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The Dynamic Potentials in Electron Diffraction

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The dynamic potentials used in the two-beam theory of electron diffraction are re-derived by using the integral equation rather than the fundamental equations. It is thereby ensured that the weak beams also satisfy the boundary conditions. The dynamic potentials thus obtained differ from the previously derived expressions in being complex and dependent on the size and shape of the crystal. As the product of wavelength and thickness tends to zero, convergence to the kinematic result is obtained. Effects of the dynamic potentials, in particular their imaginary (non-Hermitian), part, on the two-beam expressions for a parallel-plate crystal and an infinite wedge are discussed.

1. Introduction

In the two beam-treatment of the dynamic theory in electron diffraction (Bethe, 1928; MacGillavry, 1940; Pinsker, 1953; Kato, 1952*a*) the presence of weak beams is taken into account by real increments to the Fourier coefficients of the potential:

$$\begin{aligned}\Delta U_{00} &= \sum_g{}'' U_g U_{-g}/(k_g^2-k^2)\,,\\ \Delta U_{hh} &= \sum_g{}'' U_{g-h} U_{h-g}/(k_g^2-k^2)\,,\\ \Delta U_{0h} &= \Delta U_{h0}^* = \sum_g{}'' U_g U_{g-h}/(k_g^2-k^2)\,,\end{aligned} \qquad (1)$$

where the summation Σ_g is over all weak beams, i.e. excluding the strong beams, 0 and h. $\mathbf{k}_g=\mathbf{k}_0+\mathbf{g}$ is the wave vector inside the crystal of the weak beam corresponding to the reciprocal-lattice vector $\mathbf{g}/2\pi$. k is the length of the wave vector in vacuum. We have taken the Schrödinger equation in the form

$$\{\nabla^2+k^2+U\}\varphi=0, \quad U=\Sigma U_g \exp[i\mathbf{g}\mathbf{r}]\,. \qquad (2)$$

The expression for the potential obtained on including these terms is usually called the dynamic potential. It has recently been pointed out, by Miyake (1959), that the two-beam theory with inclusion of these additional terms does not converge to the kinematic theory when the product of wave length and thickness of the crystal, λH, tends to zero.

It is the purpose of the present paper to point out that, if attention is paid to the boundary conditions on deriving the ΔU's, these will generally become complex and dependent on the size and shape of the crystal. The ΔU's thus obtained can then be shown to vanish in the limit of thin crystals or short wavelength. Consequently convergence of the two-beam result to the kinematic expression is obtained. Effects of the ΔU's and in particular their imaginary parts on some of the applications of the two-beam theory are discussed.

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2. Derivation of the dynamic potentials

The aim of introducing the dynamic potentials in two-beam theory is to include 2. order interactions involving weak beams in the expressions for the strong beams. In order to achieve this let us write the solution, inside the crystal, of our Schrödinger equation (2) in the form

$$\varphi(\mathbf{r})=\psi_0 \exp[i\mathbf{k}_0\mathbf{r}]+\psi_h \exp[i\mathbf{k}_h\mathbf{r}]+\Delta\varphi\,. \qquad (3)$$

We first want an approximate expression for $\Delta\varphi$, the weak beams, in terms of the amplitudes, ψ_0 and ψ_h of the strong beams. This can be obtained from the integral equation corresponding to (2) with an incident plane wave:

$$\varphi(\mathbf{r})=\exp[ikz]+\int G(\mathbf{r}|\mathbf{r}')\varphi(\mathbf{r}')U(\mathbf{r}')\,d\tau_{\mathbf{r}'}\,. \qquad (4)$$

