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On the Principle of X-ray Interferometry

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The scattering amplitude of an X-ray interferometer is calculated using a general theory of X-ray diffraction. Analytic expressions are given for the intensities of diffracted beams in interferometry; these expressions include the effect of the positions of each crystal lattice in addition to ordinary dynamical effects. It is concluded that the fringes observed in X-ray interferometry of a lattice spacing are accounted for by an optical (Moiré) effect rather than by dynamical effects of X-ray diffraction.

1. Introduction

The first X-ray interferometer was demonstrated by Bonse & Hart (1965*a*, *b*). Their success added the new subject of X-ray interferometry to the fields of X-ray diffraction and applied X-ray optics. An experiment performed by Deslattes (1969) indicated through simultaneous X-ray and optical interferometry the possibility of measuring crystal-lattice spacings with accuracies better than one part per million.

The principle of X-ray interferometry was explained by Bonse & Hart (1965*a*, *c*) by means of a discussion based on standing wave fields caused by the dynamical effects of X-ray diffraction. Although Bonse & Hart (1965*c*) have attempted to present their explanation in an analytic form, their argument is still qualitative. Their results, though analytic for dynamical interference effects, do not contain analytic expressions which would connect dynamical wave fields with the lattice of each crystal. This shortcoming has its origin in the usual formulation of the dynamical theory of diffraction.

In the present paper, this shortcoming inherent in the ordinary formulation will be eliminated by using a more general theory of X-ray diffraction (Ashkin & Kuriyama, 1966; Kuriyama, 1967). The results will be given in an analytical form for the intensities of X-ray beams diffracted by the interferometer. It will be demonstrated that the interferometry of a lattice spacing is explained merely by ordinary optics (Moiré interference). The dynamical effects are thus not really involved in the explanation of the principle underlying interferometry. This conclusion does not exclude the role of the dynamical effects in interferometry; the Bormann effect, for example, allows one to obtain maximum contrast in lattice spacing interference patterns, though this needs not be an optimal mode of operation in practice (Deslattes, 1969; Hart, 1968).

2. The scattering amplitude of a crystal

A general theory of X-ray diffraction has been developed (Ashkin & Kuriyama, 1966; Kuriyama, 1967) wherein the generalized polarizability of a crystal is given by a non-local function $\Gamma(x_1; x_2)$ that depends upon two independent space-time coordinates. In this theory translational invariance holds for time coordinates. Therefore the Fourier transform of the generalized polarizability can be written as $\Gamma(\mathbf{k}_1,\mathbf{k}_2;\omega)$. It has been shown by Kuriyama (1967) that this quantity is given by

$$\Gamma(\mathbf{k}_1\mathbf{k}_2;\omega)=(V/N)\sum_i \gamma_i(\mathbf{k}_1\mathbf{k}_2;\omega) \exp\left[-i(\mathbf{k}_1-\mathbf{k}_2)\,.\,\mathbf{R}_i\right], \quad (2\cdot1)$$

where V is the volume of the crystal, N is the total number of atoms in the crystal, $\mathbf{R}_i$ is the position of the ith atom and $\gamma_i(\mathbf{k}_1\mathbf{k}_2;\omega)$ is the 'atomic' polarizability of the ith atom. The quantities Γ and γ_i are tensors which characterize the rotation of the polarization directions of scattered X-rays. For simplicity, however, those quantities are treated in this paper as though they are not tensors: the polarization mixing effects (Ashkin & Kuriyama, 1966) are neglected and simple polarization factors modify the atomic polarizability.

If the crystal is perfect and the unit cell contains n atoms specified by $m(=1,2,\ldots n)$, then the position of the atoms can be given by

$$\mathbf{R}_i=\mathbf{R}_l(m)=\mathbf{l}+\mathbf{r}_m\,, \quad (2\cdot2)$$

where $\mathbf{l}$ is the position of the origin of the lth unit cell, and $\mathbf{r}_m$ denotes the position of the mth atom measured from the origin of the unit cell. Equation (2·1) thus reduces to

$$\Gamma(\mathbf{k}_1,\mathbf{k}_2;\omega)=(V/n\tilde{N})\sum_{\mathbf{l}}^{\tilde{N}} \exp\left[-i(\mathbf{k}_1-\mathbf{k}_2)\,.\,\mathbf{l}\right] \times\sum_m^n \gamma_m(\mathbf{k}_1,\mathbf{k}_2;\omega)\exp\left[-i(\mathbf{k}_1-\mathbf{k}_2)\,.\,\mathbf{r}_m\right], \quad (2\cdot3)$$

where $\tilde{N}$ is the total number of unit cells in the crystal. The quantities $\gamma_m(\mathbf{k}_1,\mathbf{k}_2;\omega)$ give to lowest order the usual atomic scattering factors which depends only on $\mathbf{k}_1-\mathbf{k}_2$. Therefore we simplify them by writing $\gamma_m(\mathbf{k}_1-\mathbf{k}_2;\omega)$. One can then write

$$v(\mathbf{k}_1-\mathbf{k}_2)\equiv\sum_m \gamma_m(\mathbf{k}_1-\mathbf{k}_2;\omega) \times\exp\left[-i(\mathbf{k}_1-\mathbf{k}_2)\,.\,\mathbf{r}_m\right], \quad (2\cdot4)$$

where v is the X-ray structure factor of the unit cell (the explicit frequency (ω) dependence of v has been omitted for convenience). Thus one obtains

$$\Gamma(\mathbf{k}_1\mathbf{k}_2;\omega)=(V/n)\{(1/\tilde{N})\sum_{\mathbf{l}}\exp[-i(\mathbf{k}_1-\mathbf{k}_2)\cdot\mathbf{l}]\}\times v(\mathbf{k}_1-\mathbf{k}_2)\,. \quad (2\cdot5)$$

Since $\mathbf{l}$ represents the periodic lattice vector, $(1/\tilde{N})\sum_{\mathbf{l}}\exp[i(\mathbf{k}_1-\mathbf{k}_2)\cdot\mathbf{l}]$ is equal to the generalized Kronecker delta $\Delta(\mathbf{k}_1-\mathbf{k}_2)$ which vanishes unless $\mathbf{k}_1-\mathbf{k}_2=\mathbf{K}$ (2π times a reciprocal-lattice vector). Thus it gives the Laue interference function.

