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Theoretical Study of X-ray Diffraction in Homogeneously Bent Crystals – the Bragg Case

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Abstract

X-ray dynamical diffraction in homogeneously bent crystals is studied theoretically in the Bragg case. The study starts from the Green function given previously by Chukhovskii, Gabrielyan & Petrashen' [*Acta Cryst.* (1978), **A34**, 610-620] as an inverse Laplace transform and which can be viewed as an integral over all incident plane waves. The integrand is developed by means of an asymptotic representation of parabolic cylinder functions. Integration by the stationary-phase method leads to the evidence of curved X-ray paths and, in the case of large values of strain gradient, to the creation of a new wave field. The intensity of the new wave field is shown to be a fraction $\exp(-2\pi|\nu|)$ of the incident beam where $|\nu|$ is the inverse of the strain gradient expressed in reduced units.

1. Introduction

The propagation of X-rays in distorted crystals has been widely studied since 1961 when Penning & Polder first published their geometrical-optics theory of propagation of wave fields. Their theory was based on an analogy with the propagation of light in inhomogeneous media. Then Kato (1963, 1964) developed a more rigorous theory using the Eikonal formulation and leading to the same results. Penning & Polder and Kato considered crystals distorted by a uniform strain gradient in the transmission or Laue case. Let us mention here that all theoretical works in this field have considered uniform strain gradients, that is distortions such that the second derivative of the projection of the displacement vector $\mathbf{u}(\mathbf{r})$ on the diffraction vector $\mathbf{h}$ with respect to the incident s_0 and reflected s_h directions is constant [$\partial^2(\mathbf{h}.\mathbf{u})/\partial s_0\,\partial s_h =$ constant]. Then Bonse (1964) generalized Penning & Polder's theory in order to apply it to the reflection or Bragg case and obtained hyperbolic trajectories for incident waves outside the domain of total reflection.

The three theories mentioned above are geometrical-optics theories and can only be valid for small strain gradients. Another approach to the study of X-ray propagation in distorted crystals was developed later, on the basis of the Green-Riemann-function method which takes into account diffraction phenomena and thus can be applied to large strain gradients. The Laue case was first treated by Petrashen' (1973), Chukhovskii (1974), Katagawa & Kato (1974), Petrashen' & Chukhovskii (1975, 1976), Chukhovskii & Petrashen' (1977). The Green function they obtained is a hypergeometric function which by itself does not provide any physical insight. Using asymptotic expansions, the authors were able to retrieve the results of geometrical theories in the case of small strain gradients and kinematical theory for extremely large strain gradients. Then Balibar, Chukhovskii & Malgrange (1983) expressed the hypergeometric function as an inverse Laplace transform from which they were able to evidence the creation of a new wave field at the apex of the hyperbolic ray path for strong strain gradients. Its intensity was shown to be a fraction $\exp(-2\pi/|\alpha_0|)$ (where α_0 is proportional to the strain gradient) of the intensity of the wave field before the apex of the trajectory. These results gave a theoretical basis to the computed results obtained previously by Balibar, Epelboin & Malgrange (1975).

The Bragg case was studied somewhat later. Petrashen' (1973) obtained the Riemann function as

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an infinite series of confluent hypergeometric functions where unfortunately all the terms are of the same order. Then, Chukhovskii, Gabrielyan & Petrashen' (1978) obtained the Green function in the form of an inverse Laplace transform. They gave some characteristics of the wave fields in the case of small strain gradients but did not say anything about large values of the strain gradient. Computer integration of Takagi–Taupin equations was then performed by Gronkowski & Malgrange (1984). They obtained not only the hyperbolic trajectories of geometrical optics but also the creation of a new wave field in the case of large strain gradients and the value of its intensity, in good agreement with the value given by Balibar, Chukhovskii & Malgrange (1983) in the Laue case.

The aim of this paper is to give a theoretical basis to these computer results and more generally to describe X-ray wave field propagation in homogeneously bent crystals in the Bragg case.