Here $G(\mathbf{r}|\mathbf{r}')$ is the free-space Greens function:

$$G(\mathbf{r}|\mathbf{r}')=(1/2\pi)^3\int\frac{\exp[i\mathbf{s}(\mathbf{r}-\mathbf{r}')]}{s^2-k^2}\,d\tau_{\mathbf{s}}\,,$$

where the integration over the radial component, s, is understood to be performed along a specified contour in the complex plane (Schiff (1955) or Morse & Feshbach (1953)). Substituting (3) and the Fourier series for the potential into (4) one obtains, when neglecting $\Delta\varphi$ in the integrand,

$$\begin{aligned}\varphi(\mathbf{r})=\exp[ikz]+(1/2\pi)^3\iint\frac{\exp[i\mathbf{s}(\mathbf{r}-\mathbf{r}')]}{s^2-k^2}\\ \times\Sigma(U_g\psi_0+U_{g-h}\psi_h)\exp[i\mathbf{k}_g\mathbf{r}']\,d\tau_{\mathbf{s}}\,d\tau_{\mathbf{r}'}\,,\end{aligned}$$

where $\Delta\varphi$ obviously is to be identified with the terms for which $g\neq h, 0$. Carrying out the integration over $d\tau_{\mathbf{r}'}$,

$$\begin{aligned}\Delta\varphi(\mathbf{r})=(1/2\pi)^3\sum_g{}''\int\frac{\exp[i\mathbf{s}\mathbf{r}]}{s^2-k^2}\\ \times S(\mathbf{k}_g-\mathbf{s})(U_g\psi_0+U_{g-h}\psi_h)\,d\tau_{\mathbf{s}}\,,\end{aligned} \qquad (5)$$

where

$$S(\mathbf{s}) = \int_V \exp\,[i\mathbf{s}\mathbf{r}]\,d\tau_\mathbf{r}$$

is the shape-transform of the crystal. As the crystal size increases, the above expression approaches the expression for the weak beams given in the references; when the crystal thickness go to zero, the terms in $\Delta\varphi$ converge to their kinematic values.

Expressions for ψ_h/ψ_0 and $\mathbf{k}_0$ which include the 2-order effects due to the weak beams can now be obtained by a procedure similar to the standard two-beam treatment. Substitution of (3) with the expression (5) for $\Delta\varphi$ in the Schrödinger equation (2) gives, inside the crystal boundaries,

$$\begin{aligned}&[k^2-k_0^2]\psi_0\exp\,[i\mathbf{k}_0\mathbf{r}]+[k^2-k_h^2]\psi_h\exp\,[i\mathbf{k}_h\mathbf{r}]\\&\quad+[U_0\psi_0+U_{-h}\psi_h]\exp\,[i\mathbf{k}_0\mathbf{r}]\\&\quad+[U_h\psi_0+U_0\psi_h]\exp\,[i\mathbf{k}_h\mathbf{r}]\\&\quad+\sum_g{}''\sum_f(1/2\pi)^3\int(1/(s^2-k^2))\exp\,[i\mathbf{s}\mathbf{r}]S(\mathbf{k}_g-\mathbf{s})\\&\quad\times[U_g\psi_0+U_{g-h}\psi_h]U_f\exp\,[i\mathbf{f}\mathbf{r}]\,d\tau_s=0\,.\end{aligned}\tag{6}$$

Outside the crystal there will be in addition terms $\Sigma''(U_g\psi_0+U_{g-h})\psi_h\exp\,[i\mathbf{k}_g\mathbf{r}]$ from $U\varphi$. Within the crystal, these terms cancel with $[\nabla^2+k^2]\Delta\varphi$. Multiplication with $\exp\,[-i\mathbf{k}_0\mathbf{r}]/V$ and integration over V, and similarly with $\exp\,[-i\mathbf{k}_h\mathbf{r}]/V$ yields the standard form:

$$\begin{aligned}&[\varkappa_0^2-k_0^2]\psi_0+[U_{-h}+\Delta U_{0h}]\psi_h=0,\quad \varkappa_0^2=k^2+U_0+\Delta U_{00},\\&[U_h+\Delta U_{h0}]\psi_0+[\varkappa_h^2-k_h^2]\psi_h=0,\quad \varkappa_h^2=k^2+U_0+\Delta U_{hh},\end{aligned}\tag{7}$$

where the ΔU's now take the form

$\Delta(k)$,

$$\Delta U_{em}=\sum_g{}''U_{g-m}U_{e-g}T(\mathbf{k}_g,k)\,,\tag{7a}$$

$\Delta(k)$,

$$T(\mathbf{k}_g,k)=(1/V(2\pi)^3)\int\frac{|S(\mathbf{s}-\mathbf{k}_g)|^2}{s^2-k^2}\,d\tau_s\,,\tag{7b}$$

where the integration along the radial coordinate must be performed along the same contour as in the Green's function integral. For a general discussion of the form (7b), which is identical with the second integral in the Born series for the scattering amplitude, see Morse & Feshbach (1953).