In the scattering formalism of modern quantum mechanics, the scattering amplitude for diffracted X-rays is given by the probability amplitude of a photon in the wave packet state $|\mathbf{k},\nu,\mathbf{R};\text{in}\rangle$ to make a transition to the state $|\mathbf{k}',\nu'\mathbf{R}';\text{out}\rangle$, where $\mathbf{k}$ is momentum, $\omega=|\mathbf{k}|$ is energy (with $c=\hbar=1$), ν the polarization direction of the photon, $\mathbf{R}$ is the center position of the X-ray beam on the crystal, and the primes indicate those quantities for outgoing waves. The scattering amplitude is given (Ashkin & Kuriyama, 1966; Kuriyama, 1967) (with ν and ν' suppressed) by

$$\langle\mathbf{k}',\mathbf{R}';\text{out}\,|\mathbf{k},\mathbf{R};\text{in}\rangle=\int d^3\mathbf{p}\int d^3\mathbf{p}'A^*(\mathbf{k}',\mathbf{p}';\mathbf{R}')S(\mathbf{p}',\mathbf{p})A(\mathbf{k},\mathbf{p};\mathbf{R})\,, \quad (2\cdot6)$$

where A is the Fourier transform of the free photon wave packet depending on a parameter $\mathbf{R}$ which indicates the spatial location for the maximum intensity. This A is determined by the momentum and the energy distribution of the incoming X-ray beam. The quantity $S(\mathbf{p}',\mathbf{p})$ is the scattering matrix element. We will derive it for a crystal plate. To calculate the scattering matrix element $S(\mathbf{p}',\mathbf{p})$, it is sufficient from equation (2·6) that we need to consider only a plane wave as an incident beam.

We introduce a coordinate system which is fixed in space. In this coordinate system, the normalized plane wave $f(x;\mathbf{k})$ is written

$$f(x;\mathbf{k})=[2(2\pi)^3 4\pi|\mathbf{k}|]^{-1/2}\exp[i(\mathbf{k}\cdot\mathbf{r}-|\mathbf{k}|t)]\,, \quad (2\cdot7)$$

where x represents the space–time coordinates $(\mathbf{r},t)$. An incoming plane wave having an amplitude $S^{(0)}(\mathbf{p})$ and propagating in the $\mathbf{p}$ direction is then given by

$$\chi^i(x;\mathbf{p})=S^{(0)}(\mathbf{p})f(x;\mathbf{k}=\mathbf{p})\,. \quad (2\cdot8)$$

This wave travels in space to reach a crystal plate which occupies the region between $z=z_0$ and $z=z_0+L$, as shown in Fig. 1. After being diffracted by the crystal, the outgoing waves travel in space again like plane waves

$$\chi^f(x;\mathbf{p}')=S(\mathbf{p}',\mathbf{p})S^{(0)}(\mathbf{p})f(x;\mathbf{k}=\mathbf{p}') \quad (2\cdot9)$$

in the $\mathbf{p}'$ direction. The possible directions $\mathbf{p}'$ are those for which $S(\mathbf{p}'\mathbf{p})$ does not vanish.

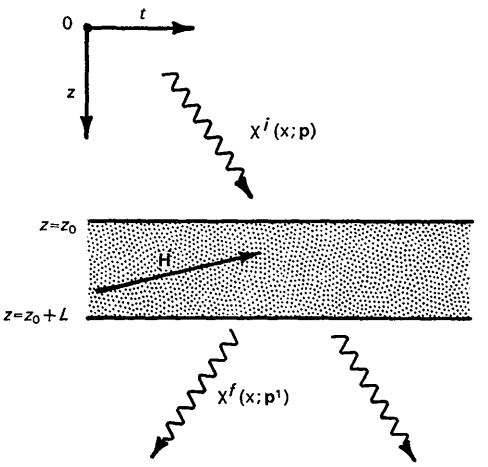

Fig. 1. Diffraction by one crystal plate. A crystal plate of thickness L is located at a distance z_0 from the position where the phase of the incoming X-ray wave is established. The wave packets $\chi^i(x;\mathbf{p})$ and $\chi^f(x;\mathbf{p}')$ represent those in the initial and the final states, respectively.

In the coordinate system fixed in space, the vector indicating the origin of the lth unit cell is given by

$$\mathbf{l}=\mathbf{d}+\mathbf{l}'+z_0\hat{z}\,, \quad (2\cdot10)$$

where $\mathbf{d}$ fixes the crystal lattice in space, and $\mathbf{l}'$ is a lattice translational vector, and $\hat{z}$ is the unit vector in the z direction. Since the location of the crystal plate in space has been already introduced by z_0, it is convenient to define the location of the lattice with respect to such a mathematically defined crystal plate.

Using the method developed by Kuriyama (1967, 1970) for an imperfect crystal and the polarizability from equation (2·5) along with equation (2·10) one obtains the scattering matrix of a perfect crystal:

$$S(\mathbf{p}',\mathbf{p})=(p_z'/|\mathbf{p}|)\delta(|\mathbf{p}|-|\mathbf{p}'|)\sum_{\mathbf{k}}\delta(\mathbf{p}_t+\mathbf{K}_t-\mathbf{p}_t')\times\exp[i(p_z+K_z-p_z')z_0]\exp[i\mathbf{K}\cdot\mathbf{d}] \quad (2\cdot11)$$
$$\times\sum_i F_{\mathbf{K}}[i;\mathbf{p}_t]\exp[i(\alpha_i(\mathbf{p}_t)+K_z-p_z')L]\,,$$

where the *subscript t* indicates the projection of a vector on the crystal surface. The quantities $F_{\mathbf{K}}[i,\mathbf{p}_t]$ are called the dynamical field functions for the mode i. Their forms are given in the Appendix. They are obtained from the photon Green's functions which characterize the propagation of quasi-photons inside the crystal (see the Appendix). These dynamical field functions depend upon the tangential component of the wave-vector of the incoming photon, $\mathbf{p}_t$. In other words, they are given in terms of the quantity which describes the deviation of the incoming photon from the Bragg condition. The quantities $\alpha_i(\mathbf{p}_t)$ can be interpreted as the z component wave-vector for a quasi-photon (internal wave field) in the crystal. They are determined by a dispersion equation [see equation (A·9)] for the given value

of the tangential component of the wave-vector of the incoming photon. Equation (2·11) gives the same result as ordinary dynamical theory, except that the phase factors, $\exp[i(p_z+K_z-p'_z)z_0]$ and $\exp[i\mathbf{K}\cdot\mathbf{d}]$ now appear. It is obvious that these phase factors do not play any significant role in the diffracted intensities for a single crystal; ordinary dynamical theory therefore is sufficient for a description of simple diffraction from a single crystal.

However, it is important to note that the S matrix consists of the sum of many terms with differing $\mathbf{K}$. For example, when the incident beam satisfies a single Bragg condition ($|\mathbf{p}|\simeq\mathbf{p}+\mathbf{H}|$), two final states ($\mathbf{p}'_t=\mathbf{p}_t$ and $\mathbf{p}_t=\mathbf{p}_t+\mathbf{H}_t$) simultaneously appear with $\mathbf{K}=\mathbf{O}$ and $\mathbf{H}$. The S matrix is therefore given by the sum of two terms, one in $\mathbf{O}$ direction and the other in the $\mathbf{H}$ direction: in other words, in diffraction the amplitudes for component waves are added with a definite phase relationship to give the total scattering amplitude. This statement is equivalent to saying that all component waves are coherent. In addition to the dynamical phase factor, $\exp[i(\alpha_t(\mathbf{p}_t)+K_z-p'_z)L]$, which results in Pendellösung fringes and other interference effects, there are two other phase factors mentioned before. In one-crystal diffraction there is no easy way of combining two beams diffracted in different directions; therefore, the phase factors are undetectable. One can, however, detect them in an ingenious arrangement of multiple diffraction due to Bonse & Hart (1965*a*, *b*). As we shall see the phase factor $\exp[i\mathbf{K}\cdot\mathbf{d}]$ is especially important in interferometry of a lattice spacing.