2. The Green function as an integral over incident plane waves

The Green function describing the diffracted wave in a crystal distorted by a uniform strain gradient has been given in the Bragg case by Chukhovskii, Gabrielyan & Petrashen' (1978) and expressed as an inverse Laplace transform which can be written

$$G_h(s_0, s_h) = \exp[-\Phi(s_0, s_h, B)](i/4B)^{1/2}(1/2i\pi) \times \int_{p_0-i\infty}^{p_0+i\infty} \exp[p(s_0+s_h)/2] \times [D_{-1-\nu}(Y)/D_{-\nu}(Y_0)]\,\mathrm{d}p \quad (1)$$

where s_0 and s_h are reduced coordinates in the direction of the incident and reflected wave vectors $\mathbf{K}_0$ and $\mathbf{K}_h$ respectively:

$$s_0 = \pi\gamma_0[s_0]/\Lambda_r \qquad s_h = \pi|\gamma_h|[s_h]/\Lambda_r$$

where $[s_0]$ and $[s_h]$ are normal coordinates along $\mathbf{K}_0$ and $\mathbf{K}_h$. Λ_r is the real part of the usual extinction distance $\Lambda = \lambda(\gamma_0|\gamma_h|)^{1/2}/[C(\chi_h\chi_{\bar{h}})^{1/2}]$, $\gamma_0 = \cos(\mathbf{s}_0, \mathbf{n})$, $\gamma_h = \cos(\mathbf{s}_h, \mathbf{n})$ (Fig. 1), $\chi_h, \chi_{\bar{h}}$ are the h and $\bar{h}$ Fourier coefficients of the electronic susceptibility, and $4B = \partial^2/\partial s_0 \partial s_h$ $(2\pi\, \mathbf{h}.\mathbf{u})$ and is related to

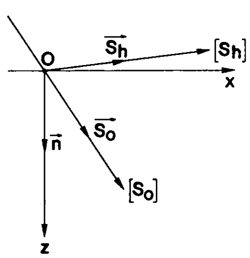

Fig. 1. Coordinate system.

the usual β parameter through the relation

$$4B = 2\Lambda_0\beta/\pi = \beta/\beta_c, \quad (2)$$

where $\beta_c = \pi/(2\Lambda_0)$ is the critical value introduced by Authier & Balibar (1970), Λ_0 being the extinction distance in the symetric Laue case. Λ_0 is an intrinsic length for a given crystal and a given reflection since it is the inverse of the distance between the two apices of the dispersion hyperbola.

Of the remaining symbols in (1),

$$\nu = i(1+2ik)/4B \quad (3)$$

where $2k$ is the ratio (assumed to be small) between the imaginary and the real part of $\chi_h\chi_{\bar{h}}$,

$$Y_0 = p\nu^{1/2}, \quad (4)$$

$$Y = [p - 4iB(s_0 - s_h)]\nu^{1/2}, \quad (4')$$

D_ν is the parabolic cylinder function of order ν, and

$$\Phi(s_0, s_h, B) = B(s_0^2 - s_h^2) + 2Bs_0s_h.$$

Let us note that the notations used here are those used by Balibar, Chukhovskii & Malgrange (1983) since, in the symmetrical Laue case, Λ_r and Λ_0 are equal and in their paper $\Lambda = \Lambda_r = \Lambda_0$. In order to simplify, let us assume *the absorption to be zero*, so that Λ is real and ν is purely imaginary. Let us write

$$p = -2i\eta_0 \quad (5)$$

where η_0 is the usual η parameter related to the departure from Bragg angle $\Delta\theta_0$ by the relation

$$\eta_0 = \frac{\Delta\theta_0 \sin 2\theta_B - \frac{1}{2}[(\gamma_h/\gamma_0) - 1]\chi_0}{C(|\gamma_h|/\gamma_0)^{1/2}(\chi_h\chi_{\bar{h}})^{1/2}} \quad (6)$$

where θ_B is the Bragg angle.

If z is the coordinate normal to the entrance surface (Fig. 1) and directed towards the inside of the crystal,

$$z = \mathbf{n}.\mathbf{r} = (s_0 - s_h)\Lambda_r/\pi. \quad (7)$$

Then, from (5) and (7),

$$p - 4iB(s_0 - s_h) = -2i(\eta_0 + 2B\pi z/\Lambda_r) = -2i[\eta_0 + (\beta z \cos\theta)/(\gamma_0|\gamma_h|)^{1/2}]. \quad (8)$$

