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The Temperature Factor in the Dynamical Theory of X-ray Interference for a Perfect Crystal with Heat Motion

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The effect of thermal vibrations on the intensity of the Laue–Bragg reflection is discussed using the dynamical theory of X-ray reflection. The temperature factor for a perfect non-absorbing crystal is shown to be of the form $\exp(-M)$ for intensity, unlike the value of $\exp(-2M)$ for a mosaic crystal. The possibility of applying this for finding out the degree of perfection of a crystal is discussed.

1. Introduction

In studying the intensity of X-ray reflection from perfect crystals, two theories are used—the kinematical theory applicable to thin and mosaic crystals and the dynamical theory, which holds good for thick perfect crystals. In the former theory, the effects of the dynamical interaction of primary and diffracted waves and of multiple scattering are neglected, whereas in the dynamical theory of Darwin and in the more general theories of Ewald & Laue, these effects are taken into account. Though Darwin & Ewald have approached the problem in different ways, their theories lead essentially to the same result (Ramachandran, 1948). Reviews of these theories are available in the books by James (1954) and Zachariasen (1945).

All these theories are strictly valid for an ideal static lattice where the atoms are at rest, whereas in the actual case, the atoms are not at rest, but are undergoing thermal oscillations. The effect due to these oscillations on the intensity of X-ray reflection has been studied, chiefly by Debye, Faxén, Waller, Born, Laval, using the kinematical theory of X-ray reflection. (For a review article, see Born, 1942; also Slater, 1958). The main effect of these oscillations of the atoms on the intensity of the Laue–Bragg scattering is to reduce it by a factor—the Debye–Waller factor, which is $\exp(-2M)$ for a mosaic crystal. However, the effect of thermal vibrations on the intensity of Bragg reflection in a perfect crystal does not seem to have been worked out. For example, both Born in his review on 'Crystal dynamics and X-ray scattering' (1942, p. 328) and James in dealing with thermal vibration in his book (1954, p. 210) state that the extension of Ewald's dynamical theory of scattering to the vibrating lattice is an important problem, but do not refer to any earlier work. The author therefore took up this problem and the results are presented below. It is found that the temperature factor for a perfect non-absorbing crystal is of the form $\exp(-M)$ for intensity, unlike the value $\exp(-2M)$ for a mosaic crystal. The author has learned from Prof. Ewald that this result has been stated by Waller (1926, 1927). However, Waller has not published the details, although he mentions that he has made an approximate solution of the problem on the basis of Ewald's theory. The derivation given below appears to be quite exact and is in fact valid even for a crystal traversed by a single acoustic wave. Only the case of a non-absorbing crystal is discussed in this paper, but it is proposed to extend this study to the case of an absorbing crystal also.

Throughout this paper the notation used is that of Zachariasen (1945) (with some minor modifications), on whose treatment the calculations are based.

2. Static and dynamic dielectric constants

As usual we may develop the dielectric constant, ε of the crystal, which is a three-dimensionally periodic quantity, as a Fourier series. Further this dielectric constant ε at any point $\mathbf{r}$ is related to the electron density function ϱ at that point by the relation (James, 1954)

$$\varepsilon(\mathbf{r}) = 1 - (e^2/\pi m v^2)\varrho(\mathbf{r}) , \tag{1}$$

where v is the frequency of the incident X-rays, and it is assumed that v is far away from any natural absorption frequency of the scattering system. Because of the fact that the atoms are vibrating ϱ and ε will not be constant and in the actual crystal, one has to consider the time dependent dynamic electron density ϱ' and dielectric constant ε'. The atomic displacements in a 'dynamic lattice' can be analyzed in terms of a number of plane waves—the 'acoustic waves' of varying frequency and amplitude. Before considering this actual case, we may first consider a simple case when the displacement of atoms can be expressed in terms of a single acoustic wave and later generalize this result to a superposition of such waves.

