

speed of $91.8 \text{ m}\cdot\text{sec}^{-1}$ (component along the neutron direction) at the examined region was used, and the transmission cross section was studied for the two cases where the specimen motion was parallel and anti-parallel to the neutron velocity. Monochromatic neutrons in this wavelength region were obtained by Bragg reflection from a mica crystal, polycrystalline beryllium being used to filter out the higher order reflected neutrons.

Fig. 6 shows the measured transmission cross sections for the stationary and moving specimen cases along with the wavelength positions where the cut-off is to be expected. Agreement between experiment and calculation is again evident. It is significant that the magnitude of the cross section discontinuity is changed in the expected manner with specimen motion. Thus it is demonstrated that the cut-off wavelength can be

easily shifted by suitable specimen motion and this can be exploited in producing window filters of adjustable width. This has been suggested independently by Iyengar (1964). In considering the case of polycrystalline specimen motion perpendicular to the incident neutron velocity, no shift in the cut-off edge is to be expected in first approximation. It is interesting that this case changes the back-reflected Debye-Scherrer circular rings into elliptical rings.

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The Role of Lattice Vibrations in Dynamical Theory of X-rays

BY A. M. AFANAS'EV AND YU. KAGAN

Kurchatov Institute of Atomic Energy, Moscow, USSR

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A consistent dynamical theory of X-rays is developed which takes into account in explicit form the processes of Thomson scattering, photoelectric absorption, and Compton scattering as well as inelastic scattering of X-rays by phonons. Special attention is paid to analysis of the role played by lattice vibrations and by temperature. Owing to inelastic scattering by phonons, the temperature dependence of the coefficients of dynamical equations is not determined by Debye-Waller factors but has a more complicated behaviour. A detailed analysis is given of the influence of lattice vibrations on the effect of anomalous transmission.

1. Introduction

In recent papers by the present authors (Afanas'ev & Kagan, 1965; Kagan & Afanas'ev, 1965, 1966) a dynamical theory has been developed which describes the motion of γ -quanta and neutrons in a regular crystal when the interaction of the particles with individual nuclei has primarily resonance character. In those papers it turned out to be possible consistently to include the vibrations of nuclei in the dynamical theory. In this aspect a considerable simplification of the problem had been achieved under an assumption that the inelastic part of the scattering cross-section by an individual nucleus was large as compared with the elastic one – as is the case in most of the situations. A complete solution of the dynamical problem in a vibrating crystal, free from this assumption, has been given in a more recent paper (Afanas'ev & Kagan, 1967).

As has been noted in the papers quoted, all the aspects of the dynamical theory of X-rays, connected with vibrations of the atoms, are identical with those of the resonance problem if the width of the resonance

level is large compared with the characteristic energy of the phonons. This circumstance made it possible to give, in the last paper (Afanas'ev & Kagan, 1967), final results for the coefficients of the dynamical theory of X-rays.

Keeping in mind the great interest attached to this problem in the physics of X-rays, we give in the present paper a detailed analysis of the influence of lattice vibrations, and thus of temperature, on the dynamical theory of X-rays and particularly on the effect of anomalous transmission (Borrmann, 1941, 1950).

2. Derivation of general equations

To describe the electromagnetic field inside the crystal we use the usual set of Maxwell equations, as in the first paper mentioned (Afanas'ev & Kagan, 1965). Converting to space and time Fourier components, we get:

$$(k^2 - \omega^2/c^2)\mathbf{E}(\mathbf{k}, \omega) - \mathbf{k}[\mathbf{k}\mathbf{E}(\mathbf{k}, \omega)] = i \frac{4\pi\omega}{c^2} \mathbf{j}(\mathbf{k}, \omega). \quad (2.1)$$

Here $\mathbf{j}(\mathbf{k}, \omega)$ is the Fourier component of the current density, which in fact is a quantum mechanical average of the Fourier component of the current density operator over the state of the system in presence of an external field (*cf. e.g. Silin & Ruhadse, 1961*).

In general case the current density operator has the form:

$$\mathbf{j}(\mathbf{r}) = -\frac{e}{2m} \sum_a (\hat{\mathcal{P}}_a \delta(\mathbf{r} - \mathbf{r}_a) + \delta(\mathbf{r} - \mathbf{r}_a) \hat{\mathcal{P}}_a),$$

$$\hat{\mathcal{P}}_a = \hat{\mathbf{P}}_a - \frac{e}{c} \hat{\mathbf{A}}(\mathbf{r}_a), \quad (2.2)$$

where the summation is performed over all the electrons in the crystal, $\hat{\mathbf{P}}_a$ stands for the a th electron momentum operator, and m is the electron mass.

Very often $\hat{\mathbf{A}}(\mathbf{r})$ was understood to represent only the vector potential of the external electromagnetic field. However $\hat{\mathbf{A}}(\mathbf{r})$ includes also a term corresponding to zero vibrations of the field, and as will be shown later the influence of this term is rather essential. Bearing this in mind we shall split $\hat{\mathbf{A}}(\mathbf{r})$ into two parts

$$\hat{\mathbf{A}}(\mathbf{r}) = \mathbf{A}_1(\mathbf{r}) + \hat{\mathbf{A}}_0(\mathbf{r}).$$

The treatment of the potential $\mathbf{A}_1(\mathbf{r})$ connected with the external field will be classical. If we set, as our gauge condition, the scalar potential equal to zero, then the Fourier components $\mathbf{E}(\mathbf{k}, \omega)$ of the electric field as determined by (2.1) will be given by the relation

$$\mathbf{E}(\mathbf{k}, \omega) = i \frac{\omega}{c} \mathbf{A}_1(\mathbf{k}, \omega). \quad (2.3)$$

On the other hand, the potential $\hat{\mathbf{A}}_0(\mathbf{r})$ is a quantum mechanical operator and can be conveniently represented in the form

$$\hat{\mathbf{A}}_0(\mathbf{r}) = \sum_{\mathbf{k}} [\hat{\mathbf{A}}(\mathbf{k}) \exp(i\mathbf{k}\mathbf{r}) + \hat{\mathbf{A}}^\dagger(\mathbf{k}) \exp(-i\mathbf{k}\mathbf{r})],$$

$$\hat{\mathbf{A}}(\mathbf{k}) = \left(\frac{2\pi c}{k} \right)^\dagger \sum_{\sigma} \eta_{\sigma} \hat{a}_{\mathbf{k}\sigma}, \quad (2.4)$$

(here and later on we set $\hbar=1$), where $\hat{a}_{\mathbf{k}\sigma}$ and $\hat{a}_{\mathbf{k}\sigma}^\dagger$ are the usual absorption and emission operators of a photon with the wave vector \mathbf{k} and polarization σ (η_{σ} is the corresponding polarization vector).

