

is determined by the expression

$$\mu_{aT} = [\mu_T^{(1)}(\mathbf{k}, \mathbf{k}) - \mu_T^{(1)}(\mathbf{k}, \mathbf{k}_1)] + \mu_T^{(2)}(\mathbf{k}, \mathbf{k}). \quad (4.9)$$

Thus, the result (4.8) contains contributions to the anomalous coefficient of absorption from every of the most essential processes of X-ray interaction with matter. This expression clearly shows that the absorption connected with the photo-effect and the Compton scattering have the same temperature dependence. (We note that the Compton scattering cross-section in the commonly used range of X-ray energies is as a rule, small compared with the photo-effect cross-section.) Such temperature dependence of absorption in the problem concerned with the anomalous transmission has for the first time been consistently derived by the present authors (Afanas'ev & Kagan, 1965) and independently by Ohtsuki (1964). (The situation considered in the paper by Afanas'ev & Kagan was equivalent to the case when $\varepsilon_0 = 1$).

The second term in (4.8) has quite another dependence on the phonon spectrum and on the temperature.

Generally speaking, this term is as a rule small compared with the first one. Nevertheless, its contribution to the total coefficient of absorption is rather important, being greater than the error with which μ_a is measured.

For example, in the case of reflexion from the plane (220) in monocrystalline germanium the magnitude of the second term in (4.8) is approximately 4% of that of the first for the line $K\alpha_1$ of copper ($\lambda = 1.5405 \text{ \AA}$). In a recent paper by Efimov (1968) refined measurements of the anomalous absorption coefficient tem-

perature dependence have been carried out for this case. As was shown by Efimov, the account of the contribution from inelastic scattering by phonons markedly affects the analysis of the relevant experimental results.

It is interesting to emphasize that the relative importance of μ_{aT} sharply increases with the increase of the ratio between the elastic scattering cross-section and the cross-section of photo-absorption. This circumstance provides interesting possibilities for carrying out experiments in which the first and the second terms in the anomalous absorption coefficient (4.8) are of the same order of magnitude.

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Ewald's and von Laue's Dynamical Theories of X-Ray Diffraction

BY H. WAGENFELD*

School of Physics, University of Melbourne, Parkville, N.2, Victoria, Australia

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Ewald's and von Laue's dynamical theories of X-ray diffraction are discussed. Ewald derived the dispersion equations with a microscopic theory (classical electron theory), whereas von Laue used a phenomenological macroscopic approach (Maxwell's theory). As is to be expected, the dispersion equations of the two theories agree if one chooses the same physical model for the electromagnetic resonators, *i.e.* point dipoles or atoms.

Introduction

Only two years after the discovery of X-ray diffraction in crystals, Darwin (1914) pointed out that von Laue's kinematical theory (von Laue, Friedrich & Knipping, 1912, 1913) does not give the correct intensities at the interference maxima. He furthermore developed a very elegant, although limited, method for the understand-

ing of X-ray diffraction in perfect crystals. In order to derive a self-consistent dynamical theory of X-ray diffraction in perfect crystals, Ewald (1917) used some of the results of his theoretical treatment of the dispersion and double refraction of light in crystals (Ewald, 1916). The theory is based on the classical electron theory. Lohr (1924) avoided any atomic theory for crystals and published a dynamical theory of X-ray diffraction which was based on Jaumann's continuum theory. It is here only assumed that the crystal has an atomic structure. However the treatment is very com-

* On sabbatical leave at the Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin-Dahlem, Germany.

plicated and was not used for any practical purpose.

Schlapp (1926) developed a dynamical theory for a linear continuous and periodic electric permittivity. The formulation of the dynamical theory of X-ray diffraction nowadays mostly used is due to von Laue (1931). He solved Maxwell's equations for a continuous and periodic electric susceptibility.

Both Ewald (1937) and von Laue (von Laue & Wagner, 1960), have been aware of the fact that their final results are identical if one uses the same model for the crystal (*i.e.* whether one uses for the electromagnetic resonators within the crystal electric point dipoles or atoms with a spatial electron-charge distribution). The difference between Ewald's and von Laue's formulation is that Ewald derived the dispersion equations with a microscopic theory, whereas von Laue used a macroscopic and phenomenological procedure. The quantum-mechanical justification for von Laue's approach was given by Kohler (1935).