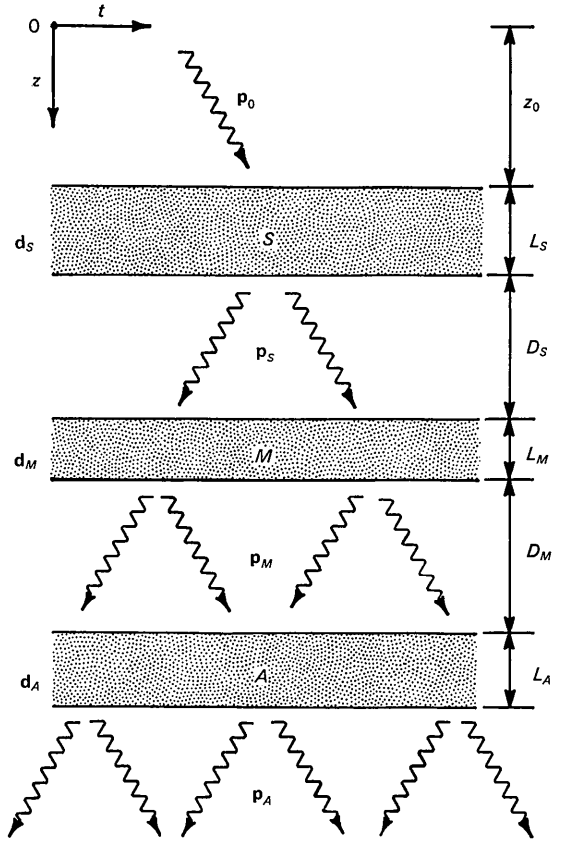

Fig. 2. Diffraction by an X-ray interferometer. A geometrical arrangement of three crystals, the splitter (S), the mirror (M) and the analyzer (A), is shown. The crystal thickness is denoted by L with a proper subscript. The mirror is located at a distance D_S away from the splitter, and D_M away from the analyzer. The wave vectors in the gaps are given by $\mathbf{p}_\sigma$ with $\sigma=0$, S, M and A. The quantities $\mathbf{d}_\sigma$ represent the spatial locations of each crystal lattice.

3. The scattering amplitude of an X-ray interferometer

The Bonse–Hart X-ray interferometer requires diffraction by more than one crystal so that X-ray beams initially diffracted in different directions can eventually be brought back together in the same direction to set up an interference pattern. Fig. 2 shows a geometrical arrangement of three crystals in an X-ray interferometer: a beam splitter (S), a transmission mirror (M) and an analyser (A). We again introduce a coordinate system fixed in space and describe the locations ($\mathbf{d}_S,\mathbf{d}_M,\mathbf{d}_A$) of the three crystals in terms of that coordinate system.

The amplitude of an incoming photon wave propagating in the $\mathbf{p}_0$ direction is denoted by $S^{(0)}(\mathbf{p}_0)$ which will be set equal to 1 in final results. Diffraction by the crystal S gives rise to outgoing waves propagating in the directions $\mathbf{p}_S$ with amplitudes $S^{(S)}(\mathbf{p}_S,\mathbf{p}_0)S^{(0)}(\mathbf{p}_0)$ as shown in equation (2·9). These diffracted waves on their arrival at the crystal M become incident beams for M. The crystal M thereby diffracts them to produce another set of waves whose amplitude [again by (2·9)] is $S^{(M)}(\mathbf{p}_M,\mathbf{p}_S)S^{(S)}(\mathbf{p}_S,\mathbf{p}_0)S^{(0)}(\mathbf{p}_0)$, since the incoming amplitude for the crystal M is $S^{(S)}(\mathbf{p}_S,\mathbf{p}_0)S^{(0)}(\mathbf{p}_0)$. We repeat the same procedure for the crystal A to obtain for the scattering amplitude of the interferometer

$$S(\mathbf{p}_A,\mathbf{p}_0)=S^{(A)}(\mathbf{p}_A,\mathbf{p}_M)S^{(M)}(\mathbf{p}_M,\mathbf{p}_S)S^{(S)}(\mathbf{p}_S,\mathbf{p}_0)S^{(0)}(\mathbf{p}_0)\,. \quad (3\cdot1)$$

The quantity $S^{(\sigma)}(p_\sigma,p_{\sigma-1})$ where $\sigma\equiv0,1\equiv S,2\equiv M$ or $3\equiv A$, is the scattering amplitude of a crystal σ, [$\sigma=0$ means no crystal: $S^{(0)}(p_0,p_{0-1})\equiv S^{(0)}(p_0)$]; the application of equation (2·11) yields

$$\begin{aligned}S^{(\sigma)}(\mathbf{p}_\sigma,\mathbf{p}_{\sigma-1})&=[\mathbf{p}_{\sigma,z}/|\mathbf{p}_{\sigma-1}|]\delta(|\mathbf{p}_{\sigma-1}|-|\mathbf{p}_\sigma|)\\&\quad\times\sum_{\mathbf{K}(\sigma)}\delta(\mathbf{p}_{\sigma-1,t}+\mathbf{K}_t(\sigma)-\mathbf{p}_{\sigma,t})\\&\quad\times\exp[i(p_{\sigma-1,z}+K_z(\sigma)-p_{\sigma,z})z(\sigma)]\exp[i\mathbf{K}(\sigma)\cdot\mathbf{d}_\sigma]\\&\quad\times\sum_{i(\sigma)}F_{\mathbf{K}(\sigma)}[i(\sigma);\mathbf{p}_{\sigma-1,t}]\\&\quad\times\exp[i\{\alpha_{i(\sigma)}(p_{\sigma-1,t})+K_z(\sigma)-p_{\sigma,z}\}L_\sigma]\,,\end{aligned} \quad (3\cdot2)$$

where $\mathbf{K}(\sigma)$ and $i(\sigma)$ are a reciprocal-lattice vector and the mode of a quasi-photon in the crystal σ, respectively. Using the notation of Fig. 2, we obtain

$$\begin{aligned} z(1)&=z(S) &&=z_0(=0)\\ z(2)&=z(M)&&=z_0+L_S+D_S \\ z(3)&=z(A) &&=z_0+L_S+D_S+L_M+D_M\,. \end{aligned} \tag{3·3}$$

Without a consequent loss of generality we can set z_0 equal to 0.