Let the displacement vector due to the acoustic wave at any point $\mathbf{r}$ be $\mathbf{u}$, given by

$$\mathbf{u} = \mathbf{a}_p \cos 2\pi(\nu_p t - \mathbf{g}_p . \mathbf{r} - \delta_p) , \tag{2}$$

where $\mathbf{a}_p$, $\mathbf{g}_p$, ν_p and δ_p are the amplitude, wave vector, frequency and phase of the acoustic wave. (The index p is put in to facilitate generalization later.) An atom, which would have been at the position $\mathbf{r}$ in the static lattice, is actually at $\mathbf{r}+\mathbf{u}$ at time t in the dynamic lattice. This indicates that the dynamic charge density function ϱ' at time t is related to the static charge density ϱ by the equation

$$\varrho'(\mathbf{r}+\mathbf{u}) = \varrho(\mathbf{r}) \quad \text{or} \quad \varrho'(\mathbf{r}) = \varrho(\mathbf{r}-\mathbf{u}) . \tag{3}$$

In writing equation (3) the approximation that is made is to neglect any distortion or any mutual penetration of electronic shells that may be produced by the vibration, which is a reasonable assumption for acoustic frequencies.* Thus, if we use $\psi'(\mathbf{r})$ and $\psi(\mathbf{r})$ to describe any physical property of the crystal in the dynamic and static conditions respectively, and *if ψ at any point* $\mathbf{r}$ *could be related to the electron density at that point* (as for instance equation (1)), then we have

$$\psi'(\mathbf{r}) = \psi(\mathbf{r}-\mathbf{u}) . \tag{4}$$

Thus

$$\varepsilon'(\mathbf{r}) = \varepsilon(\mathbf{r}-\mathbf{u}) = 1 - (e^2/\pi m v^2)\varrho(\mathbf{r}-\mathbf{u}) . \tag{5}$$

Since for a static crystal

$$\varrho(\mathbf{r}-\mathbf{u}) = \frac{1}{V}\sum_H F_H \exp\left[-2\pi i \mathbf{B}_H . (\mathbf{r}-\mathbf{u})\right] . \tag{6}$$

Equation (5) takes the form

$$\varepsilon'(\mathbf{r}) = 1 - (e^2/\pi m v^2)\frac{1}{V}\sum_H F_H \exp\left[-2\pi i \mathbf{B}_H(\mathbf{r}-\mathbf{u})\right] . \tag{7}$$

F_H is the structure amplitude corresponding to the static lattice and $\mathbf{B}_H$ is the reciprocal lattice vector for the reflection $\mathbf{H}(hkl)$. As it is more convenient to work with $1/\varepsilon'(\mathbf{r})$ we shall obtain an expansion for that. If α' and α are the dynamic and static polarizabilities per unit volume, then, since $\alpha', \alpha \ll 1$, we have

$$1/(\varepsilon'(\mathbf{r})) = 1/(1+4\pi\alpha'(\mathbf{r})) = 1 - 4\pi\alpha'(\mathbf{r}) = 1 - 4\pi\alpha(\mathbf{r}-\mathbf{u}) . \tag{8}$$

Putting $4\pi\alpha'(\mathbf{r}) = \psi'(\mathbf{r})$, $4\pi\alpha(\mathbf{r}) = \psi(\mathbf{r})$, the dielectric constant becomes

$$\varepsilon'(\mathbf{r}) = 1 + \psi'(\mathbf{r}) ,$$

where

$$\psi'(\mathbf{r}) = \psi(\mathbf{r}-\mathbf{u}) = \sum_H \psi_H \exp\left[-2\pi i \mathbf{B}_H . (\mathbf{r}-\mathbf{u})\right] \tag{9}$$

and ψ_H is the Fourier component relevant to the *static* lattice.

Further,

$$\exp\left[2\pi i \mathbf{B}_H . \mathbf{u}\right] = \exp\left[i Z_{Hp} \cos \varphi_p\right] = J_0(Z_{Hp}) + 2\sum_n i^n J_n(Z_{Hp}) \cos n\varphi_p , \tag{10}$$

where

$$Z_{Hp} = 2\pi \mathbf{B}_H . \mathbf{a}_p, \quad \varphi_p = 2\pi(\nu_p t - \mathbf{g}_p . \mathbf{r} - \delta_p) \tag{10a}$$

and J_0, J_n are Bessel functions of order 0 and n. Neglecting higher order terms than the first, we get

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* A further approximation, almost certainly of negligibly small effect, is the expansion or compression of the volume element implicit in equation (3).