In order to show that the final results of Ewald's and von Laue's theory are the same if one chooses the same crystal model, we first derive the dispersion equations for point dipoles and atoms on the basis of Ewald's microscopic theory and then we briefly discuss von Laue's theory.

For the derivation of the dispersion equations we use a simplified method which corresponds to that given recently by Ewald (1965). For a more rigorous treatment, particularly concerning the summation of lattice potentials, we refer to the papers by Ewald (1916, 1917, 1921) and Born (1923).

A formal difference between the two theories is that Ewald's dispersion equations are expressed in terms of 'vectorial structure amplitudes' (which are identical with the Fourier amplitudes of the vector of the electric polarization if the resonators are atoms), whereas von Laue formulates these equations in terms of the Fourier amplitudes of the vector of the electric displacement.

There will be no further discussion of the dispersion equations, since von Laue in general used Ewald's method here.

Ewald's treatment

In order to calculate the radiation field of an atom or an oscillating electric dipole, it is convenient to use the wave equation in terms of Hertz's vector potential \mathbf{Z} .* In Gaussian units the wave equation has the form:

* The Hertz vector \mathbf{Z} is defined by the equations

$$\mathbf{A} = -\frac{1}{c} \dot{\mathbf{Z}}, \quad -\operatorname{div} \mathbf{Z} = \frac{1}{c} \dot{\phi}$$

(\mathbf{A} vector potential, ϕ scalar potential, with $\mathbf{E} = (-1/c)\dot{\mathbf{A}} - \nabla\phi$ and fulfils the Lorentz gauge

$$\operatorname{div} \mathbf{A} = \frac{1}{c} \dot{\phi}.$$

Wave equation (1) follows from Maxwell's equations, if one puts the dissipative current term equal to zero and the magnetic permeability equal to one.

$$\nabla^2 \mathbf{Z} - \frac{1}{c^2} \ddot{\mathbf{Z}} = -4\pi \mathbf{P}. \quad (1a)$$

Here is \mathbf{P} the vector of the electric polarization of the atom. The solution of (1a) is given by

$$\mathbf{Z}(\mathbf{r}) = \int \mathbf{P}(\mathbf{r}') \frac{\exp(2\pi i K |\mathbf{r} - \mathbf{r}'|)}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}', \quad (2a)$$

with $K = 1/\lambda$ and λ vacuum wavelength. The integration has to be carried out over the spatial extension of the atom.

In Ewald's dynamical theory the atoms are replaced by point dipoles. If a point dipole of the type s and the electric moment \mathbf{p}_i^s is situated within the crystal at the position $\mathbf{r}_i^s = \mathbf{R}_l + \mathbf{r}_s$ ($\mathbf{R}_l = \sum_{i=1}^3 l_i \mathbf{a}_i$, lattice vector to the l th unit cell, l_i integers and \mathbf{r}_s the vector from the origin of the unit cell to the atom of type s within the unit cell), then equation (1a) can be written:

$$\nabla^2 \mathbf{Z} - \frac{1}{c^2} \ddot{\mathbf{Z}} = -4\pi \mathbf{p}_i^s \delta(\mathbf{r} - \mathbf{R}_l - \mathbf{r}_s). \quad (1b)$$

Here $\delta(\mathbf{r} - \mathbf{R}_l - \mathbf{r}_s)$ is Dirac's δ function.

The solution of (1b) is given by

$$\mathbf{Z}_i^s(\mathbf{r}) = \mathbf{p}_i^s \frac{\exp(2\pi i K |\mathbf{r} - \mathbf{R}_l - \mathbf{r}_s|)}{|\mathbf{r} - \mathbf{R}_l - \mathbf{r}_s|}. \quad (2b)$$

One obtains for the total radiation field at the position \mathbf{r} :

$$\mathbf{Z}(\mathbf{r}) = \sum_l \sum_s \mathbf{Z}_i^s = \sum_l \sum_s \mathbf{p}_i^s \frac{\exp(2\pi i K |\mathbf{r} - \mathbf{R}_l - \mathbf{r}_s|)}{|\mathbf{r} - \mathbf{R}_l - \mathbf{r}_s|}. \quad (3a)$$