Integration of the basic equation of geometrical-optics theory given by Kato (1963, 1964) and Penning & Polder (1961) gives for the local value of the η parameter

$$\eta = \eta_0 + (\beta z \cos\theta)/(\gamma_0|\gamma_h|)^{1/2}.$$

Then

$$p - 4iB(s_0 - s_h) = -2i\eta. \quad (9)$$

The Green function (1) is an integral over the imaginary part of p and consequently over η_0 and $\Delta\theta_0$. Equation (1) then gives the Green function as an integral of the function $P_h(\eta_0, s_0, s_h)$ over all the values of η_0:

$$G_h(s_0, s_h) = \exp[-i\Phi(s_0, s_h, B)] \int_{-\infty}^{+\infty} P_h(\eta_0, s_0, s_h)\, d\eta_0 \tag{10}$$

with

$$P_h(\eta_0, s_0, s_h) = (i/4B)^{1/2}(1/\pi)\exp[-i(s_0+s_h)\eta_0] \times[D_{-1-\nu}(Y)/D_{-\nu}(Y_0)],$$

Y_0 and Y being functions of η_0 through (4), (4′) and (5). $P_h(\eta_0, s_0, s_h)$ thus gives the behaviour, in the crystal, of an incident plane wave whose η parameter is equal to η_0.

3. Asymptotic form of the waves

In order to interpret each wave $P_h(\eta_0, s_0, s_h)$ we use here an asymptotic representation of the $D_{-n-\nu}(Y)$ functions obtained by the use of Olver's theorem (Slater, 1960) and valid for $|Y^2+4\nu|^{1/2} \gg 1$. Here n is an integer and ν is complex.

$$\begin{aligned} D_{-n-\nu}(Y) = &\{\exp[-\log(Y^2+4\nu)/4]\} \\ &\times[C(n+\nu)\exp[-\theta_{n+\nu}(Y)] \\ &+\varepsilon[n+\nu, \arg(Y^2+4\nu)^{1/2}]C^{-1}(n+\nu) \\ &\times(2\pi)^{1/2}\Gamma^{-1}(n+\nu)\exp\theta_{n+\nu}(Y)] \end{aligned} \tag{11}$$

where

$$\theta_{n+\nu}(Y) = (1/4)Y(Y^2+4\nu)^{1/2} + (n+\nu-1/2) \times\log\{[Y+(Y^2+4\nu)^{1/2}]/2\nu^{1/2}\}$$

$$C(n+\nu) = \exp[\nu/2 - (1/2)(n+\nu-1/2)\log\nu]$$

and the value of the ε function depends on the value of the argument χ of $(Y^2+4\nu)^{1/2}$,

$$(Y^2+4\nu)^{1/2} = |Y^2+4\nu|^{1/2}\exp i\chi$$

and

$$\varepsilon(n+\nu, \chi) = \begin{cases} 0 & \text{if } |\chi| \le \pi/4 \\ -\exp[-i\pi(n+\nu)] & \text{if } \pi/4 < \chi < 5\pi/4 \\ -\exp[i\pi(n+\nu)] & \text{if } -5\pi/4 < \chi < -\pi/4. \end{cases}$$

Consequently, $P_h(\eta_0, s_0, s_h)$ strongly depends on the phases of Y and Y_0 or equivalently on the phases of η_0 and η and, more simply, on their sign since we restrict ourselves to non-absorbing cases.

In order to simplify the interpretation, let us assume a *symmetric case* and choose B positive (the case B negative would be treated in the same manner and leads to identical results).

If φ_0 and φ are the respective phases of η_0 and η, χ_0 and χ those of Y_0 and Y, then

$$\chi_0 = \varphi_0 - \pi/4 \quad \text{and} \quad \chi = \varphi - \pi/4.$$

Then if η_0 (η) is positive, χ_0 (χ) is equal to $-\pi/4$ and if η_0 (η) is negative, χ_0 (χ) is equal to $3\pi/4$.

Let us write $D_{-1-\nu}(Y) = C + D$ where C and D are respectively the first and second terms in (11). The second term D which is proportional to $\varepsilon(1+\nu, \chi)$ is then equal to zero if η is positive and is different from zero if η is negative.

Similarly let us write:

$$D_{-\nu}(Y_0) = F + G$$

where G, proportional to $\varepsilon(\nu, \chi_0)$, equals zero if η_0 is positive and is different from zero if η_0 is negative.