For the Fourier component of the current density operator we have, taking account of the preceding relations

$$\mathbf{j}(\mathbf{k}) = \sum_a \left\{ \mathbf{j}_1(\mathbf{k}, a) + \frac{e^2}{mc} \exp(-i\mathbf{k}\mathbf{r}_a) [\hat{\mathbf{A}}_0(\mathbf{r}_a) + \mathbf{A}_1(\mathbf{r}_a)] \right\}, \quad (2.5)$$

$$\mathbf{j}_1(\mathbf{k}, a) = -\frac{e}{2m} [\exp(-i\mathbf{k}\mathbf{r}_a) \hat{\mathbf{P}}_a + \hat{\mathbf{P}}_a \exp(-i\mathbf{k}\mathbf{r}_a)]. \quad (2.6)$$

We can now proceed to calculate the average value of the Fourier component of the current density, mak-

ing use of the standard perturbation theory. Here the interaction Hamiltonian of the system with the external field (in linear approximation in the external field) is

$$H' = \frac{1}{2m} \sum_a \left\{ \hat{\mathbf{P}}_a - \frac{e}{c} [\hat{\mathbf{P}}_0(\mathbf{r}_a) + \mathbf{A}_1(\mathbf{r}_a)] \right\}^2$$

$$- \frac{1}{2m} \sum_a \left\{ \hat{\mathbf{P}}_a - \frac{e}{c} \hat{\mathbf{A}}_0(\mathbf{r}_a) \right\}^2$$

$$\simeq \frac{1}{2m} \sum_a \left\{ [\hat{\mathbf{P}}_a - \frac{e}{c} \hat{\mathbf{A}}_0(\mathbf{r}_a)] \mathbf{A}_1(\mathbf{r}_a) + \text{h.c.} \right\}.$$

Then, utilizing equations (2.3) and (2.5) and preserving only terms linear in the external field, we find

$$j^i(\mathbf{k}, \omega) =$$

$$\frac{i}{(2\pi)^3 \omega} \int d\mathbf{k}' E^l(\mathbf{k}', \omega) \left\{ \frac{e^2}{m} \delta^{il} \left[\sum_a \overline{\exp\{i(\mathbf{k}' - \mathbf{k})\mathbf{r}_a\}} \right]_{00} \right.$$

$$+ \sum_s' \sum_{a, a'} \frac{[\overline{[\mathbf{j}^i(\mathbf{k}, a)]_{0s}}] [\mathbf{j}_1^{i*}(\mathbf{k}', a')]_{s0}}{\omega - \omega_{s0} + i\delta}$$

$$+ \frac{e^4}{m^2 c^2} \sum_s' \sum_{a, a'} \sum_{\mathbf{k}_2} \frac{[\overline{\exp\{i(\mathbf{k}_2 - \mathbf{k})\mathbf{r}_a\}} \hat{\mathbf{A}}_0^i(\mathbf{k}_2)]_{0s} [\exp\{i(\mathbf{k}' - \mathbf{k}_2)\mathbf{r}_a\} \hat{\mathbf{A}}_0^{i*}(\mathbf{k}_2)]_{s0}}{\omega - \omega_{s0} + i\delta} \left. \right\} \quad (2.7)$$

where $\omega_{s0} = \omega_s - \omega_0$. In this expression the bar above denotes an average over the initial state; the summation over s is performed over intermediate states including the excited states of the electromagnetic field. The prime at the summation sign indicates that the terms for which the intermediate state of the crystal coincides with the initial one must be excluded from the sum.

Let us divide electrons into groups corresponding to individual atoms and let us assume that each such group vibrates together with its nucleus as one entity. Then the summation over a is transformed into a summation over n and b_n where n denotes the position of an atom in the crystal and b_n stands for the position of an electron inside the n th atom. In this case

$$\mathbf{r}_a = \mathbf{R}_n + \mathbf{u}_n + \mathbf{q}_{b_n}, \quad (2.8)$$

where \mathbf{R}_n is the equilibrium position of the n th atom, \mathbf{u}_n denotes its displacement due to vibrations and \mathbf{q}_{b_n} is the position of the b_n th electron inside the n th atom.

Using equation (2.8) one can transform the first term in parentheses in equation (2.7) to the form

$$\frac{e^2}{m} \delta^{il} \sum_n \exp\{i(\mathbf{k}' - \mathbf{k})\mathbf{R}_n\} \langle \exp\{i(\mathbf{k}' - \mathbf{k})\mathbf{u}_n\} \rangle f_n(\mathbf{k}' - \mathbf{k}). \quad (2.9)$$

Here $\langle \rangle$ denotes a thermal average over the phonon occupation numbers. The procedure of averaging over electronic system resulted in the appearance of the atomic form factor $f_n(\mathbf{k}' - \mathbf{k})$.

In complex crystalline lattices it is convenient to split the sum over n into a sum over unit cells \mathbf{n} and into a sum over atoms within the unit cell j . It is evident that $\langle \exp\{i(\mathbf{k}' - \mathbf{k})\mathbf{u}_n\} \rangle$ and $f_n(\mathbf{k}' - \mathbf{k})$ depend only on j . Moreover

$$\langle \exp\{i(\mathbf{k}' - \mathbf{k})\mathbf{u}_n\} \rangle = \exp\{-M_j(\mathbf{k}' - \mathbf{k})\}, \quad (2.10)$$

where $M_j(\mathbf{k}' - \mathbf{k})$ is the usual Debye-Waller factor. As a result, we have for (2.9)

$$\frac{e^2}{m} \left(\sum_{\mathbf{n}} \exp\{i(\mathbf{k}' - \mathbf{k})\mathbf{R}_n\} \right) \delta^{ll} F_1(\mathbf{k}' - \mathbf{k}), \quad (2.11)$$

$$F_1(\mathbf{k}) = \sum_j \exp\{i\mathbf{k}\mathbf{q}_j - M_j(\mathbf{k})\} f_j(\mathbf{k}). \quad (2.11a)$$

Here \mathbf{q}_j determines the position of the j th atom in the unit cell.