In general T will be complex due to the contribution from the pole at $|s|=k$. Only for an infinite crystal, where the transform contracts to a δ-function will we get

$$T_{\text{inf}}=1/(k_g^2-k^2)\,,$$

which leads to the previous result, equation (1). As will be shown below, however, the integrated effect of the imaginary part of the ΔU's will *not* vanish as the thickness goes to infinity.

3. Parallel-plate crystal, Laue case

A parallel-plate with the z-axis normal to the plate can be described by the shape transform,

$$S(\mathbf{s})=8\pi^2\delta(s_x)\delta(s_y)\sin\,(\tfrac{1}{2}s_zH)/s_z\,,$$

where H is the thickness of the plate. Substitution of this form in equation (7b) makes the integrations in the x- and y-directions in reciprocal space trivial. The integration in the z-direction must be performed along a contour in the complex s_z-plane, consistent with the contour for the radial integration in the Green's function, see Fujiwara (1959). The contour is shown in Fig. 1(*b*); the pole at the origin arises

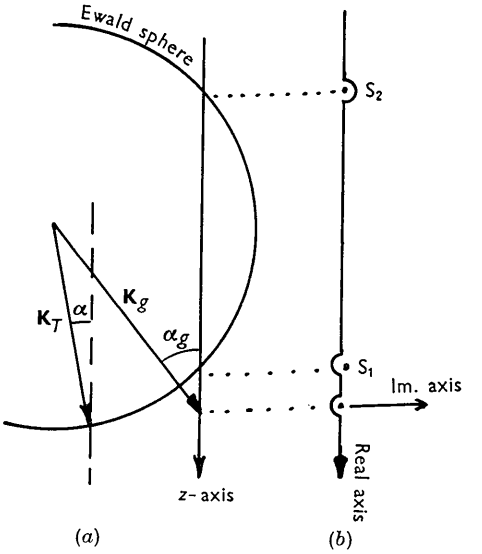

Fig. 1. (*a*) Wave vectors and angles, part 3. (*b*) Contour for integration along the z-direction in reciprocal space.

because the square of the shape-transform must be written as a sum of two terms the integrals of which vanish along infinite semi-circles in the upper and lower half plane respectively:

$$\begin{aligned}T(\mathbf{k}_g,k)&=\frac{2}{H}\int_{-\infty}^{\infty}\frac{\sin^2\,(\frac{1}{2}s_zH)\,ds_z}{\pi s_z^2[s_z^2+2s_zk_{gz}-(k^2-k_g^2)]}\\&=\frac{1}{2H}\int_{-\infty}^{\infty}\frac{(1-\exp\,[is_zH])+(1-\exp\,[-is_zH])}{\pi s_z^2[s_z-s_1][s_z-s_2]}\,ds_z\,.\end{aligned}$$

Closing the contour for the two terms in the numerator in the upper and lower half plane respectively, one obtains

$$\begin{aligned}T(\mathbf{k}_g,k)=1/(k_g^2-k^2)&+i(1-\exp\,[is_1H])/Hs_1^2(s_1-s_2)\\&+i(1-\exp\,[is_2H])/Hs_2^2(s_1-s_2)\,,\end{aligned}\tag{8}$$

where $s_{1,2}=-k_{gz}\pm(k_{gz}^2-k_g^2+k^2)^{\frac{1}{2}}$, see Fig. 1(*a*).

The last term in (8) corresponds to back-scattering and is negligible unless the s_z-axis through the end-point of k_g is nearly tangential to the Ewald sphere, a condition which for small excitation errors, $\zeta_g=|k_g|-k$, only obtains near glancing incidence, see Fig. 1(*a*).