The delta functions in equation (3·2) imply the energy and the momentum conservation rules (the Bragg reflection condition) in diffraction. Since equation (3·1) contains three of $S^{(\sigma)}$'s, the momentum of the photon in the final state must satisfy the relation

$$\mathbf{p}_{A,t}=\mathbf{p}_{0,t}+\sum_{\sigma=1}^{3}\mathbf{K}_t(\sigma)\,. \tag{3·4}$$

The final direction of a beam emerging from an interferometer depends only upon the sum of the three $\mathbf{K}_t(\sigma)$ in the successive diffractions. This implies that optical paths determined by different combinations of $\mathbf{K}(\sigma)$ can give rise to the same resultant beam. As shown above in § 2, diffracted beams with differing optical paths are coherent with each other.

We now make the realistic assumption that all three crystals in the interferometer are of the same kind crystallographically and are aligned in the same crystallographic direction. Furthermore, for this alignment an incident X-ray beam satisfies a single Bragg condition, $|\mathbf{p}_0|\simeq|\mathbf{p}_0+\mathbf{H}|$. This geometry implies that in the crystals the generalized polarizability has non-vanishing values only for $v(\mathbf{O})$, $v(+\mathbf{H})$ and consequently $v(-\mathbf{H})$. As shown in the Appendix, the possible non-vanishing dynamical field functions $F_{\mathbf{K}}$ in this case are those having $\mathbf{K}=\mathbf{O}$ and either $\mathbf{H}$ or $-\mathbf{H}$.

In practice one uses an incident beam of finite width. Thus, the scattering matrix of equation (3·1) should be substituted into the scattering amplitude formula (2·6) with an appropriate form of $A(\mathbf{k},\mathbf{p};\mathbf{R})$ that represents the location and the spectral distribution of the incident beam. The scattering amplitude of equation (2·6) is a function of $\mathbf{R}$ and $\mathbf{R}'$; the location $\mathbf{R}'$ of a diffracted beam depends upon the combination of $\mathbf{K}$'s that determines the optical path. To guarantee interference effects, the beams must come out of the third crystal almost at the same location. The exit position $\mathbf{R}'$ for the outgoing wave can be found from considerations (Ashkin & Kuriyama, 1966; Kuriyama, 1968) of classical energy flow. Of the many paths possible, the following ones give rise to interference:

Path I $[\mathbf{K}(S),\mathbf{K}(M),\mathbf{K}(A)]=(\mathbf{O},\mathbf{H},-\mathbf{H});\sum\mathbf{K}(\sigma)=\mathbf{O}$

Path II $[\mathbf{K}(S),\mathbf{K}(M),\mathbf{K}(A)]=(\mathbf{H},-\mathbf{H},\mathbf{O});\sum\mathbf{K}(\sigma)=\mathbf{O}$

Path III $[\mathbf{K}(S),\mathbf{K}(M),\mathbf{K}(A)]=(\mathbf{O},\mathbf{H},\mathbf{O});\quad\sum\mathbf{K}(\sigma)=\mathbf{H}$

Path IV $[\mathbf{K}(S),\mathbf{K}(M),\mathbf{K}(A)]=(\mathbf{H},-\mathbf{H},\mathbf{H});\sum\mathbf{K}(\sigma)=\mathbf{H}.$

Paths I and II produce outgoing photons at the same location which propagate in the transmitted direction ($\mathbf{p}_A=\mathbf{p}_0$); paths III and IV result in the photons propagating in the Bragg diffracted direction ($\mathbf{p}_A\simeq\mathbf{p}_0+\mathbf{H}$) from the same location on the third crystal.

We now calculate equation (3·1) using equation (3·2) for these combinations of the $\mathbf{K}$'s. From the momentum and the energy conservation rules in equation (3·2), the propagation vectors of the photons $\mathbf{p}_S$, $\mathbf{p}_M$, and $\mathbf{p}_A$ in gaps between the crystals are determined for each path, as listed in Table 1. In calculating $S^{(\sigma)}$ for each crystal, we need to know three exponential phase factors appearing in (3·2). Once the path is given, these phase factors are easily obtained from the table: for example, if we are interested in the mirror crystal for path I, then the block given by the row for $\sigma=2\equiv M$ and the column for path I in the Table gives the values for the tangential component $(\mathbf{p}_M)_t$ and for the z component $(\mathbf{p}_M)_z$ in terms of those for the incoming photon $\mathbf{p}_0$. The dynamical phase shift in this crystal, $\alpha_{i(M)}+K_{z(M)}-p_{M,z}$, is found also in this block to be $\delta'_{i(M)}$. The optical phase shift for this crystal, $p_{S,z}+K_{z(M)}-p_{M,z}$, is given in the last row in the path I column to be $+\Delta$. The dynamical field function for this case is found to be $F_{\mathbf{H}}[i(M),\mathbf{p}_{0,t}]$ because from the Table $\mathbf{K}(M)=\mathbf{H}$ and $\mathbf{p}_{\sigma-1,t}=\mathbf{p}_{S,t}=\mathbf{p}_{0,t}$ ($\sigma=2$ in this case). The solutions of dispersion equations, $\alpha_i(\mathbf{p}_{\sigma-1,t})$, can be expressed in terms of the solution $\alpha_i(\mathbf{p}_{0,t})$ for the incoming beam, since the tangential components of the momenta, $\mathbf{p}_{\sigma-1}$ are related to $\mathbf{p}_{0,t}$. In Table 1 we have introduced the following quantities for convenience:

$$\delta_i=\alpha_i(\mathbf{p}_{0,t})-p_{0\ z}\,, \tag{3·5}$$

and

$$\delta'_i=\alpha_i(\mathbf{p}_{0,t})+H_z-p_{H,z}\,, \tag{3·6}$$

where

$$p_{0,z}=+\sqrt{(\mathbf{p}_0)^2-(\mathbf{p}_{0,t})^2} \tag{3·7}$$

and

$$p_{H,z}=+\sqrt{(\mathbf{p}_0)^2-(\mathbf{p}_{0,t}+\mathbf{H}_t)^2}\,. \tag{3·8}$$

If we set

$$2\varepsilon=\mathbf{p}_0^2-(\mathbf{p}_0+\mathbf{H})^2+(1-\tau)v(\mathbf{O})\,, \tag{3·9}$$

$$R=\sqrt{\varepsilon^2+\tau v(+\mathbf{H})v(-\mathbf{H})}\,, \tag{3·10}$$

and

$$\tau=1+(H_z/p_{0,z})\,, \tag{3·11}$$

then the solution of a dispersion equation for the initial state ($\mathbf{p}_0$) is given by

$$\alpha_i(p_{0,t})-p_{0,z}=\frac{1}{2p_{0,z}}\left[v(\mathbf{O})+\frac{1}{\tau}\{\varepsilon+(-1)^iR\}\right], \tag{3·12}$$

where the mode with $i=1$ is the anomalous transmission mode while the mode with $i=2$ is the anomalous (strong) absorption mode.