Before we discuss this expression, we formulate the corresponding equation for an atom. According to equation (2a) this is given by

$$\mathbf{Z}(\mathbf{r}) = \sum_l \sum_s \int \mathbf{P}_i^s(\mathbf{r}') \frac{\exp(2\pi i K |\mathbf{r} - \mathbf{r}' - \mathbf{R}_l - \mathbf{r}_s|)}{|\mathbf{r} - \mathbf{r}' - \mathbf{R}_l - \mathbf{r}_s|} d^3 \mathbf{r}'. \quad (3b)$$

Ewald writes for the dipole moment of an oscillator at the position \mathbf{r}_i^s :

$$\mathbf{p}_i^s = \mathbf{p}_s \exp(2\pi i \mathbf{k}_0 \cdot \mathbf{r}_i^s) = \mathbf{p}_s \exp[2\pi i \mathbf{k}_0 \cdot (\mathbf{R}_l + \mathbf{r}_s)]. \quad (4)$$

An equivalent relation then holds also for the vector of the electric polarization of an atom at the same position. If we introduce the Fourier transform for the spherical wave into equation (3a), then we obtain:

$$\mathbf{Z}(\mathbf{r}) = \frac{1}{\pi} \sum_l \sum_s \mathbf{p}_s \exp[2\pi i \mathbf{k}_0 (\mathbf{R}_l + \mathbf{r}_s)] \int \frac{\exp[2\pi i \mathbf{k} \cdot (\mathbf{r} - \mathbf{R}_l - \mathbf{r}_s)]}{k^2 - K^2} d^3 \mathbf{k}, \quad (5a)$$

and consequently for equation (3b)

$$\mathbf{Z}(\mathbf{r}) = \frac{1}{\pi} \sum_l \sum_s \exp(2\pi i \mathbf{k}_0 \cdot (\mathbf{R}_l + \mathbf{r}_s)) \int \int \frac{\exp[2\pi i \mathbf{k} \cdot (\mathbf{r} - \mathbf{r}' - \mathbf{R}_l - \mathbf{r}_s)]}{k^2 - K^2} \mathbf{P}_i^s(\mathbf{r}') d^3 \mathbf{r}' d^3 \mathbf{k}. \quad (5b)$$

In both equations (5a) and (5b) the summation over l leads to the relation

$$\sum_l \exp[2\pi i(\mathbf{k}_0 - \mathbf{k}) \cdot \mathbf{R}_l] = \frac{1}{V_a} \delta^3(\mathbf{k} - \mathbf{k}_0). \quad (6)$$

$V_a = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)$ is the volume of a unit cell. Because of equation (6), the integration over \mathbf{k} space is changed into a summation over the reciprocal lattice and consequently one obtains for \mathbf{k} the relation

$$\mathbf{k} = \mathbf{k}_h = \mathbf{k}_0 + \mathbf{h}. \quad (7)$$

$\mathbf{h} = \sum_{i=1}^3 h_i \mathbf{b}_i$ is a reciprocal lattice vector.

It follows now for (5a):

$$\mathbf{Z}(\mathbf{r}) = \frac{1}{\pi V_a} \sum_h \frac{\exp(2\pi i \mathbf{k}_h \cdot \mathbf{r})}{k_h^2 - K^2} \left\{ \sum_s \mathbf{p}_s \exp(-2\pi i \mathbf{h} \cdot \mathbf{r}_s) \right\}, \quad (8a)$$

and accordingly for (5b):

$$\mathbf{Z}(\mathbf{r}) = \frac{1}{\pi V_a} \sum_h \frac{\exp(2\pi i \mathbf{k}_h \cdot \mathbf{r})}{k_h^2 - K^2} \left\{ \sum_s \exp(-2\pi i \mathbf{h} \cdot \mathbf{r}_s) \int \mathbf{P}_s(\mathbf{r}') \exp(-2\pi i \mathbf{k}_h \cdot \mathbf{r}') d^3 \mathbf{r}' \right\}. \quad (8b)$$

