,\frac{\sin\psi[1+\gamma_0\gamma_h(1+\nu)]}{2\pi\gamma_0\gamma_h},$$

$$C=+\frac{\Lambda^2}{dR}\,\frac{2\gamma_h\sin\theta_B-\sin\psi[1+\gamma_h^2(1+\nu)]}{2\pi\gamma_h^2}, \quad (AI.3)$$

where d is the lattice spacing, ν is the Poisson ratio.

(b) The same direction of strain gradient. The crystal is bent because of a temperature gradient. The coefficients A, B, C can be formally obtained from (AI.3) by putting $\nu=-1$;

(c) The strain gradient is directed along the x axis. Also, the crystal is bent because of a temperature gradient.

$$A=\frac{\Lambda^2}{dR}\,\frac{2\gamma_0\cos\theta_B-\cos\psi}{2\pi\gamma_0^2}$$

$$B=\frac{\Lambda^2}{dR}\,\frac{\cos\psi}{2\pi\gamma_0\gamma_h},$$

$$C=-\frac{\Lambda^2}{dR}\,\frac{2\gamma_h\cos\theta_B+\cos\psi(1-4\gamma_h^2)}{2\pi\gamma_h^2}. \quad (AI.4)$$

APPENDIX II

Derivation of the asymptotic expansion in §3 by the Olver method

Let us consider the function

$$W(v)=\left(\frac{\mathrm{d}t}{\mathrm{d}v}\right)^{-1/2}\exp(-2i\kappa t)(4i\kappa t)^{n/2}\times{}_1F_1\left(\frac{n}{2}+i\kappa,n;4i\kappa t\right) \quad (AII.1)$$

with

$$v(t)=i\frac{\kappa}{|\kappa|}\{\sqrt{[t(1+t)]}+\ln[\sqrt{(1+t)}+\sqrt{t}]\},\, t=B^2\varrho^2/\tilde{\sigma}^2.$$

$W(v)$ satisfies the equation

$$\frac{\mathrm{d}^2W}{\mathrm{d}v^2}=[4|\kappa|^2+f(v)]W \quad (AII.2)$$

where

$$f(v)=f(t)=-\frac{|\kappa|^2}{\kappa^2}\left[\frac{n(n-2)}{4t(1+t)}+\frac{8t+3}{16t(1+t)^3}\right].$$

According to the first Olver theorem (Slater, 1960), (AII.2) has two linearly independent asymptotic solutions:

$$W_1=\exp(2|\kappa|v)\left\{\sum_{s=0}^{M-1}\frac{A_s}{(2|\kappa|)^s}+O[(2|\kappa|)^{-M}]\right\},$$

$$W_2=\exp(-2|\kappa|v)\left\{\sum_{s=0}^{M-1}\frac{(-1)^sA_s}{(2|\kappa|)^s}+O[(2|\kappa|)^{-M}]\right\}. \quad (AII.3)$$

Here the functions A_s are determined by the recurrence relations:

$$A_0 = 1,$$

$$A_1 = i\frac{|\kappa|}{\kappa}\left\{\frac{4n(n-2)+3}{16\sqrt{t}[\sqrt{(1+t)}+\sqrt{t}]} - \frac{5t}{48(1+t)\sqrt{[t(1+t)]}} - \frac{1}{48\sqrt{(1+t)}[\sqrt{(1+t)}+\sqrt{t}]}\right\},$$

$$A_{s+1}(t) = -\tfrac{1}{2}\frac{dt}{dv}\frac{dA_s(t)}{dt} - \tfrac{1}{2}\int_t^\infty f(t)A_s(t)\frac{dv}{dt}dt. \qquad (AII.4)$$

The limits of the integration in (AII.4) are chosen in such a way that A_s tends to zero as $t \to \infty$. The functions W, W_1 and W_2 are solutions of the same equation, so there should be a linear relation of the form: $W = C_1W_1 + C_2W_2$.

The coefficients C_1, C_2 can be found from the asymptotic behaviour of W, W_1, W_2 for $t \to \infty$. As a result, one obtains

$$ {}_1F_1\left(\frac{n}{2}+i\kappa, n; 4i\kappa t\right) \sim \Gamma(n)\exp(2i\kappa t)(4\kappa t)^{-n/2}\left(1+\frac{1}{t}\right)^{1/4} \times \left[\frac{(i\kappa)^{i\kappa}\exp\left(-i\kappa - i\pi\frac{n}{4}\right)}{\Gamma\left(\frac{n}{2}+i\kappa\right)}W_1 + \frac{(-i\kappa)^{-i\kappa}\exp\left(i\kappa + i\pi\frac{n}{4}\right)}{\Gamma\left(\frac{n}{2}-i\kappa\right)}W_2\right]. \qquad (AII.5)$$

Notice that the same result could be obtained from (2.19) and the Taylor asymptotic representation of $\psi(a,c;x)$ (*Higher Transcendental Functions*, 1953), but without the higher-order terms.