We shall assume for calculations of the second term in parentheses in equation (2.7) that the excited electronic states which give the main contribution to the sum over s are the excited states of the individual atoms μ . Accordingly, the intermediate state will be characterized by the index μ and by the set of the phonon occupation numbers $\{v\}$ (the equilibrium phonon state is characterized by the occupation numbers $\{v^0\}$). It is obvious that the operator \hat{j}_1 does not stimulate photon transitions. Then (cf. the analogous expression in Afanas'ev & Kagan, 1965) we arrive at equation (2.11) with $\delta^{ll} F_1(\mathbf{k}' - \mathbf{k})$ substituted for

$$\begin{aligned} F_2^H(\mathbf{k}, \mathbf{k}') &= \frac{m}{e^2} \sum_j \exp\{i(\mathbf{k}' - \mathbf{k})\mathbf{q}_j\} \\ &\left\langle \sum_{\mu\{v\}} \frac{[\hat{j}_{1j}(\mathbf{k})]_{0\mu} [\hat{j}_{1j}^*(\mathbf{k}')]_{\mu 0}}{\omega - \omega_\mu - \sum_{\beta} \omega_{\beta}(v_{\beta} - v_{\beta}^0) + i\Gamma_{\mu 2}} \right. \\ &\times [\exp(-i\mathbf{k}\mathbf{u}_j)_{\{v^0\}\{v\}} \exp(i\mathbf{k}'\mathbf{u}_j)_{\{v\}\{v^0\}}] \rangle, \quad (2.12) \\ \hat{j}_{1j}(\mathbf{k}) &= \sum_{b_j} \hat{j}_1(\mathbf{k}, b_j). \end{aligned}$$

The index μ runs over a continuous, as well as a discrete row of values. Having in mind the discrete part of the spectrum we have introduced into the denominator the width Γ_μ of the corresponding level. For the continuous spectrum $\Gamma_\mu \rightarrow 0$. In this formula we can omit the phonon term $\sum_{\beta} \omega_{\beta}(v_{\beta} - v_{\beta}^0)$ in the denominator. For the discrete part of the sum over μ this possibility is provided simply by the large width of the levels, corresponding to X-ray transitions. (Γ_μ is larger than the characteristic energy of the phonon spectrum ω_{ph} .) On the other hand, when summation over the continuous part of the electronic spectrum is performed, the expression being summed over μ turns out to vary only slightly over distances of the order of ω_{ph} . (It should be noted that here a characteristic parameter over which the expression being integrated changes markedly is represented by the difference $\omega - \omega_e$, where ω_e is the energy of the absorption edge of the corresponding transition. Of course, it is possible in principle to conjure up a situation when

$\omega - \omega_e \sim \omega_{ph}$, but practically it is impossible to realize such a case.)

Thus omitting $\sum_{\beta} \omega_{\beta}(v_{\beta} - v_{\beta}^0)$ in the denominator of equation (2.12) and using the relation

$$\sum_{\{v\}} [\exp(-i\mathbf{k}\mathbf{u}_j)]_{\{v^0\}\{v\}} \exp\{i(\mathbf{k}'\mathbf{u}_j)\}_{\{v\}\{v^0\}} = [\exp\{i(\mathbf{k}' - \mathbf{k})\mathbf{u}_j\}]_{\{v^0\}\{v^0\}}$$

one finds easily

$$F_2(\mathbf{k}, \mathbf{k}') = \sum_j \exp\{i(\mathbf{k}' - \mathbf{k})\mathbf{q}_j - M_j(\mathbf{k}' - \mathbf{k})\} f_{2j}^H(\mathbf{k}, \mathbf{k}') \quad (2.13)$$

where

$$f_{2j}^H(\mathbf{k}, \mathbf{k}') = \frac{m}{e^2} \sum_{\mu} \frac{[\hat{j}_{1j}(\mathbf{k})]_{0\mu} [\hat{j}_{1j}^*(\mathbf{k}')]_{\mu 0}}{\omega - \omega_{\mu} + i\delta} \quad (2.14)$$

In fact f_{2j}^H describes the dispersion of the atomic form factor; the imaginary part of f_{2j}^H is completely determined by the processes of photoelectric absorption. (For the purpose of simplicity we assume in further treatment that $|f_{2j}^H| \ll |f_j|$.)

It should be mentioned that a relation, analogous to equation (2.12), and the transition to equation (2.14) were obtained in Afanas'ev & Kagan (1965) just for the case of the resonant scattering on broad lines. It is interesting to note that in the opposite limiting case $\Gamma_\mu \ll \omega_{ph}$ characteristic for the resonant interaction of the Mössbauer γ -quanta with nuclei, the temperature dependence turns out to be principally different from that given by equation (2.13). Instead of the Debye-Waller factor $M_j(\mathbf{k}' - \mathbf{k})$ in the exponent in (2.13) there appears a term $\frac{1}{2}[M_j(\mathbf{k}) + M_j(\mathbf{k}')] (cf. Afanas'ev & Kagan (1965) for further details).$

Owing to the existence of the operator \hat{A}_0 , the intermediate state in the last term in parentheses in equation (2.7) will be characterized, in addition to the excited state of the crystal ($\mu, \{v\}$) by a virtual photon with the momentum \mathbf{k}_2 . Taking it into account, we have directly for this term:

$$\begin{aligned} &\frac{e^4}{m^2 c^2} \sum_{n, n'} \sum_{\mathbf{k}_2} \{ \exp[i(\mathbf{k}_2 - \mathbf{k})\mathbf{R}_n + i(\mathbf{k}' - \mathbf{k}_2)\mathbf{R}_{n'}] \times \\ &\left(\sum \exp\{i(\mathbf{k}_2 - \mathbf{k})\mathbf{q}_{b_n}\}_{0\mu} \left(\sum \exp\{i(\mathbf{k}' - \mathbf{k}_2)\mathbf{q}_{b_{n'}}\}_{\mu 0} \right) \right. \\ &\left. \left\langle \sum_{\mu\{v\}} \frac{b_n}{\omega - \omega_{\mu} + \sum_{\beta} \omega_{\beta}(v_{\beta} - v_{\beta}^0) - \omega_{\mathbf{k}_2} + i\delta} \right. \right. \\ &\times (\exp\{i(\mathbf{k}_2 - \mathbf{k})\mathbf{u}_n\})_{\{v\}\{v^0\}} (\exp\{i(\mathbf{k}' - \mathbf{k}_2)\mathbf{u}_{n'}\})_{\{v^0\}\{v\}} \rangle \\ &\left. \times \left[\sum_{\sigma} [\hat{A}_0^{\dagger}(\mathbf{k}_2)]_{0, \sigma \mathbf{k}_2} [\hat{A}_0^{\dagger}(\mathbf{k}_2)]_{\sigma \mathbf{k}_2, 0} \right] \right\}. \quad (2.15) \end{aligned}$$

Using equation (2.4), one readily gets for the expression standing in the square brackets (cf. e.g. Schiff, 1955)

$$\sum_{\sigma} [\hat{A}_0^{\dagger}(\mathbf{k}_2)]_{0, \sigma \mathbf{k}_2} [\hat{A}_0^{\dagger}(\mathbf{k}_2)]_{\sigma \mathbf{k}_2, 0} = \frac{2\pi c^2}{\omega_{\mathbf{k}_2}} \left(\delta_{ll} - \frac{\mathbf{k}_2^l \mathbf{k}_2^l}{k_2^2} \right). \quad (2.16)$$