If we now introduce the common notation for point dipoles and for atoms:

$$S_h = \begin{cases} \frac{1}{V_a} \sum_s \mathbf{p}_s \exp(-2\pi i \mathbf{h} \cdot \mathbf{r}_s) & \text{(point dipoles),} \\ \frac{1}{V_a} \sum_s \exp(-2\pi i \mathbf{h} \cdot \mathbf{r}_s) \\ \int \mathbf{P}_s(\mathbf{r}') \exp(-2\pi i \mathbf{k}_h \cdot \mathbf{r}') d^3 \mathbf{r}' & \text{(atoms),} \end{cases} \quad (9a)$$

then equations (8a) and (8b) take the simple form:

$$\mathbf{Z}(\mathbf{r}) = \frac{1}{\pi} \sum_h \frac{\exp(2\pi i \mathbf{k}_h \cdot \mathbf{r})}{k_h^2 - K^2} S_h. \quad (10)$$

Ewald (1937) calls S_h the 'vectorial structure amplitude of the cell'. We see that (10) is a Fourier expansion of the Hertz vector \mathbf{Z} .

$$\mathbf{Z} = \sum_h \mathbf{Z}_h \exp(2\pi i \mathbf{k}_h \cdot \mathbf{r}), \quad (11)$$

with

$$\mathbf{Z}_h = \frac{1}{\pi} \frac{S_h}{k_h^2 - K^2}. \quad (12)$$

In order to calculate the electric field vector \mathbf{E} , we use the relation

$$\mathbf{D} = \text{curl curl } \mathbf{Z}$$

which connects the vector of the electric displacement \mathbf{D} with the Hertz vector \mathbf{Z} . Since for X-rays \mathbf{D} and \mathbf{E} are nearly the same, we obtain

$$\mathbf{E} \simeq \mathbf{D} = \text{curl curl } \mathbf{Z} = -4\pi \sum_h \frac{\mathbf{k}_h \times (\mathbf{k}_h \times \mathbf{S}_h)}{k_h^2 - K^2} \exp(2\pi i \mathbf{k}_h \cdot \mathbf{r}). \quad (13)$$

This is now the Fourier expansion for \mathbf{E} .

$$\mathbf{E} = \sum_h \mathbf{E}_h \exp(2\pi i \mathbf{k}_h \cdot \mathbf{r}), \quad (14)$$

with

$$\mathbf{E}_h = -4\pi \frac{\mathbf{k}_h \times (\mathbf{k}_h \times \mathbf{S}_h)}{k_h^2 - K^2}. \quad (15)$$

The reaction of the radiation field towards an atom of type s at the position $\mathbf{r}_l^s = \mathbf{R}_l + \mathbf{r}_s$ is given by*

$$4\pi \mathbf{p}_l^s = \alpha_s \mathbf{E}(\mathbf{r}_l^s). \quad (16)$$

Here is α_s the polarizability for an atom of type s . From this, together with equation (4), it follows that:

$$4\pi \mathbf{p}_s = \alpha_s \mathbf{E}(\mathbf{r}_s^s) \exp[-2\pi i \mathbf{k}_0(\mathbf{R}_l + \mathbf{r}_s)]. \quad (17)$$

If one introduces equation (17) into equation (9a) or (9b), then one obtains the following expressions for the structure amplitude S_h .

$$S_h = \begin{cases} \frac{1}{4\pi} \sum_{h'} \mathbf{E}_{h'} \left\{ \frac{1}{V_a} \sum_s \exp[-2\pi i(\mathbf{h} - \mathbf{h}') \cdot \mathbf{r}_s] \alpha_s \right\} \\ \frac{1}{4\pi} \sum_{h'} \mathbf{E}_{h'} \left\{ \frac{1}{V_a} \sum_s \exp[-2\pi i(\mathbf{h} - \mathbf{h}') \cdot \mathbf{r}_s] \right. \\ \left. \int \alpha_s(\mathbf{r}') \exp[-2\pi i(\mathbf{h} - \mathbf{h}') \cdot \mathbf{r}'] d^3 \mathbf{r}' \right\}. \end{cases} \quad (18a)$$

The coefficient in the bracket of (18b) is a Fourier coefficient $\chi_{h-h'}$ of the Fourier expansion of the electric susceptibility χ .

$$\chi = \sum_h \chi_h \exp(-2\pi i \mathbf{h} \cdot \mathbf{r}), \quad (19a)$$

with

$$\chi_h = \frac{1}{V_a} \sum_s \exp(-2\pi i \mathbf{h} \cdot \mathbf{r}_s) \int \alpha_s(\mathbf{r}') \exp(-2\pi i \mathbf{h} \cdot \mathbf{r}') d^3 \mathbf{r}'. \quad (19b)$$

In the last expression the integration over the unit cell is separated into a summation over the atoms at positions \mathbf{r}_s within the unit cell and integrations over the atomic polarizabilities α_s .