Now, the condition for (11) to be valid, which is $|Y^2+4\nu|^{1/2} \gg 1$, can be satisfied in two different cases:

(a) if $|\nu| \ll 1$ (*i.e.* for large values of the strain gradient), the condition implies $|Y|$ and then $|\eta| \gg 1$;

(b) if $|\nu| \gg 1$ (*i.e.* for small values of the strain gradient) the condition is fulfilled without any restriction on $|Y|$ and then on $|\eta|$.

In case (a) (large strain gradients), G which is inversely proportional to $\Gamma(\nu)$ tends to zero and can be neglected. Then

$$P_h(\eta_0, s_0, s_h) = (\nu^{1/2}/\pi)\exp[-i\eta_0(s_0+s_h)] \times[C/F + D/F]. \tag{12}$$

In case (b) (small strain gradients) it can be shown that $G/F < 1$ and then $P_h(\eta_0, s_0, s_h)$ can be expanded as a series:

$$\begin{aligned} P_h(\eta_0, s_0, s_h) = &(\nu^{1/2}/\pi)\exp[-i\eta_0(s_0+s_h)] \\ &\times[C/F + D/F - CG/F^2 \\ &- DG/F^2 + \dots]. \end{aligned} \tag{13}$$

Then, in both cases, it is necessary to study the terms C/F and D/F. Their value is given in the Appendix.

4. X-ray beams

The Green function $G_h(s_0, s_h)$ gives the amplitude of the electric field D_h at a point (s_0, s_h) due to a unit point source placed at the origin on the entrance surface. $G_h(s_0, s_h)$ [equation (10)] is obtained through the integration of $P_h(\eta_0, s_0, s_h)$ which is itself a sum of terms [see (12) and (13) for large and small strain gradients respectively]. Then $G_h(s_0, s_h)$ is a sum of integrals. The first and second integrals can be written (neglecting for the moment the factor $\nu^{1/2}/\pi$)

$$I_1 = \int \exp[-i\eta_0(s_0+s_h)][C/F]\, d\eta_0 = \int R_1 \exp(i\varphi_1)\, d\eta_0 \tag{14}$$

$$I_2 = \int \exp[-i\eta_0(s_0+s_h)][D/F]\, d\eta_0 = \int R_2 \exp(i\varphi_2)\, d\eta_0 \tag{15}$$

where R_1 and R_2 are real, all the phases being included in φ_1 and φ_2. I_1 and I_2 can be integrated using the stationary-phase method. The condition for the phase to be stationary gives the trajectory corresponding to an incident beam whose departure from the Bragg angle corresponds to η_0. Let us remind ourselves that I_2 is zero if η is positive; φ_1 and φ_2 can be written

$$\varphi_1 = S(\eta) - S(\eta_0) - \eta_0(s_0 + s_h) \qquad (16)$$

$$\varphi_2 = -S(\eta) - S(\eta_0) - \eta_0(s_0 + s_h) \qquad (17)$$

where

$$S(\eta) = \{|\eta|(\eta^2-1)^{1/2} - \log[|\eta| + (\eta^2-1)^{1/2}]\}/4B$$

(see Appendix).

Then $\partial S/\partial\eta = [\operatorname{sign}(\eta)(\eta^2-1)^{1/2}]/2B$ where $\operatorname{sign}(\eta)$ equals 1 if $\eta > 0$ and -1 if $\eta < 0$.

The conditions for φ_1 and φ_2 to be stationary give the trajectories. These conditions depend on the sign of η_0 and η.

Let us remark that, in the symmetric Bragg case, (8) and (9) give

$$\eta = \eta_0 + 2B\pi z/\Lambda = \eta_0 + \beta z/\tan\theta \qquad (18)$$

and let us remember that B has been chosen positive.

(a) If η_0 is positive, then η is positive and the integral I_2 is zero. The phase φ_1 is stationary if

$$2B(s_0 + s_h) = (\eta^2-1)^{1/2} - (\eta_0^2-1)^{1/2}$$

or

$$\beta x = (\eta^2-1)^{1/2} - (\eta_0^2-1)^{1/2} \qquad (19)$$

using (2) and $(s_0 + s_h) = \pi x/\Lambda_0$ in the symmetric Bragg case, where x is the coordinate along the entrance surface (Fig. 1). Equations (18) and (19) can be viewed as parametric equations of a hyperbola (Fig. 2) whose equation is

$$[(\beta z/\tan\theta) + \eta_0]^2 - [\beta x + (\eta_0^2-1)^{1/2}]^2 = 1$$

or

$$[\beta(z+z_0)/\tan\theta]^2 - [\beta(x+x_0)]^2 = 1 \qquad (20)$$

where $z_0 = \eta_0\tan\theta/\beta$ and $x_0 = (\eta_0^2-1)^{1/2}/\beta$.