Neglecting this case, however, we can introduce the usual approximations:

$$k_g^2-k^2\simeq 2k\zeta_g,\ \cos\alpha\simeq\cos\alpha_g,$$
$$s_1\simeq-\zeta_g/\cos\alpha,\ s_2\simeq-2k_{gz},$$

and obtain

$$T(\mathbf{k}_g,k)\simeq(1/2k\zeta_g)\times[1+(i\cos\alpha/H\zeta_g)(1-\exp[-iH\zeta_g/\cos\alpha])]\,. \quad (9)$$

The limiting form of T as H decreases is found by expanding the exponential as a power series in H:

$$T=iH/4k_{gz}+O(H^2)\,, \quad (9b)$$

which shows that the ΔU's go to zero as the thickness goes to zero. The same limiting form obtains when the wave-length goes to zero in such a way that $k_g^2-k^2\simeq 2k\zeta_g$ stays finite. It is found quite generally that

$$U_{00},\ U_{hh}\to U_0 \quad\text{and}\quad U_{h0},\ U_{0h}\to U_h \quad\text{as}\quad \lambda H\to 0\,,$$

from which it may be concluded that the kinematic expression for the diffracted intensity is also a limiting case for the two-beam dynamic result including the second-order interaction with the weak beams.

A limiting form similar to (9*b*) can also be obtained from the expression (8) which includes back scattering. Expanding both exponentials as power series one finds

$$T(\mathbf{k}_g,k)\to iH/(s_1-s_2)\,.$$

This result is, however, meaningless unless s_2H as well as $s_1H\ll 1$. For realistic thicknesses this condition can only be obtained when $\mathbf{k}_g$ is nearly parallel to the plate (cf. Fig. 1(*a*)).

To investigate the effect on the diffracted intensity of the complex ΔU's, these must be introduced in the dispersion equation corresponding to (7), a procedure adopted by Yoshioka (1957) in his study of complex potentials arising from inelastic interactions. The real parts can be incorporated in the Fourier coefficients as in standard treatments (see for example Pinsker (1953), Kato (1952)). We shall below assume this to be done.

On writing the wave vectors inside the crystal in the form

$$\mathbf{k}_0+i\mathbf{l},\ \mathbf{k}_0+\mathbf{h}+i\mathbf{l}\,,$$

where $\mathbf{k}_0$ and $\mathbf{l}$ are real, we can collect real and imaginary terms from the dispersion equation when the imaginary terms are small, so that their squares and products can be neglected, we obtain

$$Re:\ [\varkappa_0^2-k_0^2][\varkappa_h^2-k_h^2]=(Re\{U_{0h}\})^{2*}$$
$$Im:\ 2\mathbf{l}.\mathbf{k}_0(\varkappa_h^2-k_h^2)+2\mathbf{l}.\mathbf{k}_h(\varkappa_0^2-k_0^2)$$
$$=Im\{\Delta U_{00}\}(\varkappa_0^2-k_0^2)+Im\{\Delta U_{hh}\}(\varkappa_h^2-k_h^2)\mp 2Im\{\Delta U_{0h}\}Re\{U_{0h}\}\,. \quad (10)$$

* This appiies strictly speaking to centrosymmetric crystals only. For noncentrosymmetric crystals we should have to write "the Hermitian part of U_{0h}."

The first of these equations gives the same dispersion surface as would be obtained if the imaginary parts were neglected. The second equation gives the imaginary part of the wave vector in the direction of wave propagation, as the left-hand side can be written as a scalar product of $\mathbf{l}$ and a vector normal to the dispersion surface. The two signs correspond to the two branches of the dispersion surface, the upper sign relating to the branch nearest to the Laue point. In practical cases $\mathbf{k}_0$ and $\mathbf{k}_h$ are nearly parallel and hence

$$\mathbf{l}.\mathbf{k}.\simeq\mathbf{l}.\mathbf{k}_h\simeq(1/2|\xi+\eta|)\sum_g{}''(|U_g|^2.|\xi|+|U_{h-g}|^2|\eta|\mp 2|U_g|.|U_{g-h}|Im\{T(\mathbf{k}_g;k)\}$$
$$=\sum_g{}''\frac{(|U_g|\sqrt{|\xi|}\mp|U_{h-g}|\sqrt{|\eta|})^2}{4|\xi+\eta|k\zeta_g^2H/\cos\alpha}(1-\cos[\zeta_gH/\cos\alpha])\,, \quad (10a)$$

where we have substituted the expressions (7*a*) for ΔU_{00} etc., taken T from equation (9) and introduced the usual approximations (see Kato, 1952*a*)

$$\varkappa_0^2-k_0^2=2k(\varkappa_0-|k_0|)=2k\xi,\ \varkappa_h^2-k_h^2=2k\eta\,.$$