We shall omit the term $\sum_{\beta} \omega_{\beta}(v_{\beta} - v_{\beta}^0)$ in the denominator of equation (2.15) for the same reasons that we

had in mind when obtaining equations (2.13) and (2.14) from (2.12). Besides, it is convenient to split Σ in (2.15) into two parts treating the terms with $\mu=0$ separately. After taking equation (2.16) into account this term gives

$$\begin{aligned} & \frac{2\pi e^4}{m^2} \sum_{n,n'} \sum_{\mathbf{k}_2} \{ \exp\{i(\mathbf{k}_2 - \mathbf{k})\mathbf{R}_n + i(\mathbf{k}' - \mathbf{k}_2)\mathbf{R}_{n'}\} \times \\ & f_n(\mathbf{k}_2 - \mathbf{k})f_{n'}(\mathbf{k}' - \mathbf{k}_2) [\langle \exp\{i(\mathbf{k}_2 - \mathbf{k})\mathbf{u}_n + i(\mathbf{k}' - \mathbf{k}_2)\mathbf{u}_{n'}\} \rangle \\ & - \langle \exp\{i(\mathbf{k}_2 - \mathbf{k})\mathbf{u}_n\} \rangle \langle \exp\{i(\mathbf{k}' - \mathbf{k}_2)\mathbf{u}_{n'}\} \rangle] \\ & \times \frac{1}{\omega_{\mathbf{k}_2}} \cdot \frac{\delta^{il} - k_2^i k_2^l / k_2^2}{\omega - \omega_{\mathbf{k}_2} + i\delta} \}. \quad (2.17) \end{aligned}$$

The second term in the square brackets has appeared here because the terms with $\{v\} = \{v^0\}$ must be excluded from the sum over $\{v\}$, when $\mu=0$. The rest of the terms in the sum over μ in (2.15) give, under the same assumptions that were used in obtaining equations (2.12) to (2.14), the contribution given by equations (2.11) and (2.13) with $f_{3j}^{il}(\mathbf{k}, \mathbf{k}')$ having been substituted by

$$\begin{aligned} f_{3j}^{il}(\mathbf{k}, \mathbf{k}') &= \frac{2\pi e^2}{m} \sum_{\mu \neq 0} \sum_{\mathbf{k}_2} \\ & \left(\sum_{b_j} \exp\{i(\mathbf{k}_2 - \mathbf{k})\mathbf{Q}_{b_j}\} \right)_{0\mu} \left(\sum_{b_j} \exp\{i(\mathbf{k}' - \mathbf{k}_2)\mathbf{Q}_{b_j}\} \right)_{\mu 0} \\ & \times \frac{1}{\omega_{\mathbf{k}_2}(\omega - \omega_{\mu} - \omega_{\mathbf{k}_2} + i\delta)} \\ & \times \left(\delta^{il} - \frac{k_2^i k_2^l}{k_2^2} \right). \quad (2.18) \end{aligned}$$

We note that in deriving equation (2.18) as well as equation (2.13) the intermediate excited state of the electronic system was supposed to be that of an individual atom, so that in equation (2.15) it was put $n=n'$ ($\mathbf{n}, j=\mathbf{n}', j'$) when $\mu \neq 0$.

This expression describes an additional contribution to the atomic form factor due to the Compton scattering.

Direct calculations, taking account of equation (2.10), give the following result for the temperature-dependent factor in (2.17)

$$\begin{aligned} & \langle \exp(i(\mathbf{k}_2 - \mathbf{k})\mathbf{u}_n + i(\mathbf{k}' - \mathbf{k}_2)\mathbf{u}_{n'}) \rangle \\ & - \langle \exp(i(\mathbf{k}_2 - \mathbf{k})\mathbf{u}_n) \rangle \langle \exp(i(\mathbf{k}' - \mathbf{k}_2)\mathbf{u}_{n'}) \rangle \\ & = \exp\{-M_j(\mathbf{k}_2 - \mathbf{k}) - M_{j'}(\mathbf{k}' - \mathbf{k}_2)\} \\ & \times \langle \exp\{Y_{jj'}(\mathbf{k}, \mathbf{k}', \mathbf{R}_n - \mathbf{R}_{n'})\} - 1 \rangle, \quad (2.19) \end{aligned}$$

where

$$\begin{aligned} Y_{jj'}(\mathbf{k}, \mathbf{k}', \mathbf{R}_n - \mathbf{R}_{n'}) &\equiv \langle [i(\mathbf{k} - \mathbf{k}_2)\mathbf{u}_n][i(\mathbf{k}' - \mathbf{k}_2)\mathbf{u}_{n'}] \rangle \\ &= \Omega_0 \sum_{\alpha, \mathbf{q}} \varphi_{jj'}(\mathbf{k}, \mathbf{k}', \mathbf{k}_2; \alpha, \mathbf{q}) \cdot \frac{2\bar{v}(\alpha, \mathbf{q}) + 1}{\omega(\alpha, \mathbf{q})} \\ & \times \exp\{i\mathbf{q}(\mathbf{R}_n - \mathbf{R}_{n'})\}, \quad (2.20) \end{aligned}$$

and

$$\begin{aligned} \varphi_{jj'}(\mathbf{k}, \mathbf{k}', \mathbf{k}_2; \alpha, \mathbf{q}) &= \frac{1}{2A_i A_j} [(\mathbf{k} - \mathbf{k}_2) \mathbf{V}_j(\alpha, \mathbf{q}) \\ & [(\mathbf{k}' - \mathbf{k}_2) \mathbf{V}_{j'}^*(\alpha, \mathbf{q})]]. \quad (2.21) \end{aligned}$$

Here \mathbf{q}, α are the wave vector and the branch number of a phonon; $\omega(\alpha, \mathbf{q}), \bar{v}(\alpha, \mathbf{q})$ are the frequencies and average occupation numbers of the phonons; A_j is the mass of the j th atom; $\mathbf{V}_j(\alpha, \mathbf{q})$ is the polarization vector of the j th atom in the α, \mathbf{q} th normal mode, Ω_0 is the unit-cell volume.