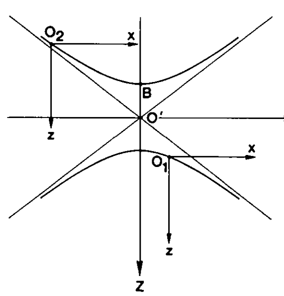

Fig. 2. Hyperbola giving the ray paths for a given value of the strain gradient β. The origin of the path on the hyperbola depends on the value of the parameter η_0 related to the departure from the Bragg angle of the incident beam.

Let us recall that the origin of coordinates is the entrance point of the incident beam. Let us choose the point $O'(z = -z_0, x = -x_0)$ as the origin for a new coordinate system: $Z = z + z_0$ and $X = x + x_0$ (Fig. 2). Then (20) for the hyperbola becomes

$$(\beta Z/\tan\theta)^2 - (\beta X)^2 = 1. \qquad (21)$$

The coordinates of the origin O_1 for the path are now $Z = z_0$ and $X = x_0$ (since at the origin $z = 0$ and $x = 0$). Both are here positive (Figs. 2 and 3a). The path does not contain the apex of the hyperbola and as z increases tends more and more towards the asymptote.

(b) If η_0 is negative, then η can be either negative or positive depending on the value of z:

(i) If $z < -(\eta_0\tan\theta)/\beta$, η is negative; the condition for φ_1 to be stationary is then

$$x = [(\eta_0^2-1)^{1/2} - (\eta^2-1)^{1/2}]/\beta. \qquad (22)$$

The trajectory is again a part of hyperbola (20) [or equivalently (21)] where $z_0 = \eta_0\tan\theta/\beta$ and $x_0 = -(\eta_0^2-1)^{1/2}/\beta$. They are both negative. The trajectory goes from the origin O_2 towards the apex B of the

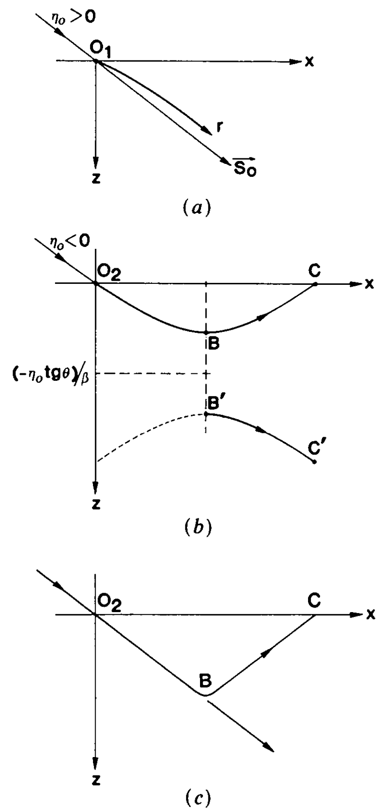

Fig. 3. Ray paths for different values of η_0, β being chosen positive. (a) Case $\eta_0 > 0$ (origin O_1 in Fig. 2). (b) Case $\eta_0 < 0$ (origin O_2 in Fig. 2). The intensity of the new wave field $B'C'$ is different from zero for large values of the strain gradient only. (c) Realistic path when the strain gradient is large enough to give rise to a new wave field.

hyperbola (Figs. 2 and 3*b*). Since η is negative, the integral I_2 is not zero and the stationary condition for φ_2 is

$$x=[(\eta_0^2-1)^{1/2}+(\eta^2-1)^{1/2}]/\beta, \quad (23)$$

which corresponds to the part BC of the hyperbola. These results could also be obtained using geometrical optics [see, for example, Gronkowski & Malgrange (1984)].

(ii) If $z>-(\eta_0\tan\theta)/\beta$ then η is positive and the second term I_2 is zero. φ_1 is stationary if

$$x=[(\eta_0^2-1)^{1/2}+(\eta^2-1)^{1/2}]/\beta, \quad (24)$$

which gives the trajectory $B'C'$ on the other branch of the hyperbola (Fig. 3*b*).