Boundary conditions for the parallel plate can now be applied in the standard way. In the notation used by Kato (1952*a*) we obtain the amplitude of the diffracted beam

$$\psi_h=C\sum_{j=1}^{2}(-1)^j\exp[i(\mathbf{k}_h^{(j)}+i\mathbf{l}^{(j)})\mathbf{n}H],\quad C=c^{(1)}c^{(2)}/(c^{(1)}-c^{(2)})\,, \quad (11)$$

where $c^{(j)}=\psi_h^{(j)}/\psi_0^{(j)}$. The superscripts refer to the two branches of the dispersion surface and $\mathbf{n}$ is a unit vector normal to the crystal plate. From the tangential continuity of the wave vectors, $\mathbf{l}$ is parallel to $\mathbf{n}$. When the imaginary parts are small, as assumed above, the effect of $Im\{\Delta U_{00}\}$ etc. on C is negligible, and the intensity is found to be:

$$I_h=|U_{0h}|^2/(\zeta_h^2+|U_{0h}|^2)\times[\exp[-(l^{(1)}+l^{(2)})H]\sin^2(|k_h^{(1)}-k_h^{(2)}|\cdot\tfrac{1}{2}H)+\tfrac{1}{2}(\exp[-l^{(1)}H]-\exp[-l^{(2)}H])]\,.$$

The second term in the parenthesis will usually be small, so that the main effect of the imaginary part of the apparent or dynamic potential will be a modulation of the $\sin^2$ or pendulum solution by the first exponential. The argument of the exponential must be computed from equation (10*a*). To study the magnitude of the modulation, consider the case when the incident beam is nearly normal to the plate. Then $\xi^{(1)}\simeq-\eta^{(2)}$, $\xi^{(1)}\simeq-\eta^{(2)}$, and hence

$$H(l^{(1)}+l^{(2)})\simeq\sum_g{}''(|U_g|^2+|U_{g-h}|^2)\times(1-\cos[H\zeta_g])/4k^2\zeta_g^2\,. \quad (12)$$

Inserting the typical values of 1 Å^{-2} ($\sim$ 4 volt) for each of the Fourier coefficients U_g and U_{g-h} and $\zeta_g=0{\cdot}02$, a probable value for a 'systematic interaction' (Hoerni (1956)), we find the corresponding

term in the sum to be of the order 0·25, when $H\zeta_g = (2n+1)\pi$, i.e. with a thickness period of ~ 300 Å. This period is of the same order of magnitude as that of the pendulum solution for strong reflections. For non-systematic interaction an estimate of the average effect as a function of thickness can be obtained by integrating (12) over ζ_g. When the argument (12) is small for all ζ_g the average turns out to be

$$\exp\left[-(l^{(1)}+l^{(2)})H\right]_{(non\text{-}syst.)} \simeq \exp\left[-\sum_g \left[(|U_g|^2+|U_{g-h}|^2)H/2k^2 s_g\right]\right],$$

where s_g is the distance from the reciprocal-lattice point $(1/2\pi)\mathbf{g}$ to the line through the reciprocal lattice-point $(1/2\pi)\mathbf{h}$ and the origin. This latter form is seen to be an absorption term of standard type.

It may be mentioned that the thickness-dependent part of the real part of the ΔU's (cf. equation (9)) gives rise to an oscillating increment in the argument of the $\sin^2$ in the pendulum solution. This increment is readily found to be

$$\sum_g (|U_g|^2+|U_{h-g}|^2)\sin(H\zeta_g)/8k^2\zeta_g^2,$$

under the conditions when (12) is valid. The order of magnitude may amount to a few degrees.

4. Crystal wedge

The most general two-beam treatment of electron diffraction from a wedge is given by Kato (1952*a*, *b*), and we shall make extensive use of his results. It will be assumed throughout that the wave vectors involved have appreciable components along both normals to the wedge faces in order that back-scattering terms can be neglected, and that the Ewald sphere may be approximated by a plane in the vicinity of the reciprocal lattice point g.