The fact that equation (2.19) depends only on the difference $\mathbf{R}_n - \mathbf{R}_{n'}$ permits us to transform equation (2.17) to the form of equation (2.11) with the substitution of $F_I(\mathbf{k}' - \mathbf{k})\delta^{il}$ for

$$\begin{aligned} F_I^{il}(\mathbf{k}, \mathbf{k}') &= \frac{2\pi e^2}{m} \sum_{j,j'} \sum_{\mathbf{k}_2} \{ \exp[i(\mathbf{k}_2 - \mathbf{k})\mathbf{Q}_j \\ & + i(\mathbf{k}' - \mathbf{k}_2)\mathbf{Q}_{j'}] \Phi_{jj'}^{il}(\mathbf{k}, \mathbf{k}', \mathbf{k}_2) \times [\sum_n \exp\{i(\mathbf{k}_2 - \mathbf{k})\mathbf{R}_n \} \\ & \times (\exp\{Y_{jj'}(\mathbf{k}, \mathbf{k}', \mathbf{R}_n)\} - 1)] [\omega_{\mathbf{k}_2}(\omega - \omega_{\mathbf{k}_2} + i\delta)^{-1}] \}, \quad (2.22) \end{aligned}$$

where

$$\begin{aligned} \Phi_{jj'}^{il}(\mathbf{k}, \mathbf{k}', \mathbf{k}_2) &= f_j(\mathbf{k}_2 - \mathbf{k})f_{j'}(\mathbf{k}' - \mathbf{k}_2) \\ & \times \exp\{-M_j(\mathbf{k}_2 - \mathbf{k}) \\ & - M_{j'}(\mathbf{k}' - \mathbf{k}_2)\} (\delta^{il} - k_2^i k_2^l / k_2^2). \quad (2.23) \end{aligned}$$

F_I^{il} describes the contribution to the structure amplitude due to the scattering processes with absorption (emission) of phonons (later on we shall refer to this scattering as the phonon scattering).

Thus, the expression in parentheses in equation (2.7) is brought to the form

$$\frac{e^2}{m} \left(\sum_n \exp\{i(\mathbf{k}' - \mathbf{k})\mathbf{R}_n\} \right) [F_0^{il}(\mathbf{k}, \mathbf{k}') + F_I^{il}(\mathbf{k}, \mathbf{k}')], \quad (2.24)$$

where

$$\begin{aligned} F_0^{il}(\mathbf{k}, \mathbf{k}') &= \sum_j \exp\{i(\mathbf{k}' - \mathbf{k})\mathbf{Q}_j - M_j(\mathbf{k}' - \mathbf{k})\} \\ & [\delta^{il} f_j(\mathbf{k}' - \mathbf{k}) + f_{2j}^{il}(\mathbf{k}, \mathbf{k}') + f_{3j}^{il}(\mathbf{k}, \mathbf{k}')]. \quad (2.25) \end{aligned}$$

Now making use of the relation

$$\sum_n \exp\{i(\mathbf{k}' - \mathbf{k})\mathbf{R}_n\} = \frac{2\pi}{\Omega_0} \sum_h \delta(\mathbf{k}' - \mathbf{k}_h), \quad \mathbf{k}_h = \mathbf{k} + \mathbf{K}_h,$$

where \mathbf{K}_h is the reciprocal lattice vector multiplied by 2π , we find

$$j^i(\mathbf{k}, \omega) = \sum_h \sigma_{\omega}^{il}(\mathbf{k}, \mathbf{k}_h) E^l(\mathbf{k}_h, \omega). \quad (2.27)$$

Here σ_{ω}^{il} in accordance with equation (2.24) is

$$\sigma_{\omega}^{il}(\mathbf{k}, \mathbf{k}') = \frac{i}{\omega \Omega_0} \frac{e^2}{m} [F_0^{il}(\mathbf{k}, \mathbf{k}') + F_I^{il}(\mathbf{k}, \mathbf{k}')]. \quad (2.28)$$

Now inserting (2.27) into the initial equation (2.1), we arrive after a number of simple transformations at the following set of dynamical equations:

$$\begin{aligned} (k_h^2 / \kappa^2 - 1) E^i(\mathbf{k}_h, \omega) &= \\ \sum_{h'} g^{ih}(h, h') E^l(\mathbf{k}_{h'}, \omega) &+ \frac{k_h^i [\mathbf{k}_h E(\mathbf{k}_h, \omega)]}{\kappa^2}, \quad (2.29) \end{aligned}$$

where

$$g^{ih}(h, h') = \frac{4\pi i}{\omega} \sigma_{\omega}^{il}(\mathbf{k}_h, \mathbf{k}_{h'})$$

$$= -\frac{4\pi r_0}{\kappa^2 \Omega_0} [F_0^{ii}(\mathbf{k}_h, \mathbf{k}_{h'}) + F_T^{ii}(\mathbf{k}_h, \mathbf{k}_{h'})] \\ \equiv g_0^{ii}(h, h') + g_T^{ii}(h, h'); \quad \kappa = \omega/c, \quad r_0 = e^2/mc^2. \quad (2.30)$$

We note that in view of the small value of interaction between the X-ray and an individual atom the electric field inside the crystal remains practically transverse so that the last term in the right-hand part of equation (2.29) is negligibly small and can be safely omitted.

Expression (2.30), together with equations (2.25), (2.14), (2.18), (2.20) and (2.22), completely solves the problem of how the coefficients of the dynamical set of equations depend on temperature. In accordance with (2.30) the coefficients g^{ii} are divided into the sum of two terms, the first one, g_0^{ii} , having the temperature dependence governed only by the Debye-Waller factors [cf. (2.25)]. (In monatomic crystals with one or two atoms per unit cell $g_0^{ii}(h, h') \sim \exp\{-M(\mathbf{k}_h - \mathbf{k}_{h'})\}$). This part of the structure amplitude is connected with the processes of the Thomson scattering, photoelectric absorption, and the Compton scattering [respectively the first, the second, and the third terms of the right-hand part of equation (2.25)]. The second term in (2.30) g_T^{ii} is determined by the scattering processes on phonons and has, as may be seen from equations (2.22), (2.23), (2.20), a fairly complex temperature dependence. If g_T^{ii} is small compared with g_0^{ii} then the temperature dependence of the g^{ii} coefficients is determined simply by the Debye-Waller factors in accordance with the expression (2.25) for the structure amplitude. Such a result has been obtained by Afanas'ev & Kagan (1965) and Kagan & Afanas'ev (1965, 1966) for the case of a broad resonant level (equivalent, as we have already mentioned, to the case of the X-ray scattering from electrons) just on the assumption that the elastic part of the scattering cross-section is small compared with the inelastic one (which is equivalent to $|g_T^{ii}| \ll |g_0^{ii}|$).