This is a new result which was not given by geometrical-optics theory: there can exist a new wave field; since η has to change sign, the wave field jumps from one branch to the other. The amplitude of the wave contains a factor $\alpha(\chi,\chi_0)$ which depends on the phases of η and η_0 (see the Appendix). If η_0 and η are of the same sign as in case (i), α is only a phase factor whereas when η_0 is negative and η positive, $\alpha=\exp(-\pi|\nu|)$, which means that if $|\nu|$ is large (small strain gradient) the amplitude tends to zero. By contrast if $|\nu|$ is small (strong strain gradient), then the amplitude of the new wave field can no longer be neglected. This demonstrates the creation of a new wave field when the strain gradient is large. Its intensity is a fraction $\exp(-2\pi|\nu|)$ of the normal wave field. Since we have considered the non-absorbing case, $|\nu|=1/4B=\beta_c/\beta$ from (2) and (3). The curvature of the hyperbola close to its apex is very strong for high values of $|\beta|$ and outside the neighbourhood of the apex of the hyperbola the paths are practically straight lines parallel to either $\mathbf{s}_0$ or $\mathbf{s}_h$ (Fig. 3*c*).

The stationary-phase method has provided us with the energy path going through a given point (s_0, s_h) when a spherical wave is incident at the origin O. It has given the value of the parameter η_0 of the associated incident plane wave. This result can also be considered as giving the trajectory of a quasi-plane-wave beam with incidence $\Delta\theta_0$ and parameter η_0. At a depth z, the local value of η is given by (18) and the trajectory is made of one branch of the hyperbola (20) [where $z_0=\eta_0\tan\theta/\beta$ and $x_0=\operatorname{sign}(\eta_0)\times(\eta_0^2-1)^{1/2}$] for the normal wave field and of the other branch for the new wave field. The squared modulus of the amplitudes $R_1(\eta_0,\eta)$ or $R_2(\eta_0,\eta)$ gives the intensity of the reflected beam issued from the wave field. $R_1(\eta_0,\eta)$ and $R_2(\eta_0,\eta)$ both contain a factor $\nu^{-1/2}$ which has not to be taken into account since it disappears when multiplied by the factor $\nu^{1/2}$ which appears in $P_h(\eta_0,s_0,s_h)$, (12) and (13). It is worthwhile noticing that $|C/F|^2$ and $|D/F|^2$ both contain the factor $(\eta_0^2-1)^{1/2}[|\eta_0|+(\eta_0^2-1)^{1/2}]^{-1}$ which is (apart from a factor of 2) the fraction of the incident beam which goes into the crystal and could be deduced easily from boundary conditions at the entrance surface. The factors which depend on η could be deduced also from boundary conditions at a fictitious exit surface at the point under consideration. For the new wave field the factor $|\alpha|^2=\exp(-2\pi|\nu|)$ gives the fraction of the initial wave field which goes into the new wave field and the factor $|A(\nu)|^2$ in $|D/F|^2$ shows that along BC (Fig. 3*c*) the intensity is decreased by a factor $1-\exp(2\pi|\nu|)$ as required by the conservation of energy.

Returning to the case of small strain gradients, we see that the form (13) of $P_h(\eta_0,s_0,s_h)$ is valid whatever $|\eta_0|$ and $|\eta|$ are and cannot be restricted to the two first terms. Let us consider the third and fourth terms respectively equal to $-CG/F^2$ and $-DG/F^2$ (see Appendix) and leading to two integrals:

$$\begin{aligned}I_3&=\int\exp[-i\eta_0(s_0+s_h)][-CG/F^2]\,\mathrm{d}\eta_0\\&=\int R_3\exp(i\varphi_3)\,\mathrm{d}\eta_0 \quad (25)\\I_4&=\int\exp[-i\eta_0(s_0+s_h)][-DG/F^2]\,\mathrm{d}\eta_0\\&=\int R_4\exp(i\varphi_4)\,\mathrm{d}\eta_0. \quad (26)\end{aligned}$$

These integrals are different from zero only if η_0 is negative, since if η_0 is positive G is equal to zero. The condition for φ_3 to be stationary depends on the sign of η. If $z<-(\eta_0\tan\theta)/\beta$, η is negative and this condition is:

$$\beta x=3(\eta_0^2-1)^{1/2}-(\eta^2-1)^{1/2} \quad (27)$$

which can be written

$$\beta(x-x_c)=(\eta_0^2-1)^{1/2}-(\eta^2-1)^{1/2} \quad (28)$$

where

$$x_c=2(\eta_0^2-1)^{1/2}/\beta. \quad (29)$$

x_c is the x coordinate of the intersection C of the hyperbolic trajectory OBC with the surface (Fig. 3*b*).