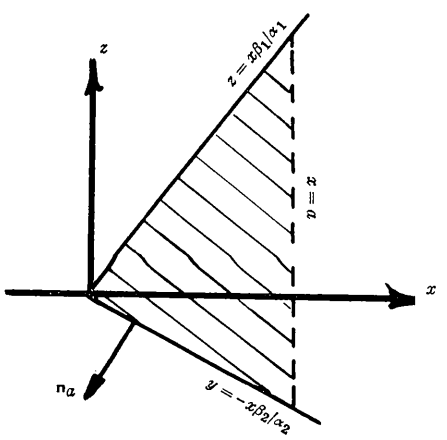

Fig. 2. Coordinates and notations for the wedge, part 4.

Introducing the shape transform of the wedge, Fig. 2

$$S(\mathbf{s}) = 2\pi\delta(s_y)/(\alpha_1 s_x+\beta_1 s_z)(\alpha_2 s_x-\beta_2 s_z), \quad \alpha_1\beta_2+\alpha_2\beta_1 = 1,$$

and performing the integrations in (5), we obtain

$$\Delta\varphi(r) = -\sum_g{}''[1-\exp[i\zeta_{gz}(z-x\beta_1/\alpha_1)]] \quad (U_g\psi_0+U_{g-h}\psi_h)\exp[i\mathbf{k}_g\mathbf{r}]/2k\zeta_g$$

by a suitable definition of contours. To obtain T we shall integrate over part of the wedge, defined by $x<a$ cf. Fig. 2. The rest of the wedge may be considered to be covered by an opaque screen, following Kato (1952*a*). There results

$$T = [1+2i/\zeta_{gz}H_m - 2(1-\exp[-i\zeta_{gz}H_m])/\zeta_{gz}^2 H_m^2]/2k\zeta_g$$

where H_m is the thickness in the z-direction at $x=a$.

Again it is seen that T and hence the ΔU's vanish as the dimension of the crystal goes to zero. For a crystal of appreciable size, the last term will be negligible, whereas the second term will give rise to an integrated effect, as in the case of a parallel plate. To find this effect, we may follow the procedure given by Kato (1952*b*) for calculation of the refraction effects from a limited wedge. It will be assumed that ΔU is a slowly varying function of the position on the dispersion surface.

Kato's (1952*a*, *b*) procedure leads to the integral expression

$$\psi_h^{(j)} = \frac{(-1)^{(j)}}{(2\pi)^4} C \iiint \exp[i(\mathbf{K}_r-\mathbf{k}_0^{(i)})\mathbf{r}_e + (\mathbf{k}_h^{(j)}-\mathbf{K}_h)\mathbf{r}_a]\, df_{ra}\, df_{re}\, df_{k_0^{(j)}}, \quad (13)$$

where C has the same mening as in equation (11), $\mathbf{K}_r$ and K_h are the wave vectors in vacuum of the incident and reflected beams respectively, $\mathbf{k}_0^{(j)}$ and $\mathbf{k}_h^{(j)}$ are wave vectors in the crystal and $\mathbf{r}_e$ and $\mathbf{r}_a$ are position vectors on the entrance and exit face. Kato shows this to transform into (apart from uninteresting phase factors)

$$\psi_h^{(j)} = \frac{(-1)^{(j)}}{(2\pi)^2 n_{az}} C \int \exp[i\Delta^{(j)}\sigma]\, df_\sigma, \quad (14)$$

where $\Delta^{(j)}$ is the vectorial difference between $\mathbf{k}_h^{(j)}$ and the wave-vector $\mathbf{k}_{h0}^{(j)}$ determined by the boundary conditions for an infinite wedge, and σ is a vector parallel to the plane tangential to the dispersion surface at the wave point corresponding to an infinite wedge. Substituting $\mathbf{k}_0^{(j)}+i\mathbf{l}^{(j)}$ for $\mathbf{k}_0^{(j)}$ and similarly for $\mathbf{k}_h^{(j)}$ in equation (13) we obtain in the same way,