3. Analysis of the contribution from the phonon scattering

If one compares (2.22) with (2.11a), then one easily concludes that $|F_T^{ii}| \ll |F_1|$. As a result, the contribution to the scattering properties of the system is small. However, from the point of view of absorption the picture changes. Indeed, the Thomson term F_1 does not contribute to the absorption, the latter being thus determined only by the rest of the terms in the structural factor F_0^{ii} . Therefore the importance of the term F_T^{ii} has to be estimated according to its contribution to the absorption. It turns out that in many cases this contribution may prove to be comparable to that from F_0^{ii} and thus it can introduce noticeable corrections into all effects in which the absorption is essential, and particularly into the effect of anomalous transmission.

In crystals with one atom per unit cell the absorption is determined simply by the imaginary part of the structure amplitude, and in complex crystals by a com-

bination of the form

$$\tilde{F}^{ii}(\mathbf{k}, \mathbf{k}') = \frac{1}{2}[F^{ii}(\mathbf{k}, \mathbf{k}') - F^{ii*}(\mathbf{k}', \mathbf{k})]. \quad (3.1)$$

Now, \tilde{F}_T^{ii} will be determined by equation (2.22) with the substitution of $(\omega - \omega_{\mathbf{k}_2} + i\delta)^{-1}$ for $-i\pi\delta(\omega - \omega_{\mathbf{k}_2})$. It is this part that we shall be interested in in later discussion. Before going into its analysis we shall consider the physical nature of the additional absorption appearing in the dynamical problem in the vibrating crystal.

Let us consider, for simplicity, a crystal with one atom per unit cell. In this case the structure amplitude (2.25) of the rigid lattice may be directly shown to be simply proportional to the amplitude for elastic scattering of a photon by an individual atom.

In the dynamical problem only the amplitudes for true elastic scattering must play an important role. This explains why in the case of a vibrating lattice the factors of the form $\exp\{-M(\mathbf{k} - \mathbf{k}')\}$ appear which characterize the probability that phonons are not excited during the scattering process. However, this does not cover all the role that lattice vibrations play.

The fact is that even in the case of a pure elastic scattering by an isolated atom the amplitude for elastic scattering at zero angle has an imaginary part due to the well known optical theorem. In a rigid regular crystal the imaginary part of this amplitude turns to zero in the absence of absorption. In the presence of lattice vibrations inelastic scattering by phonons changes the amplitude for elastic scattering resulting in a partial reappearance of the imaginary part. In the limit of high temperatures the imaginary part of the scattering amplitude reaches a value corresponding to that of an isolated atom. It is this circumstance that explains the presence of the additional term F_T^{ii} .

We now turn to expression (2.22) and separate out of it the term with $\mathbf{n} = 0$. We expand $(\exp Y_{jj'} - 1)$ in a series in terms of the powers of $Y_{jj'}$ and confine ourselves to the first non-vanishing term of the series. As a result we get

$$\tilde{F}_T^{ii}(\mathbf{k}, \mathbf{k}') = -i \frac{2\pi^2 e^2}{m\omega} \sum_{j, j'} \sum_{\mathbf{k}_2} (\exp\{i(\mathbf{k}_2 - \mathbf{k})\mathbf{e}_j \\ + i(\mathbf{k}' - \mathbf{k}_2)\mathbf{e}_{j'}\}) \Phi_{jj'}^{ii}(\mathbf{k}, \mathbf{k}', \mathbf{k}_2) \{(\exp[Y_{jj'}(\mathbf{k}, \mathbf{k}', 0)] - 1) \\ + \sum_{\mathbf{n} \neq 0} Y_{jj'}(\mathbf{k}, \mathbf{k}', \mathbf{R}_n)\} \delta(\omega - \omega_{\mathbf{k}_2}). \quad (3.2)$$

In our further treatment we consider only the case when the wave length λ of X-rays is small compared with the distance a between atoms, that is when

$$\lambda/a \ll 2\pi. \quad (3.3)$$

In this case the contribution to $\tilde{F}_T^{ii}(\mathbf{k}, \mathbf{k}')$ from the first term in parentheses in (3.2) is determined mainly by the terms with $j = j'$ in the sum over j, j' . The rest of the terms in the sum will give only a small contribution, if the condition (3.3) is satisfied, because in these terms there remains a rapidly oscillating phase factor of the form $\exp\{i(\mathbf{k}_2 - \mathbf{k})(\mathbf{e}_j - \mathbf{e}_{j'})\}$ in the sum over \mathbf{k}_2 ,

and therefore these terms can be safely neglected. As a result, we find the following expression for the part of $g_T^{II}(h, h')$ connected with the first term in parentheses (3.2):

$$g_T^{II}(h, h') \simeq i \frac{4\pi r_0^2}{\Omega_0 \omega} \sum_j \exp\{i(\mathbf{k}_h - \mathbf{k}_{h'}) \cdot \mathbf{e}_j\} \\ \times \int f_j(\mathbf{k} - \mathbf{k}_h) f_j(\mathbf{k}_{h'} - \mathbf{k}) (\delta^{il} - k^i k^l / k^2) \\ \times [\exp\{-M_j(\mathbf{k}_{h'} - \mathbf{k}_h)\} \\ - \exp\{-M_j(\mathbf{k} - \mathbf{k}_h) - M_j(\mathbf{k}_{h'} - \mathbf{k})\}] \frac{d\Omega_{\mathbf{k}}}{4\pi} \Big|_{k=\kappa}. \quad (3.4)$$

In obtaining (3.4) we went over from the summation over \mathbf{k}_2 to an integration, and also have made use of the relation

$$M_j(\mathbf{k}_2 - \mathbf{k}) + M_j(\mathbf{k}' - \mathbf{k}_2) - Y_{jj}(\mathbf{k}, \mathbf{k}', 0) \equiv M_j(\mathbf{k}' - \mathbf{k}).$$

For crystals with one atom per unit cell (in this case $\mathbf{e}_j = 0$) the expression (3.4) is naturally exact.

We note that if all of the atoms vibrated independently, then the second term in (3.2) would turn to zero, and g_T^{II} would be strictly determined by the expression (3.4). Thus, the second term in (3.2) reflects a coherent character of the inelastic scattering of X-rays by phonons. The contribution of this term under the condition (3.3) is in practice always less than the contribution which is determined by the first term. It must be pointed out that, as we shall see later, this term is essentially singled out in its value. However, the rest of the terms in the expansion of the exponent in a series in terms of $Y_{jj'}$ give a negligible contribution when $\mathbf{n} \neq 0$.