The coefficient in equations (18a) can be interpreted in the same manner, but now for point dipoles.

If the frequency of the electromagnetic radiation field is large in comparison with the frequency which corresponds to a K shell eigenvalue, then $\alpha_s(\mathbf{r})$ is given by

$$\alpha_s(\mathbf{r}) = - \frac{e^2 q_s(\mathbf{r})}{m\pi v^2}. \quad (20)$$

* Here we have to write strictly

$$4\pi \mathbf{p}_l^s = \alpha_s \mathbf{E}(\mathbf{r}_l^s)$$

where $\mathbf{E}'(\mathbf{r}_l^s) = \mathbf{E}(\mathbf{r}_l^s) - \mathbf{E}_l^s(\mathbf{r}_l^s)$ is the exciting field at the position \mathbf{r}_l^s , but Ewald (1917, 1921) showed that, particularly for X-rays, equation (16) is a very good approximation. In Gaussian units we have

$$\mathbf{p}_l^s = \alpha_s \mathbf{E}(\mathbf{r}_l^s),$$

but in order to identify von Laue's quantity χ with the electric susceptibility of the crystal, we have to write

$$4\pi \mathbf{p}_l^s = \alpha_s \mathbf{E}(\mathbf{r}_l^s),$$

and we therefore use the notation (16).

$\varrho_s(\mathbf{r})$ is the electron charge distribution of the atom. If one introduces this equation into (19b), one obtains*

$$\chi_h = - \frac{e^2 F_h}{V_a \pi m v^2}, \quad (21)$$

with

$$F_h = \sum_s f_s \exp(-2\pi i \mathbf{h} \cdot \mathbf{r}_s) \quad (22)$$

the structure factor and

$$f_s = \int \varrho_s(\mathbf{r}) \exp(-2\pi i \mathbf{h} \cdot \mathbf{r}) d^3\mathbf{r} \quad (23)$$

the atomic scattering factor for an atom with the atomic number Z_s .

For point dipoles α_s has within the above-mentioned approximation the form

$$\alpha_s = - \frac{e^2 Z_s}{m v^2 \pi}, \quad (24)$$

and Ewald (1937) calls the Fourier coefficients corresponding to (19b) A_h .

$$\begin{aligned} A_h &= \frac{1}{V_a} \sum_s \alpha_s \exp[-2\pi i (\mathbf{h} \cdot \mathbf{r}_s)] \\ &= - \frac{e^2}{\pi v^2 m V_a} \sum_s Z_s \exp(-2\pi i \mathbf{h} \cdot \mathbf{r}_s). \end{aligned} \quad (25)$$

The two expressions (21) and (25), together with (22), agree if one replaces Z_s by f_s and *vice versa*. This has already been pointed out by Ewald (1937).

Ewald's structure amplitudes now take the form:

$$\mathbf{S}_h = \begin{cases} \frac{1}{4\pi} \sum_{h'} \mathbf{E}_{h'} A_{h-h'} & (26a) \\ \frac{1}{4\pi} \sum_{h'} \mathbf{E}_{h'} \chi_{h-h'} & (26b) \end{cases}$$

If one inserts into these equations the expression (15) for \mathbf{E}_h , then one obtains the following equations:

$$\mathbf{S}_h = \begin{cases} \sum_{h'} \frac{\mathbf{k}_{h'} \times (\mathbf{k}_{h'} \times \mathbf{S}_{h'})}{k_{h'}^2 - K^2} A_{h-h'} & (27a) \\ \sum_{h'} \frac{\mathbf{k}_{h'} \times (\mathbf{k}_{h'} \times \mathbf{S}_{h'})}{k_{h'}^2 - K^2} \chi_{h-h'} & (27b) \end{cases}$$