As seen from Table 1, $F_{\mathbf{O}}[i;\mathbf{p}_{0,t}]$, $F_{\mathbf{H}}[i,\mathbf{p}_{0,t}]$, $F_{\mathbf{O}}[i;\mathbf{p}_{0,t}+\mathbf{H}_t]$ and $F_{-\mathbf{H}}[i;\mathbf{p}_{0,t}+\mathbf{H}_t]$ are the dynamical field functions necessary for evaluating equation (3·1). After performing several steps of calculation on equations (A.6) to (A.8) one obtains

$$F_{\mathbf{O}}[i;\mathbf{p}_{0,t}]=\tfrac{1}{2}\left[1-(-1)^i\frac{\varepsilon}{R}\right], \tag{3·13}$$

$$F_{\mathbf{H}}[i,\mathbf{p}_{0,t}]=\frac{(-1)^i}{2}\,\frac{v(+\mathbf{H})}{R} \tag{3·14}$$

and

$$F_{\mathbf{O}}[i;\mathbf{p}_{0,t}+\mathbf{H}_t]=\tfrac{1}{2}\left[1+(-1)^i\frac{\varepsilon}{R}\right], \tag{3·15}$$

$$F_{-\mathbf{H}}[i;\mathbf{p}_{0,t}+\mathbf{H}_t]=\frac{(-1)^i}{2}\,\tau\,\frac{v(-H)}{R}. \tag{3·16}$$

In equation (3·1) there appear only products of three of these functions with a proper combination of $\mathbf{K}(\sigma)$. To express them, it is convenient to define the following quantities:

$$\mathscr{F}(i)=(2R)^{-3}(R^2-\varepsilon^2)\,[R-(-1)^i\varepsilon], \tag{3·17}$$

$$\mathscr{G}=(2R)^{-3}(R^2-\varepsilon^2)v(+\mathbf{H}) \tag{3·18}$$

and

$$f(i,j)=\frac{R-(-1)^i\varepsilon}{R-(-1)^j\varepsilon}. \tag{3·19}$$

Furthermore, we denote the energy momentum conservation equation by $\delta_{\mathbf{K}}$ with $\mathbf{K}=\mathbf{O}$ for the transmitted direction and $\mathbf{K}=\mathbf{H}$ for the Bragg diffracted direction, and reduce it to

$$\begin{aligned}\delta_K&\equiv(p_{A,z}/|p_0|)\delta(p_A-p_0)\delta(\mathbf{p}_{A,t}+\mathbf{K}_t-\mathbf{p}_{0,t})\\&=\delta(p_{A,z}+K_z-p_{K,z})\delta(\mathbf{p}_{A,t}+\mathbf{K}_t-\mathbf{p}_{0,t}),\end{aligned} \tag{3·20}$$

where $p_{K,z}$ are given by equations (3·7) and (3·8).

A detector set at a proper distance from the interferometer receives only photons propagating in the transmitted direction ($\sum\mathbf{K}(\sigma)=\mathbf{O}$) or those in the Bragg diffracted direction ($\sum\mathbf{K}(\sigma)=\mathbf{H}$). The scattering amplitude observed by the detector in the O direction, $\langle\mathbf{p}_A;\text{ out}|\mathbf{p}_0;\text{ in}\rangle\equiv S_0$ is given by

$$\begin{aligned}S_0=&\text{I}\exp[i\{\mathbf{H}\,.\,(\mathbf{d}_M-\mathbf{d}_A)-\Delta D_M\}]\\&+\text{II}\exp[i\{\mathbf{H}\,.\,(\mathbf{d}_S-\mathbf{d}_M)-\Delta D_S\}],\end{aligned} \tag{3·21}$$

while the one in the $\mathbf{H}$ direction, $\langle\mathbf{p}_A;\text{ out}|\mathbf{p}_0;\text{ in}\rangle\equiv S_{\mathbf{H}}$, is

$$\begin{aligned}S_H=&[\text{III}\exp[-i\{\mathbf{H}\,.\,(\mathbf{d}_S-\mathbf{d}_M)-\Delta D_S\}]+\text{IV}\\&\exp(-i\{\mathbf{H}\,.\,(\mathbf{d}_M-\mathbf{d}_A)-\Delta D_M\})]\exp[i\mathbf{H}\,.\,\mathbf{d}_S],\end{aligned} \tag{3·22}$$

where

$$\text{I}=\sum_{i(A)}\sum_{i(M)}\sum_{i(S)}(-1)^{i(M)+i(A)}\mathscr{F}[i(S)]\exp[i\{\delta_{i(A)}L_A+\delta_{i(M)}L_{(M)}+\delta_{i(S)}L_S\}] \tag{3·23}$$

$$\text{II}=\sum_{i(A)}\sum_{i(M)}\sum_{i(S)}(-1)^{i(M)+i(S)}\mathscr{F}[i(A)]\exp[i\{\delta_{i(A)}L_A+\delta_{i(M)}L_M+\delta_{i(S)}L_S\}] \tag{3·24}$$

$$\text{III}=\mathscr{G}\sum_{i(A)}\sum_{i(M)}\sum_{i(S)}(-1)^{i(M)}f(i(S),i(A))\exp[i\{\delta'_{i(A)}L_A+\delta'_{i(M)}L_M+\delta'_{i(S)}L_S\}] \tag{3·25}$$

$$\text{IV}=\mathscr{G}\sum_{i(A)}\sum_{i(M)}\sum_{i(S)}(-1)^{i(M)+i(A)+i(S)}\exp[i\{\delta'_{i(A)}L_A+\delta'_{i(M)}L_M+\delta'_{i(S)}L_S\}] \tag{3·26}$$

$$\Delta=\delta'_1-\delta'_1=\delta_2-\delta_2\,. \tag{3·27}$$

In evaluating the scattering amplitude equation (2·6) in terms of equation (3·1) the δ function (3·20) merely determines the possible momenta for the final state.

4. Conclusion and discussion

(a) *The principle of the X-ray interferometer*

The results obtained in the previous section are the same as those expected from the ordinary dynamical theory, except that the phase factors, $\exp[i\mathbf{H}\,.\,(\mathbf{d}_S-\mathbf{d}_M)]$ and $\exp[i\mathbf{H}\,.\,(\mathbf{d}_M-\mathbf{d}_A)]$ appear in the present results. As discussed in § 2, there is a definite phase shift in the scattered wave (only for $\mathbf{K}\neq\mathbf{O}$) due to the position of the crystal lattice. It is not detectable in intensity measurements in diffraction by one crystal. However, in diffraction by several crystals the phase shifts due to the relative positions of the crystal lattices explicity influence the resultant intensities of diffracted waves.