Similarly the phase φ_4 is stationary if

$$\beta(x-x_c)=(\eta_0^2-1)^{1/2}+(\eta^2-1)^{1/2}. \quad (30)$$

Equations (28) and (30) are identical to (22) and (23) where x has been replaced by $x-x_c$. As the fundamental equation (18) still holds, the trajectory is the same arc of a hyperbola as OBC but with its origin at C, giving the trajectory CB_1C_1 (Fig. 4). We obtain here, as expected, the reflexion of the beam at the surface. It can be shown easily that the other terms in the development (13) lead to successive reflexions at the surface. The case $z>-(\eta_0\tan\theta)/\beta$ does not need to be considered here; it would lead to a new wave field created after B_1 but its amplitude is non-negligible only if $|\nu|$ is small [because of $A(\nu)$ in C/F] and then G tends to zero so that the integrals are zero. This is not surprising: if $|\nu|$ is small, then the curvature of the hyperbola is strong. The beam arriving at C is quite parallel to $\mathbf{K}_h$ and is not reflected at the surface. All its energy goes out of the crystal.

5. Amplitude of the reflected wave at the surface

Although the stationary phase is an integration method, we have used it, up to now, to determine ray paths. It will be used now to determine the amplitude of the reflected wave at the crystal surface for an incident spherical wave at the origin O. We need then the values of the integrals $I_1, I_2, I_3, \dots$ [where we reintroduce the factor $\nu^{1/2}/\pi$ dropped just before (14)] at the surface, that is at every point for which $s_0 = s_h$ and then $\beta x = 4Bs_0$.

For I_1 the phase is not stationary at the surface since the corresponding ray paths go inside the crystal [ray paths of type O_1r and O_2B in Figs. 3(*a*) and (*b*) respectively] but I_1 can be integrated exactly for points at the surface for which $z=0$ and then $\eta=\eta_0$. Its value derived from tables (*e.g.* Bateman, 1954) is

$$J_1(2s_0)/(2s_0) = J_1(\pi x/\Lambda_0)/(\pi x/\Lambda_0) \qquad (31)$$

which is the value for the perfect crystal (J_1 is the Bessel function of order 1).

The phases φ_2 and φ_3, in I_2 and I_3 respectively, are equal for $\eta=\eta_0$ and stationary for a value of η_0 given by

$$(\eta_0^2-1)^{1/2} = \beta x/2 \qquad (32)$$

which is identical to (29).

Integration by the stationary-phase method then gives

$$I_2 = \exp(-i\pi/4)\pi^{-1}(\Lambda_0\beta)^{1/2}u^{1/2}(1+u^2)^{-1/4} \times f(\beta)\exp[-2iS(u)] \qquad (33)$$

where $f(\beta)=1$ for small values of the strain gradient and $f(\beta)=[1-\exp(-2\pi|\beta_c/\beta|)]^{1/2}$ for large values of the strain gradient, and

$$I_3 = -[u+(1+u^2)^{1/2}]^{-2}I_2 \qquad (34)$$

with

$$S(u) = (\beta_c/\beta)\{u(1+u^2)^{1/2} - \log[u+(1+u^2)^{1/2}]\}$$

and $u=\beta x/2$. The corresponding stationary paths are BC and CJ (Fig. 5).

For small or intermediate values of the strain gradient the following terms I_4 and I_5 have to be considered. They correspond to stationary paths GC and CH and a stationary value η_0' such that

$$(\eta_0'^2-1)^{1/2} = \beta x/4. \qquad (35)$$

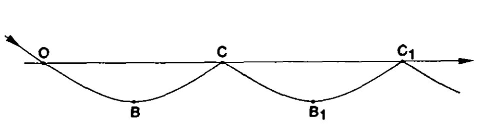

Fig. 4. Beam trajectory showing the reflexion at the crystal surface.