The expressions for $A_s(t)$ when $s > 1$ are complicated. Nevertheless, it is easy to show that

$$A_s(t) = O(\{\sqrt{[t(1+t)]}\}^{-1})$$

and the expansions (AII.3) are in powers of

$$\{4|\kappa|\sqrt{t}[(1+t)]\}^{-1} \simeq [\varrho\sqrt{(1+B^2\varrho^2)}]^{-1}.$$

So far, no assumption about the value of k has been made. Taking into account $|k| \ll 1$ one has

$$(\tilde{\sigma}^2 + B^2\varrho^2)^{1/2} \simeq (1+B^2\varrho^2)^{1/2} + \frac{i\tilde{k}}{(1+B^2\varrho^2)^{1/2}} \qquad (AII.6)$$

if, of course, $\varrho(1+B^2\varrho^2)^{1/2} \gg 1$.

Now, making use of (AII.6) as well as the known relations for the Γ-function,

$$\Gamma(1+z) = z\Gamma(z), \quad \Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin \pi z},$$

one readily obtains the asymptotic representation (3.1).

References

ANDO, Y. & KATO, N. (1970). *J. Appl. Cryst.* **3**, 74–89.
ANDO, Y., PATEL, J. R. & KATO, N. (1973). *J. Appl. Phys.* **44**, 4405–4412.
BALIBAR, F. (1969). *Acta Cryst.* A**25**, 650–658.
BONSE, U. (1964). *Z. Phys.* **177**, 385–423.
CHUKHOVSKII, F. N. (1974*a*). *Kristallografia*, **19**, 482–488.
CHUKHOVSKII, F. N. (1974*b*). Collected Abstracts, 2nd Eur. Crystallogr. Meeting, Keszthely, Hungary, 26–29 August, p. 61
CHUKHOVSKII, F. N. & PETRASHEN', P. V. (1975). *Dokl. Akad. Nauk. SSSR*, **222**, 599–602.
FISHMAN, YU. M. & LUTZAU, V. G. (1973). *Phys. Stat. Sol.* (*a*), **18**, 443–449.
FUKUSHIMA, E., HAYAKAWA, K. & NIMURA, H. (1963). *J. Phys. Soc. Japan*, **18**, Suppl. II, 348–351.
HART, M. (1966). *Z. Phys.* **189**, 269–291.
HASHIZUME, H., & KOHRA, K. (1972). *Phys. Stat. Sol.* (*a*), **13**, K9–K11.
Higher Transcendental Functions (1953). Vol. I. New York: McGraw-Hill.
KATAGAWA, T. & KATO, N. (1974). *Acta Cryst.* A**30**, 830–836.
KATO, N. (1964). *J. Phys. Soc. Japan*, **19**, 971–985.
KATO, N. & ANDO, Y. (1966). *J. Phys. Soc. Japan*, **21**, 964–968.
KATO, N. & PATEL, J. R. (1973). *J. Appl. Phys.* **44**, 965–970.
LITZMAN, O. & JANACEK, Z. (1974). *Phys. Stat. Sol.* (*a*), **25**, 663–665.
MEIERAN, E. S. & BLECH, I. A. (1965). *J. Appl. Phys.* **36**, 3162–3167.
PATEL, J. R. & KATO, N. (1973). *J. Appl. Phys.* **44**, 971–977.
PENNING, P. (1966). Thesis, Eindhoven.
PENNING, P. & POLDER, D. (1961). *Philips Res. Rep.* **16**, 419–440.
PETRASHEN', P. V. (1973). *Fis. Tverd. Tela*, **15**, 3131–3132.
PETRASHEN', P. V. & CHUKHOVSKII, F. N. (1975). *JETP*, **69**, 477–487.
PETRASHEN', P. V. & CHUKHOVSKII, F. N. (1976). *Kristallografia*, **21**, 283–292.
SCHWUTTKE, G. H. & HOWARD, J. K. (1968). *J. Appl. Phys.* **39**, 1581–1591.
SLATER, L. J. (1960). *Confluent Hypergeometric Functions*. Cambridge Univ. Press.
TAKAGI, S. (1962). *Acta Cryst.* **15**, 1311–1312.
TAKAGI, S. (1969). *J. Phys. Soc. Japan*, **26**, 1239–1253.