Table 1. *Propagation vectors of photons in gaps between the crystals*

		Transmitted direction		Bragg diffracted direction	
Crystals (σ)	Paths	Path I	Paths II	Path III	Path IV
	$\mathbf{K}(S)$, $\mathbf{K}(M)$, $\mathbf{K}(A)$	**O, H, −H**	**H, −H, O**	**O, H, O**	**H, −H, H**
$\sigma=1\equiv S$	$(\mathbf{p}_S)_t=\mathbf{p}_{S,t}$	$\mathbf{p}_{0,t}$	$\mathbf{p}_{0,t}+H_t$	$\mathbf{p}_{0,t}$	$\mathbf{p}_{0,t}+\mathbf{H}_t$
	$(\mathbf{p}_S)_z=p_{S,z}$	$p_{0,z}$	$p_{H,z}$	$p_{0,z}$	$p_{H,z}$
	$\alpha_{t(S)}+K_z(S)-p_{S,t}$	$\delta_{i(S)}$	$\delta'_{i(S)}$	$\delta_{i(S)}$	$\delta'_{i(S)}$
$\sigma=2\equiv M$	$(\mathbf{p}_M)_t=p_{M,T}$	$\mathbf{p}_{0,t}+\mathbf{H}_t$	$\mathbf{p}_{0,t}$	$\mathbf{p}_{0,t}+\mathbf{H}_t$	$\mathbf{p}_{0,t}$
	$(\mathbf{p}_M)_z=p_{M,z}$	$p_{H,z}$	$p_{0,z}$	$p_{H,z}$	$p_{0,z}$
	$\alpha_{t(M)}+K_z(M)-p_{M,z}$	$\delta'_{i(M)}$	$\delta_{i(M)}$	$\delta'_{i(M)}$	$\delta_{i(M)}$
$\sigma=3\equiv A$	$(\mathbf{p}_A)_t=\mathbf{p}_{A,t}$	$\mathbf{p}_{0,t}$	$\mathbf{p}_{0,t}$	$\mathbf{p}_{0,t}+\mathbf{H}_t$	$\mathbf{p}_{0,t}+\mathbf{H}_t$
	$(\mathbf{p}_A)_z=p_{A,z}$	$p_{0,z}$	$p_{0,z}$	$p_{H,z}$	$p_{H,z}$
	$\alpha_{t(A)}+K_z(A)-p_{A,z}$	$\delta_{i(A)}$	$\delta_{i(A)}$	$\delta'_{i(A)}$	$\delta'_{i(A)}$
	$p_{S,z}+K_z(M)-p_{M,z}$	$\Delta(\equiv\delta'_i-\delta_i)$	$-\Delta$	Δ	$-\Delta$
	$p_{M,z}+K_z(A)-p_{A,z}$	$-\Delta$	0	0	Δ

The intensities of the beams diffracted by the interferometer are given by modulus square of S_0 and S_H and contain only the relative shifts of the crystal lattices, $\mathbf{d}_{SM} \equiv \mathbf{d}_S - \mathbf{d}_M$ and $\mathbf{d}_{MA} \equiv \mathbf{d}_M - \mathbf{d}_A$. These observable intensities are

$$I_0 = |S_0|^2 = |\mathrm{I} \exp\{i\mathbf{H}\mathbf{d}_{MA}\} \exp\{-i\Delta D_M\} + \mathrm{II} \exp\{i\mathbf{H}\mathbf{d}_{SM}\} \exp\{-i\Delta D_S\}|^2 \quad (4\cdot1)$$

and

$$I_H = |S_H|^2 = |\mathrm{IV} \exp\{-i\mathbf{H}\mathbf{d}_{MA}\} \exp\{+i\Delta D_M\} + \mathrm{III} \exp\{-i\mathbf{H}\mathbf{d}_{SM}\} \exp\{+i\Delta D_S\}|^2 . \quad (4\cdot2)$$

The quantities I, II, III, and IV, defined by equations (3·23) to (3·26), contain all of the dynamical effects in each optical path. For instance, the quantity I includes every possible quasi-particle mode which occurs as a result of dynamical interactions in the optical path I through all the crystals. On the other hand, the phase factors appearing in equations (4·1) and (4·2) do not depend on those dynamical modes; therefore it is concluded that the presence of these phase factors is merely the consequence of an optical effect (*i.e.* the difference in optical path lengths depends on different wave-vectors), and is not accounted for by the dynamical effects. It is the presence of these phase factors, especially those related to $\mathbf{d}_{MA}$ and $\mathbf{d}_{SM}$, that leads to the interference effect in which the lattice spacings of the crystals are revealed, as has been demonstrated experimentally (Hart, 1968; Deslattes, 1969).

Since the dynamical effects are built in the quantities I–IV, the Pendellösung effect or the effect caused by inserting a different crystal (medium) is completely reproduced in the present formulation to give the same results as discussed by Bonse & Hart (1965*a*) and Kato & Tanemura (1967). Therefore, further discussions are centered exclusively on interferometry of a lattice spacing.

(*b*) *Interferometry of a lattice spacing*

To demonstrate the observations of a lattice spacing by interference, we consider first the original Bonse–Hart diffraction arrangement. In this arrangement, the crystals are so thick that only the anomalous transmission mode ($i(A) = i(M) = i(S) = 1$) passes through the crystals. Furthermore, the interferometer is assumed to be tuned to give maximum *efficiency* of transmission. As seen from equations (4·1) and (4·2) the maximum dynamical intensity* is not necessarily obtained in that tuning, because of the presence of $\mathbf{d}_{MA}$ and $\mathbf{d}_{SM}$. We can only obtain the maximum *efficiency* of transmission in a given arrangement of the crystals. It may be obtained when D_M is set equal to D_S: (the crystals are equally spaced). This equidistance condition was obtained in previous argument (Ashkin & Kuriyama, 1966; Kuriyama, 1968) concerning exit locations of the outgoing waves to secure the maximum overlapping of different paths. Under the equidistance condition we obtain

$$I_0 = 4|\mathscr{F}(1)|^2 \cos^2 \tfrac{1}{2}\{\mathbf{H}(\mathbf{d}_{MA} - \mathbf{d}_{SM})\} , \quad (4\cdot3)$$

and

$$I_H = 4|\mathscr{G}|^2 \cos^2 \tfrac{1}{2}\{\mathbf{H}(\mathbf{d}_{MA} - \mathbf{d}_{SM})\} , \quad (4\cdot4)$$

since

$$\mathrm{I} = \mathrm{II} = \mathscr{F}(1) \exp[i\delta_1(L_A + L_M + L_S)] \quad (4\cdot5)$$

and

$$\mathrm{III} = \mathrm{IV} = -\mathscr{G} \exp[i\delta_1'(L_A + L_M + L_S)] . \quad (4\cdot6)$$

It is immediately observed from equations (4·3) and (4·4) that the scattered intensity changes from its maximum value to its minimum if either the splitter crystal ($\mathbf{d}_{SM}$) or the analyzer ($\mathbf{d}_{MA}$) is shifted with respect to the remaining crystals by the amount of half a Bragg spacing in the direction parallel to **H**. Bonse & Hart (1965*c*) predicted this result using an intuitive argument. The motion of the crystal can be in any direction. Only the projection of the motion toward the **H** direction determines the positions of the alternate maxima and minima. If the mirror crystal is shifted instead with respect to the other crystals, then the scattered intensity repeats its maximum and minimum at every crystal move of a quarter a Bragg spacing. Since the mirror is moved rather than the splitter or analyzer, the optical path length on both sides of the mirror crystal changes as in ordinary optical interferometers, and causes a doubly dense interference pattern. When the three crystals are thick permitting only the anomalous transmission modes to pass the interferometer, the contrast factor reaches 100%.