We transform the second term in parentheses (3.2) as follows:

$$\tilde{F}_T^{II}(\mathbf{k}, \mathbf{k}') = \\ - i \frac{2\pi^2 e^2}{m\omega} \left\{ \sum_{h''} P^{II}(\mathbf{k}, \mathbf{k}', \mathbf{K}_{h''}) - \frac{\Omega_0}{(2\pi)^3} \int P^{II}(\mathbf{k}, \mathbf{k}', \mathbf{K}_2) d\mathbf{K}_2 \right\} \quad (3.5)$$

where

$$P^{II}(\mathbf{k}, \mathbf{k}', \mathbf{k}_2) = \sum_{\alpha\mathbf{q}} \sum_{jj'} \{ \exp[i(\mathbf{k}_2 - \mathbf{k} + \mathbf{q}) \cdot \mathbf{e}_j] \\ + i(\mathbf{k}' - \mathbf{k}_2 - \mathbf{q}) \cdot \mathbf{e}_{j'} \} \Phi_{jj'}^{II}(\mathbf{k}, \mathbf{k}', \mathbf{k}_2 + \mathbf{q}) \\ \times \varphi_{jj'}(\mathbf{k}, \mathbf{k}', \mathbf{k}_2 + \mathbf{q}; \alpha, \mathbf{q}) \cdot \frac{2\bar{v}(\alpha, \mathbf{q}) + 1}{\omega(\alpha, \mathbf{q})} \cdot \delta(\omega - \omega_{\mathbf{k}_2 + \mathbf{q}}). \quad (3.6)$$

In those cases, when $\mathbf{k}' \neq \mathbf{k}$, $P^{II}(\mathbf{k}, \mathbf{k}, \mathbf{k}_2)$ is a smooth function of \mathbf{k}_2 , and if the condition (3.3) is satisfied, then the sum over h'' and the integral in (3.5) compensate each other to a considerable degree. In this case one can neglect the term (3.5) and then $g_T^{II}(h, h')$ at $h \neq h'$ is described with good accuracy by the expression (3.4).

If $\mathbf{k}' = \mathbf{k}$, then the terms with $\mathbf{k}_{h''}$ will be singled out in the sum over h'' , and these are the terms which are responsible for the Bragg reflection and for which the following condition is satisfied

$$k_{h''}^2 \simeq k^2. \quad (3.7)$$

We preserve only these terms in (3.5) (the remaining terms will be compensated by corresponding integrals as was the case in the preceding treatment). If the condition (3.7) is satisfied, then the main contribution to P^{II} , when the summation over α, \mathbf{q} is performed, comes from the region of small $\omega(\alpha, \mathbf{q})$, that is from the acoustic vibrations with small \mathbf{q} . Owing to this circumstance we can set $\mathbf{q} = 0$ in the first and in the second factors of (3.6) and change $\varphi_{jj'}(\mathbf{k}, \mathbf{k}', \mathbf{k}_2 + \mathbf{q}; \alpha, \mathbf{q})$ and $2\bar{v}(\alpha, \mathbf{q}) + 1$ respectively for $\varphi_{jj'}(\mathbf{k}, \mathbf{k}', \mathbf{k}_2; \alpha, \mathbf{q})$ and $2T/\omega(\alpha, \mathbf{q})$. Besides, the polarization vector $\mathbf{V}_j(\alpha, \mathbf{q})$ of the acoustic modes is connected with the polarization vector $\mathbf{V}(\alpha, \mathbf{q})$ of the sound wave by the relation

$$\mathbf{V}_j(\alpha, \mathbf{q}) = (A_j/A)^{1/2} \mathbf{V}(\alpha, \mathbf{q}); \quad A = \sum_j A_j. \quad (3.8)$$

As a result, we obtain

$$F_T^{II}(\mathbf{k}, \mathbf{k}') \simeq \\ - i \frac{2\pi^2 e^2}{m\omega} \sum_{h''} \left\{ |F_1(\mathbf{K}_{h''})|^2 \cdot \left(\delta^{il} - \frac{k_{h''}^i k_{h''}^l}{k_{h''}^2} \right) \cdot \frac{T}{A} \right. \\ \left. \times \sum_{\alpha'} \int \frac{|\mathbf{K}_{h''} \cdot \mathbf{V}(\alpha', \mathbf{q})|^2}{\omega^2(\alpha', \mathbf{q})} \delta(\omega - \omega_{\mathbf{k}_{h''} + \mathbf{q}}) \frac{d\mathbf{q}}{(2\pi)^3} \right\} \delta_{\mathbf{k}, \mathbf{k}'}. \quad (3.9)$$

Here α' labels only the acoustic modes; the summation over h'' is carried out only over the reciprocal lattice vectors, satisfying the condition (3.7).

The appearance of the term (3.9) is connected with the existence of the anomalous diffusive scattering in the vicinity of the Bragg peaks. The right hand part of (3.9) is proportional to the total cross section of the one-phonon scattering near the Bragg angles. The integration over $d\mathbf{q}$ in (3.9) leads to a logarithmic divergence at $\mathbf{q} \rightarrow 0$. This fact is in complete correspondence with the behaviour of the anomalous diffusive scattering difference cross section, which is known (see, e.g. Landau & Lifschitz, 1957) to be proportional to $1/\Theta^2$, where Θ is a scattering angle measured from the direction corresponding to the Bragg scattering. In order to avoid this divergency one must take into account that at small Θ the motion of the scattered wave bears a dynamical character; in other words, the state into which the wave comes as a result of scattering is not that of a plane wave but rather a superposition of plane waves in accordance with a solution of the dynamical set of equations (2.29).

Having taken this into account, we are led to the conclusion that the expression being integrated in (3.9) preserves its form only for $\Theta \gtrsim q_{\min}/k$ where

$$q_{\min} = k |g_0(h, h)| \quad (3.10)$$

and the region of smaller q , now having no divergency, gives a negligible contribution. Cutting the integration over $d\mathbf{q}$ in (3.9) at the level q_{\min} , we find for the part of g_T^{II} connected with (3.9):

$$g_T^{II}(h, h') = \frac{6\pi r_0^2}{\Omega_0 k} \left\{ \sum_{h'' \neq h} |F_1(\mathbf{K}_{h''})|^2 \cdot \frac{T}{Ac^2} \right.$$

$$g_T^{(2)ll}(h, h') = \frac{6\pi r_0^2}{\Omega_0 \kappa} \left\{ \sum_{h'' \neq h} |F_1(\mathbf{K}_{h''})|^2 \cdot \frac{T}{Ac_s^2} \right. \\ \left. \times \frac{k_{h''}^2}{\kappa^2} \ln(q_0/q_{\min})(\delta^{ll} - k_{h''}^l k_{h''}^l / k_{h''}^2) \right\} \delta_{h, h'}, \quad (3.11)$$

where q_0 is a value of the order of the limiting momentum of phonons and

$$\frac{1}{c_s^2} = \frac{1}{3} \sum_{\alpha'} \int_0^{2\pi} \frac{|\mathbf{n}_{h''} \mathbf{V}(\alpha', \varphi)|^2}{c^2(\alpha', \varphi)} \cdot \frac{d\varphi}{2\pi}. \quad (3.12)$$

The integration over $d\varphi$ in (3.12) is carried out over all directions perpendicular to the vector $\mathbf{k}_{h''}$, $c(\alpha', \varphi)$ is the velocity of sound of the α' th acoustic branch in the corresponding direction, and $\mathbf{n}_{h''} = \mathbf{K}_{h''}/K_{h''}$.