One obtains

$$I_4 = \exp(-3i\pi/4)\pi^{-1}(\Lambda_0\beta/2)^{1/2}(u')^{1/2}(1+u'^2)^{-1/4} \times[u'+(1+u'^2)^{1/2}]^{-1}\exp[-4iS(u')] \qquad (36)$$

$$I_5 = -[u'+(1+u'^2)^{1/2}]^{-2}I_4 \qquad (37)$$

where $u'=\beta x/4$.

The following terms in expansion (13) would give stationary paths in C corresponding to $3, 4, 5, \dots$ successive reflexions at the surface. The corresponding intensities decrease as the number of reflexions increases.

6. Concluding remarks

We have here demonstrated the creation of a new wave field in the Bragg case for highly distorted crystals. This has been done starting from the Green function given by Chukhovskii, Gabrielyan & Petrashen' (1978) and using a new asymptotic form for the cylindric functions $D_{-n-\nu}(Y)$. This new development can describe both cases: strong and slight distortions of the crystal. The principle is then the same as that used by Balibar, Chukhovskii & Malgrange (1983). The Green function is written as an integral over the angles of incidence. The integrand can then be considered as the wave in the crystal resulting from a given incident plane wave. The integrand is a sum of terms and ray paths are obtained from the condition that the phase of each term be stationary. Successive reflexions on the surface are obtained in the case of small strain gradients and the main result for high strain gradients is the creation of a new wave field close to the apex of the hyperbola. This new wave field takes a fraction $\exp(-2\pi/|\alpha_0|)$ out of the normal wave field where α_0 is the strain gradient expressed in a unit equal to $\beta_c = \pi/2\Lambda_0$ where Λ_0 is the intrinsic extinction distance (equal to the inverse of the distance of the apices of the dispersion hyperbola). This is exactly the same result as the one found theoretically in the Laue case (Balibar, Chukhovskii & Malgrange, 1983) and shown in the Bragg case by computer experiments by Gronkowski & Malgrange (1984).

APPENDIX

Let us write

$$P_0 = \eta_0^2 - 1 \quad P = \eta^2 - 1$$

$$Q_0 = |\eta_0| + (\eta_0^2-1)^{1/2} \quad Q = |\eta| + (\eta^2-1)^{1/2}$$

$$S(\eta) = (1/4B)\{|\eta|(\eta^2-1)^{1/2} - \log[|\eta| + (\eta^2-1)^{1/2}]\}.$$

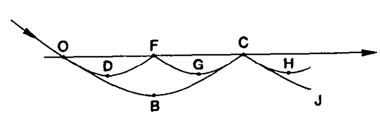

Fig. 5. Stationary paths at a point C on the surface when the incident wave is spherical.

Then

$$C/F=\nu^{-1/2}(P_0/P)^{1/4}(Q_0Q)^{-1/2}\times\alpha(\chi_0,\chi)\exp\{i[S(\eta)-S(\eta_0)]\}$$

where

$$\alpha(\chi_0,\chi)=\begin{cases}\exp(i\pi/2) & \text{if } \eta_0>0 \text{ and } \eta>0\\ \exp(-i\pi/2) & \text{if } \eta_0<0 \text{ and } \eta<0\\ \exp(-\pi|\nu|) & \text{if } \eta_0<0 \text{ and } \eta>0\end{cases}$$

$$D/F=A(\nu)(P_0/P)^{1/4}(Q/Q_0)^{1/2}\times\exp\{i[-S(\eta)-S(\eta_0)]\}$$

where

$$A(\nu)=\begin{cases}\nu^{-1/2} & \text{if } |\nu|\to\infty\\ |\nu|^{-1/2}[1-\exp(2i\pi\nu)]^{1/2} & \\ \quad=\exp(i\pi/4)\nu^{-1/2}[1-\exp(-2\pi|\nu|)]^{1/2} & \text{if } |\nu|\to 0\end{cases}$$

$$-CG/F^2=-\nu^{-1/2}(P_0/P)^{1/4}Q_0^{-3/2}Q^{-1/2}\times\exp\{i[S(\eta)-3S(\eta_0)]\}$$

$$-DG/F^2=\nu^{-1/2}\exp(-i\pi/2)\times(P_0/P)^{1/4}Q^{1/2}Q_0^{-3/2}\times\exp\{i[-S(\eta)-3S(\eta_0)]\}.$$

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