It has become obvious in the above derivation that the assumptions of thick crystals and of equidistance condition are not really necessary to obtain an interference pattern due to a lattice spacing. At a slight loss of fringe visibility, but with an increase in resultant intensities one can obtain, from an interferometer consisting of the crystals of arbitrary thickness, an interference pattern of the same spacing as discussed above. To prove this, we next consider a general case. The quantities I to IV can be written generally as $|\mathrm{I}| \exp[i\Phi_\mathrm{I}]$ and $|\mathrm{II}| \exp[i\Phi_\mathrm{II}]$ *etc.* Equation (4·1) for example, then reduces to

$$I_0 = |\mathrm{I}|^2 + |\mathrm{II}|^2 + 2|\mathrm{I}||\mathrm{II}| \cos\{\mathbf{H}(\mathbf{d}_{MA} - \mathbf{d}_{SM}) - \Delta(D_M - D_S) + \Phi_\mathrm{I} - \Phi_\mathrm{II}\} . \quad (4\cdot7)$$

Since the quantities |I| and |II| do not depend upon the variable $\mathbf{d}_{MA} - \mathbf{d}_{SM}$, the spacing between a maximum and its adjacent minimum, $\mathbf{X} = (\mathbf{d}_{MA} - \mathbf{d}_{SM})_\mathrm{Max} - (\mathbf{d}_{MA} - \mathbf{d}_{SM})_\mathrm{Min}$ satisfies the condition

$$\mathbf{H} \cdot \mathbf{X} = \pi , \quad (4\cdot8)$$

regardless of the values of crystal thickness, of $D_M - D_S$ and of $\Phi_\mathrm{I} - \Phi_\mathrm{II}$. The same argument holds for I_H obviously.

* In the Bonse & Hart (1965*a*) calculation, the intensities of diffracted beams in maximum transmission always become equal to the maximum dynamical intensity.

(*c*) *Fringe visibility in thin crystal cases*

Contrast factors for fringe visibility may be defined by equations (4·1) and (4·2) as

$$C_0=4|\mathrm{I}||\mathrm{II}|/|\mathrm{I}|^2+|\mathrm{II}|^2 \tag{4·9}$$

in the transmitted direction and

$$C_H=4|\mathrm{III}||\mathrm{IV}|/|\mathrm{III}|^2+|\mathrm{IV}|^2 \tag{4·10}$$

in the Bragg diffracted direction, where | | indicates the modulus of the quantities I to IV. When the crystals are thin, all the modes in each path must be taken into account to evaluate equations (4·9) and (4·10). In general it is tedious to calculate these contrast factors. However, it can be concluded generally that the contrast factors in both directions may be different. In certain special cases (for instance, if the splitter has the same thickness as the analyzer), it can be shown that in both path I and path II a change of mode cannot occur; that is, the mode (say, $i(S)=1$) in the splitter cannot excite a different mode (say, $i(A)=2$) in the analyzer. On the other hand, for paths III and IV such an exchange is allowed. This case gives $|\mathrm{I}|=|\mathrm{II}|$ so that the contrast factor can reach 100% for the transmitted direction. However, the contrast factor for the Bragg diffracted direction cannot reach 100%.

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APPENDIX

Dynamical field functions

In the derivation of the scattering amplitude one needs first to solve the photon Green's function equation, and to evaluate the complex integrals appreaing in the amplitude in terms of their residues. The photon Green's function is a basic quantity describing how a 'photon' propagates in the material especially when the Bragg conditions are nearly satisfied. It is also called the Bragg diffracted propagator. In this paper we are concerned with the case of a single Bragg diffraction where for a given wave-vector $\mathbf{p}$ there is only one reciprocal-lattice vector, either $\mathbf{H}$ or $-\mathbf{H}$, such that the Bragg condition $|\mathbf{p}|=|\mathbf{p}+\mathbf{H}|$ or $|\mathbf{p}-\mathbf{H}|$ is approximately satisfied. In this case, the Fourier transform of the photon Green's function equations can be written

$$\mathrm{M}\mathbf{D}=4\pi\mathbf{E}\,, \tag{A.1}$$

where

$$\mathrm{M}=\begin{pmatrix}\Omega(\mathbf{q}-\mathbf{H}) & -v(-\mathbf{H}) & 0\\ -v(+\mathbf{H}) & \Omega(\mathbf{q}) & -v(-\mathbf{H})\\ 0 & -v(+\mathbf{H}) & \Omega(\mathbf{q}+\mathbf{H})\end{pmatrix}, \tag{A.2}$$

$$\mathbf{D}=\begin{pmatrix}D_{-\mathbf{H}}(\mathbf{q})\\ D_{\mathbf{O}}(\mathbf{q})\\ D_{+\mathbf{H}}(\mathbf{q})\end{pmatrix} \tag{A.3}$$

and

$$\mathbf{E}=\begin{pmatrix}0\\ 1\\ 0\end{pmatrix}. \tag{A.4}$$

The quantity $\Omega(\mathbf{q}+\mathbf{K})$ is given by

$$\Omega(\mathbf{q}+\mathbf{K})=(\mathbf{q}+\mathbf{K})^2-\omega^2-v(\mathbf{O})\,, \tag{A.5}$$

where ω is the energy of the incoming photon, that is, $|\mathbf{p}|$. The solutions $D_{\mathbf{K}}$ are then substituted into the scattering amplitude. They appear as part of integrands, since the scattering amplitude is given in an integral form. The scattering amplitude is then evaluated by contour integration. The residues contain the following functions

$$F_{-\mathbf{H}}[i;\mathbf{p}^t]=(\beta_i+p_z)\times\left[\Omega(\mathbf{q}+\mathbf{H})v(-\mathbf{H})/\frac{\partial}{\partial q_z}\det\mathrm{M}\right]_{\mathbf{q}_t=\mathbf{p}_t;\ q_z=\beta_i} \tag{A.6}$$

$$F_{\mathbf{O}}[i;\mathbf{p}_t]=(\beta_i+p_z)\times\left[\Omega(\mathbf{q}-\mathbf{H})\Omega(\mathbf{q}+\mathbf{H})/\frac{\partial}{\partial q_z}\det\mathrm{M}\right]_{\mathbf{q}_t=\mathbf{p}_t;q_z=\beta_i} \tag{A.7}$$

$$F_{\mathbf{H}}[i;\mathbf{p}_t]=(\beta_i+p_z)\times\left[\Omega(\mathbf{q}-\mathbf{H})v(+\mathbf{H})/\frac{\partial}{\partial q_z}\det\mathrm{M}\right]_{\mathbf{q}_t=\mathbf{p}_t;\ q_z=\beta_i} \tag{A.8}$$