With the notation

$$\mathbf{k}_{h'} \times (\mathbf{k}_{h'} \times \mathbf{S}_{h'}) = -k_{h'}^2 \mathbf{S}_{h' \perp \mathbf{k}_{h'}} \quad (28)$$

one obtains finally:

$$\mathbf{S}_h = \begin{cases} \sum_{h'} \frac{k_{h'}^2 A_{h-h'}}{k_{h'}^2 - K^2} \mathbf{S}_{h' \perp \mathbf{k}_{h'}} & (29a) \\ \sum_{h'} \frac{k_{h'}^2 \chi_{h-h'}}{k_{h'}^2 - K^2} \mathbf{S}_{h' \perp \mathbf{k}_{h'}} & (29b) \end{cases}$$

Both equations (29a) and (29b) represent a system of linear and homogenous equations in terms of Ewald's

structure amplitude \mathbf{S}_h . The set of equations (29a) are Ewald's dispersion equations for point dipoles. The system (29b) are the generalized equations for atoms. The result, that for both types of resonators (dipoles and atoms) the structure of the dispersion equations is the same, can be expected and is already mentioned by Ewald (1937).

If we now want to express the equations (29) in terms of \mathbf{E}_h , then we have to apply equation (15) to (26). We obtain:

$$(k_h^2 - K^2) \mathbf{E}_h = \sum_{h'} k_h^2 A_{h-h'} \mathbf{E}_{h' \perp \mathbf{k}_h} \quad (30a)$$

for point dipoles and

$$(k_h^2 - K^2) \mathbf{E}_h = \sum_{h'} k_h^2 \chi_{h-h'} \mathbf{E}_{h' \perp \mathbf{k}_h} \quad (30b)$$

for atoms. In both equations we have used the notation

$$\mathbf{k}_h \times (\mathbf{k}_h \times \mathbf{E}_h) = -k_h^2 \mathbf{E}_{h \perp \mathbf{k}_h}. \quad (31)$$

Let us now briefly review von Laue's treatment (von Laue, 1931; von Laue & Wagner, 1960).

Von Laue's treatment

Von Laue solves the wave equation

$$\nabla^2 \mathbf{D} - \frac{1}{C^2} \ddot{\mathbf{D}} = -4\pi \text{curl curl } \mathbf{P} \quad (32)$$

for the interior of the crystal and assumes that the electric susceptibility has the periodicity of the crystal lattice. Then χ can be expanded in a Fourier series (19a) and the solutions for (32) are vector Bloch waves.

$$\mathbf{D} = \sum_h \mathbf{D}_h \exp(2\pi i \mathbf{k}_h \cdot \mathbf{r}) \quad (33)$$

and

$$\mathbf{P} = \sum_h \mathbf{P}_h \exp(2\pi i \mathbf{k}_h \cdot \mathbf{r}). \quad (34)$$

Equation (32) takes now the form

$$(k_h^2 - K^2) \mathbf{D}_h = -4\pi \mathbf{k}_h \times (\mathbf{k}_h \times \mathbf{P}_h). \quad (35)$$

In order to express these equations only in terms of \mathbf{D}_h , von Laue uses instead of the equation

$$4\pi \mathbf{P} = \chi \mathbf{E}, \quad (36)$$

the approximation*

$$4\pi \mathbf{P} = \chi \mathbf{D}. \quad (37)$$

Together with

$$4\pi \mathbf{P}_h = \sum_{h'} \chi_{h-h'} \mathbf{D}_{h'} \quad (38)$$

and the notation

$$\mathbf{k}_h \times (\mathbf{k}_h \times \mathbf{D}_h) = -k_h^2 \mathbf{D}_{h \perp \mathbf{k}_h}, \quad (39)$$

it follows finally that

$$(k_h^2 - K^2) \mathbf{D}_h = \sum_{h'} k_h^2 \chi_{h-h'} \mathbf{D}_{h' \perp \mathbf{k}_h}. \quad (40)$$

These are von Laue's dispersion equations.

* Equation (21) is identical with von Laue's equation (26.49) (von Laue & Wagner, 1960).