Thus, the final expression for g_T^{ll} has the following form:

$$g_T^{ll}(h, h') \simeq g_T^{(1)ll}(h, h') + g_T^{(2)ll}(h, h'), \quad (3.13)$$

where $g_T^{(1)ll}$ and $g_T^{(2)ll}$ are determined by equations (3.4) and (3.11) respectively.

It should be noted that in the case when the condition (3.3) is not strictly satisfied and at not very high temperatures, a linear expansion of the exponent in the first term in parenthesis (3.2) may prove to be a good approximation. In this case \bar{F}_T^{ll} is determined simply by the first term in parenthesis (3.5).

Expression (3.13), being approximated, has nevertheless the advantage that all of its constituent parts can be directly calculated in a comparatively simple way.

For a numerical calculation of g_T^{ll} in this approximation one has to know only the atomic scattering amplitudes, the Debye-Waller factors, as well as the elastic constants for determination of c_s^2 . As a rule, all these values are known accurately enough. On the other hand, an accurate calculation of g_T^{ll} with the help of equations (2.30), (2.22) and (2.20) demands detailed information about lattice vibrations, and in particular it needs the knowledge of polarization vectors of the normal modes for all the range of wave vectors.

4. Influence of lattice vibrations on the effect of 'anomalous transmission'

The results obtained above make possible a complete analysis of the problem of 'anomalous transmission' of X-rays through a crystal with a vibrating lattice. As usual, we restrict ourselves to a case in which only one Bragg reflexion (with a corresponding vector \mathbf{K}_1 of the reciprocal lattice) exists, and we consider only the polarization $\boldsymbol{\eta}$ perpendicular to the plane of scattering for which the effect of 'anomalous transmission' takes place. In this case the dynamical set of equations is confined to a set of two equations for corresponding amplitudes of the electric field with scalar coefficients of the form $g(h, h') = \eta^i \eta^l g^{il}(h, h')$, $h, h' = 0, 1$.

For the sake of simplicity we further restrict our treatment to the case of a crystal with either one or

two similar atoms in a unit cell and we choose the reflexion in such a way that in the case of two atoms in a unit cell $\exp(i\mathbf{K}_1 \mathbf{Q}_j) = 1$. We shall consider a symmetrical reflexion and in addition we assume that the plane of reflexion is one of the crystal symmetry planes.

The latter assumption simplifies the analysis to some extent since in this case it is always the case that

$$g(0, 0) = g(1, 1), \quad (4.1) \\ g(0, 1) = g(1, 0).$$

In accordance with the results of the preceding sections [see equations (2.30), (2.25), (3.13), (3.11), (3.4)] we get, having taken into account the restrictions made above,

$$g(0, 0) = - \frac{4\pi r_0}{\Omega_0 \kappa^2} [f(0) + f_2(\mathbf{k}, \mathbf{k}) + f_3(\mathbf{k}, \mathbf{k}) + i\mu_T(\mathbf{k}, \mathbf{k})/\kappa], \quad (4.2)$$

$$g(0, 1) = - \frac{4\pi r_0}{\Omega_0 \kappa^2} [f(\mathbf{K}_1) + f_2(\mathbf{k}, \mathbf{k}_1) + f_3(\mathbf{k}, \mathbf{k}_1)] \\ \times \exp[-M(\mathbf{K}_1)] + i\mu_T(\mathbf{k}, \mathbf{k}_1)/\kappa, \quad (4.3)$$

$$f_{2,3}(\mathbf{k}, \mathbf{k}') = \eta^i \eta^l f_{2,3}^{il}(\mathbf{k}, \mathbf{k}'). \quad (4.4)$$

The last terms on the right hand side of equations (4.2) and (4.3) are connected with inelastic scattering of X-rays by phonons and are determined as follows

$$\mu_T(\mathbf{k}, \mathbf{k}') = \mu_T^{(1)}(\mathbf{k}, \mathbf{k}') + \mu_T^{(2)}(\mathbf{k}, \mathbf{k}'), \quad (4.5)$$

$$\mu_T^{(1)}(\mathbf{k}, \mathbf{k}') \simeq 4\pi N_0 r_0^2 \int f(\mathbf{k}_2 - \mathbf{k}) f(\mathbf{k}' - \mathbf{k}_2) (1 - (\boldsymbol{\eta} \mathbf{k}_2)^2 / k_2^2) \\ \times (\exp\{-M(\mathbf{k}' - \mathbf{k})\} \\ - \exp\{-M(\mathbf{k}_2 - \mathbf{k}) - M(\mathbf{k}' - \mathbf{k}_2)\}) \frac{d\Omega_{\mathbf{k}_2}}{4\pi} |_{k_2=k}, \quad (4.6)$$

$$\mu_T^{(2)}(\mathbf{k}, \mathbf{k}') \simeq \delta_{\mathbf{k}, \mathbf{k}'} \cdot 6\pi N_0 r_0^2 \sin^2 \theta_B \cdot \frac{4T}{Ac_s^2} \\ \times f^2(\mathbf{K}_1) \exp\{-2M(\mathbf{K}_1)\} \ln(q_0/q_{\min}). \quad (4.7)$$

Here N_0 is the number of atoms per unit volume; θ_B is the Bragg angle.

The expression for the coefficient of anomalous absorption is known to have the form

$$\mu_a = \kappa [g''(0, 0) - g''(0, 1)]$$

where g'' denotes the imaginary part of the corresponding coefficient. Then, taking account of (4.2)–(4.7), we find

$$\mu_a = (\mu_2 + \mu_3)(1 - \varepsilon_0 \exp\{-M(\mathbf{K}_1)\}) + \mu_a T. \quad (4.8)$$

Here

$$\mu_{2,3} = - \frac{4\pi r_0}{\Omega_0 \kappa} f_{2,3}''(\mathbf{k}, \mathbf{k})$$

are the absorption coefficients of X-rays which are determined by the photo-absorption and the Compton scattering respectively, and

$$\varepsilon_0 = \frac{f_2''(\mathbf{k}, \mathbf{k}_1) + f_3''(\mathbf{k}, \mathbf{k}_1)}{f_2''(\mathbf{k}, \mathbf{k}) + f_3''(\mathbf{k}, \mathbf{k})}.$$

The contribution to the anomalous coefficient of absorption which is due to inelastic scattering by phonons

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.