$$\psi_h^{(j)} = \frac{(-1)^j}{(2\pi)^2 n_{az}} C \int \exp[i\Delta^{(j)}\sigma]\exp[-l^{(j)}z']\, df_\sigma, \quad (14a)$$

where z' is the length inside the crystal of the normal to df_σ. This normal will be nearly parallel to the z-axis, and so we make approximation

$$z' \simeq (\alpha_1/\beta_1+\alpha_2/\beta_2)x, \quad df_\sigma \simeq dx\,dy,$$

to obtain

$$\psi_h^{(j)} \simeq \frac{(-1)^j}{n_{az}} C \frac{\exp[i\Delta_x^{(j)}a]\exp[-l^{(j)}H_m]-1}{i\Delta_x^{(j)}-l^{(j)}H_m/a}.$$

Omitting the factors in front, the integrated intensity is found to be

$$I^{(j)} \sim [1-\exp(-2l^{(j)}H_m)]/2l^{(j)}H_m ,$$

which is the correction factor to the integrated intensity of the two dynamic refraction spots. From the first of equations (10*a*) it is seen that this factor may differ appreciably for the two spots. Considering, as a very simple example, the same numerical values as used in the end of section 3, we find that near the Bragg angle the outer refraction spot, $j=2$, will be reduced in intensity by a factor $\sim 0{\cdot}8$ whereas the inner spot will be only very slightly reduced in intensity. Such differences in intensity between the refraction spots are frequently observed, the outer spot invariably being the weaker (Honjo & Mihama (1954)). An explanation for this effect in terms of inelastic interaction has been offered by Yoshioka (1957), but the intensity differences calculated from his theory appears considerably smaller.

5. Conclusion

The above derivation of the dynamic potentials in the two-beam theory appears to resolve the discrepancy pointed out by Miyake (1959) between the limiting results as $\lambda H \to 0$ for the two-beam theory and the n-beam theories of Cowley & Moodie (1957), Fujiwara (1959) and Fujimoto (1959). It may be well to point out, however, that the limit $H \to 0$ will not always have a clear physical meaning, especially for crystals containing more than one kind of atom, as demonstrated experimentally and theoretically by Cowley & Kuwabara (1962), the limit $H \to 0$ being then purely formal.

It may appear surprising that complex wave vectors appear in a problem which is known to be soluble in terms of (an infinite number) of real wave vectors. This apparent contradiction is superficial; in the multiple wave-field picture the imaginary parts of the wave vectors represent the effect of interference between the neglected wave fields and the two wave fields of the two-beam theory. This effect can evidently be described by a periodic reduction in amplitude, as seen from equation (12). The effect of the imaginary parts of the ΔU's is thus a 'beating' of the two-beam solution, not an absorption, except for very thin crystals, where T is proportional to H.

In the 'multiple elastic scattering' picture (Fujiwara, 1959) the description is different; there the present theory for the direct and the diffracted beam, h, includes all terms which contain the beams $g \neq h, 0$, less than three times and hence all second-order terms. The present results must accordingly converge to the kinematic result *in the same way* as in the phase-object approximation (Cowley & Kuwabara op. cit.) or a Born series. This is indeed found to be so by comparing e.g. equation (9) with corresponding terms from these theories.

The difference between the present treatment and the one given in the references (Pinsker, 1953; MacGillavry, 1940; Kato, 1952*a*) lies in the method of expressing the weak beams in terms of the two strong ones. This has usually been accomplished by solving the g'th fundamental equation with regard to ψ_g, thereby introducing weak beams which fail to satisfy the boundary conditions. We have instead employed the integral equation corresponding to the problem, and hence ensured that the weak beams also conform to the boundary conditions. In addition we find it questionable whether the terms

$$\sum_{f \neq g, h, 0} U_{g-f}\psi_f$$

neglected in the fundamental equation will always be less than the diagonal term $U_0\psi_g$.

It may finally be mentioned that the procedure employed here can be considered as a first step in an iterative procedure, as the $\Delta\varphi$ as given by equation (5) may be reinserted in the integral equation to provide a better approximation for $\Delta\varphi$ and hence for the strong beams. Such a procedure may proceed along lines similar to the Born-series treatment carried out by Fujiwara (1959).

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