* Since $\mathbf{D} = \mathbf{E} + 4\pi \mathbf{P} = (1 + \chi) \mathbf{E}$, it follows from (37) that $4\pi \mathbf{P}_h = \sum_{h'} \chi_{h-h'} \mathbf{D}_{h'} = \sum_{h'} \chi_{h-h'} \mathbf{E}_{h'} + \sum_{h' m} \chi_{h-h'} \chi_{h'-m} \mathbf{E}_m + \dots$. The error in (37) is therefore of the order $|\chi_h| \approx 10^{-5}$.

Alternatively one can express the dispersion equations in terms of \mathbf{P}_h . In order to do this, we multiply equation (35) by $\chi_{h-h'}$, divide by $(k_h^2 - K^2)$ and sum over h . It follows from this, together with equation (38), and after we have interchanged h with h' , that

$$\mathbf{P}_h = \sum_{h'} \frac{k_{h'}^2 \chi_{h-h'}}{k_h^2 - K^2} \mathbf{P}_{h' \perp \mathbf{k}_{h'}}. \quad (41)$$

Here we have used the notation

$$\mathbf{k}_{h'} \times (\mathbf{k}_{h'} \times \mathbf{P}_{h'}) = -k_{h'}^2 \mathbf{P}_{h' \perp \mathbf{k}_{h'}}. \quad (42)$$

If one introduces δ functions inside the integrals of the Fourier amplitudes

$$\mathbf{P}_h = \frac{1}{V_a} \int \mathbf{P}(\mathbf{r}) \exp(-2\pi i \mathbf{k}_h \cdot \mathbf{r}) d^3\mathbf{r}, \quad (43)$$

then the equations (41) are identical with Ewald's dispersion equations (29a) for point dipoles. Otherwise the equations (41) are the same as Ewald's dispersion equations generalized for atoms. Therefore Ewald's structure amplitude \mathbf{S}_h is identical with the Fourier amplitude \mathbf{P}_h of the vector of the electric polarization, if one chooses the same physical model. This follows as well from a comparison between equations (26b) and (38). One has of course to replace \mathbf{D}_h by \mathbf{E}_h in (38). In order to come back to the equations (30b), one has now to replace in (40) the Fourier amplitudes \mathbf{D}_h by \mathbf{E}_h . These interchanges of \mathbf{E} and \mathbf{D} occur because the two authors use different approximations, Ewald the approximation (13) and von Laue the approximation (37). It seems to be better to express von Laue's dispersion equations in terms of \mathbf{D}_h , since

$$\mathbf{k}_h \cdot \mathbf{D}_h = 0, \quad \text{but} \quad \mathbf{k}_h \cdot \mathbf{E}_h \neq 0. \quad (44)$$

The equations (44) follow from the relations

$$\text{div } \mathbf{D} = 0 \quad \text{and} \quad \text{div } \mathbf{E} = 4\pi Q. \quad (45)$$

Discussion

We have seen that Ewald's microscopic theory leads for the interior of the crystal to the same result as von Laue's theory if one chooses the same model for the resonators. This holds as long as one neglects possible overlapping of the electron charges of adjacent atoms and, in the case of absorption, the Kronig fine structure of the absorption edges. Von Laue neglected such effects in his original paper as well, but absorption can be introduced into Ewald's theory as easily (complex atomic polarizability) as in von Laue's theory (complex susceptibility) (Kohler, 1933). Molière (1939) generalized von Laue's treatment for the case where the Kronig fine structure of the absorption edge becomes important.

For the half crystal von Laue's theory leads to the boundary conditions of Maxwell's theory. Ewald has shown that in his theory one obtains for the half crystal two different fields \mathbf{E}_m and \mathbf{E}_e . \mathbf{E}_m is called the 'mesofield', which is identical with the one obtained for the infinite crystal. The second field, \mathbf{E}_e , is called the 'epifield'. It travels with vacuum velocity through the crystal. The existence of the epifield contradicts the self-consistency of the fields within the crystal. But it can be expressed so that it is cancelled by the incident vacuum wave and we are therefore left, within the crystal, with the mesofield only. This leads to the same relations for the amplitudes and wave vectors as in von Laue's theory. Apart from his other publications Ewald (1925) discussed the boundary conditions in his paper about the 'reflexion and refraction of light as a problem of electron theory' and at the Kyoto Conference (Ewald, 1962).

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