They are called dynamical field functions. The quantity $\beta_i\equiv\beta_i(\mathbf{p}_t)$ which is a function of $\mathbf{p}_t$ is a pole of the complex integrals, and is determined by

$$[\det\mathrm{M}]_{\mathbf{q}_t=\mathbf{p}_t;\,q_z=\beta_i}=0\,. \tag{A.9}$$

This equation is called a dispersion equation which determines the possible modes of the dressed photon created by the incoming photon and the crystal electrons nation. Equation (A.9) can be written in either one of the following forms:

$$\det\mathrm{M}=\begin{cases}\Omega(\mathbf{q}-\mathbf{H})\det m_H(\mathbf{q}) & \text{(A.10)}\\ \Omega(\mathbf{q}+\mathbf{H})\det m_{-H}(\mathbf{q}) & \text{(A.11)}\end{cases}$$

depending on whether $\Omega(\mathbf{q}-\mathbf{H})\gg\Omega(\mathbf{q}+\mathbf{H})$, or $\Omega(\mathbf{q}+\mathbf{H})\gg\Omega(\mathbf{q}-\mathbf{H})$, where

$$\det m_H(\mathbf{q})=\Omega(\mathbf{q})\Omega(\mathbf{q}+\mathbf{H})-v(\mathbf{H})v(-\mathbf{H}) \tag{A.12}$$

and

$$\det m_{-H}(\mathbf{q})=\Omega(\mathbf{q}-\mathbf{H})\Omega(\mathbf{q})-v(\mathbf{H})v(-\mathbf{H})\,. \tag{A.13}$$

In § 3, we have encountered the situation where $\mathbf{p}_t$ in (A.6) to (A.8) is either $\mathbf{p}_{0,t}$ or $\mathbf{p}_{0,t}+\mathbf{H}_t$. If the modes for $\mathbf{p}_{0,t}$ are denoted by $\beta_i(\mathbf{p}_{0,t})\equiv\alpha_i$, then it follows from equations (A.12) and (A.13) that $\beta_i(\mathbf{p}_{0,t}+\mathbf{H}_t)=\alpha_i+H_z$, since

$$[\det m_H(\mathbf{q})]_{\mathbf{q}_t=\mathbf{p}_{0,t};\,q_z=\alpha_i}=[\det m_{-H}(\mathbf{q})]_{\mathbf{q}_t=\mathbf{p}_{0,t}+\mathbf{H}_t;q_z=\alpha_i+H_z}\,. \tag{A.14}$$

Therefore, only one set of α_t's is required to describe $F_{\mathbf{O}}[i,\mathbf{p}_{0,t}]$, $F_{\mathbf{H}}[i,\mathbf{p}_{0,t}]$, $F_{\mathbf{O}}[i,\mathbf{p}_{0,t}+\mathbf{H}_t]$ and $F_{-\mathbf{H}}[i,\mathbf{p}_{0,t}+\mathbf{H}_t]$. Using the quantities defined by equations (3·5) to (3·12) we obtain

$$\left[\frac{\partial}{\partial q_z}\det m_H(\mathbf{q})\right]_{q_t=p_{0,t};\ q_z=\alpha_i} = 4(-1)^i\alpha_i R \qquad (A.15)$$

$$[\Omega(\mathbf{q})]_{q_t=p_{0,t};\ q_z=\alpha_i} = [\Omega(\mathbf{q}-\mathbf{H})]_{q_t=p_{0,t};\ \alpha_i+H_z} = \frac{1}{\tau}\,[\varepsilon+(-1)^i R] \qquad (A.16)$$

$$[\Omega(\mathbf{q}+\mathbf{H})]_{q_t=p_{0,t};\ q_z=\alpha_i} = -[\varepsilon-(-1)^i R]\,. \qquad (A.17)$$

Substituting these results in (A.6) to (A.8) we can obtain equations (3·13) to (3·16) for dynamical field functions.

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Some Properties of the Single-Crystal Rocking Curve in the Bragg Case

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In the present article (i) a new formula for the single-crystal rocking curve for both the centrosymmetric and polar Bragg case is given; (ii) a geometrical construction is derived, whence many properties of the rocking curve are easily visualized; (iii) the different analytical expressions introduced by several authors are shown to be a consequence of different definitions of the variable 'y'.

1. Introduction

The rocking curve (RC) for perfect crystals in the Bragg case has been discussed by many authors. A list of references may be found in well-known books (*e.g.* Zachariasen, 1945; Laue, 1960; James, 1950) or in the articles of Hirsch & Ramachandran (1950), Batterman & Cole (1964) and Bucksch, Otto & Renninger (1967). Although many of these authors follow the treatment of Zachariasen, the expressions in the 'normalized variable y'* differ slightly one from the other.

The first difference was pointed out by Hirsch & Ramachandran (1950). Their expression is more general than that of Zachariasen, and the discrepancy is shown to be a consequence of some approximations. Cole & Stemple (1962) derived a general expression for both the centrosymmetric and polar case and Bucksch, Otto & Renninger (1967) made a physical analysis of it. In their paper (p. 508) one reads (in a loose translation) – 'For small g and κ† the tails of the RC approach the Darwin curve asymptotically from below. But for greater g and κ they rise above this curve.'

On the other hand, Battermann & Cole (1964, p. 707) state 'The Darwin–Prins curve matches the Darwin curve only at a point close to the low angle slope of the peak. It is less than the Darwin curve at all other points'. Since they also use some approximations (κ) the last statement seems to be their consequence. These two statements are rather contradictory. Therefore in the first part of the present article we shall follow Batterman & Cole's (1964) (hereafter BC) derivation, showing that their statement is quite general, and we shall derive a modified formula for the RC.

In the second part we shall give a simple geometrical construction by means of which one can visualize many interesting properties of the RC.

Finally we shall show, that by redefining the 'normalized variable y' by means of a linear transformation, one gets the formulae of Hirsch & Ramachandran and Cole & Stemple, and thus the statement of Bucksch, Otto & Renninger will be brought into agreement with that of BC.

2. Derivation of the general formula

By definition the RC is the ratio of the diffracted and incident power plotted as a function of deviation from the Bragg angle $\theta-\theta_B$, *i.e.*

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* By 'normalized y' we mean a linear transform of the deviation from the Bragg angle such that the range of total reflexion lies between $y=-1$ and $y=1$

† Defined as

$$\kappa = \left|\frac{F_H''}{F_{H'}}\right|,\quad g = -\tfrac{1}{2}\,\frac{1-b}{|b|^{1/2}|P|}\cdot\frac{F_0''}{|F_{H'}|}\,.$$