$$\exp [2\pi i \mathbf{B}_H . \mathbf{u}] = J_0(Z_{Hp}) + 2iJ_1(Z_{Hp}) \cos \varphi_p = T^p_H + iC^p_H T^p_H (\exp (i\varphi_p) + \exp (-i\varphi_p)), \tag{10b}$$

where

$$T^p_H = J_0(Z_{Hp}),\ C^p_H = J_1(Z_{Hp})/J_0(Z_{Hp}) . \tag{10c}$$

Putting (10*b*) in equation (9), $\psi'(\mathbf{r})$ becomes

$$\begin{aligned}\psi'(\mathbf{r}) &= \sum_H \psi_H \exp [-2\pi i \mathbf{B}_H . \mathbf{r}][T^p_H + iT^p_H C^p_H \\ &\qquad \times (\exp (i\varphi_p) + \exp (-i\varphi_p))] \\ &= \sum_H \psi'_H \exp [-2\pi i \mathbf{B}_H . \mathbf{r}] + \sum_H \psi'^p_H [\exp (i\varphi_p) \\ &\qquad + \exp (-i\varphi_p)] \exp [-2\pi i \mathbf{B}_H . \mathbf{r}] ,\end{aligned} \tag{11}$$

where

$$\psi'_H = \psi_H T^p_H,\ \psi'^p_H = i\psi_H T^p_H C^p_H . \tag{11a}$$

From (11*a*) we get for the forward scattering for which $H=0$, $B=0$, $T_0=1$ that

$$\psi'_0 = \psi_0 . \tag{11b}$$

3. Dispersion relations

The field vectors ($\mathbf{D}'$, the displacement vector, $\mathbf{H}'$, the magnetic vector, $\mathbf{E}'$, the electric vector) must everywhere satisfy Maxwell's equation for an electromagnetic field in an insulating medium.

$$\text{Curl } \mathbf{H}' = (1/c)\, (\partial \mathbf{D}'/\partial t) . \tag{12a}$$

$$\left.\begin{array}{l}\text{Curl } \mathbf{E}' \\ \text{Curl } \mathbf{D}'/\varepsilon' \\ \text{Curl } (1-\psi')\mathbf{D}'\end{array}\right\} = -(1/c)\, (\partial \mathbf{H}'/\partial t) . \tag{12b}$$

In order to get a solution, in the case of the static crystal, $\mathbf{D}$ and $\mathbf{H}$ are expanded in terms of plane waves as

$$\mathbf{D} = \exp [2\pi i \nu t] \sum_H \mathbf{D}_H \exp [-2\pi i \boldsymbol{\beta}_H . \mathbf{r}] . \tag{13}$$

$$\mathbf{H} = \exp [2\pi i \nu t] \sum_H \mathbf{H}_H \exp [-2\pi i \boldsymbol{\beta}_H . \mathbf{r}] . \tag{14}$$

This expansion is guessed at, knowing from Ewald's theory that the wave field consists of plane waves, the wave vectors of any two of which differ by a reciprocal lattice vector. In order to guess the correct expansions for $\mathbf{D}'$ and $\mathbf{H}'$ pertinent to the dynamic case, we remember the result of the Faxén–Waller theory that in the diffracted beam, in addition to the unmodified wave of frequency ν and wave vector $\boldsymbol{\beta}_H$, modified waves of frequency $\nu \pm \nu_p$ and wave vectors $\boldsymbol{\beta}_H \pm \mathbf{g}_p$ are produced. This fact and the form of equation (11) suggest that $\mathbf{D}'$ and $\mathbf{H}'$ may be written as follows:

$$\begin{aligned}\mathbf{D}' &= \exp [2\pi i \nu t] \sum_H \mathbf{D}'_H \exp [-2\pi i \boldsymbol{\beta}_H . \mathbf{r}] + \exp [2\pi i \nu t] \\ &\quad \times \sum_H \mathbf{D}'^p_H \exp [-2\pi i \boldsymbol{\beta}_H . \mathbf{r}] [\exp (i\varphi_p) + \exp (-i\varphi_p)] .\end{aligned} \tag{15}$$

$$\begin{aligned}\mathbf{H}' &= \exp [2\pi i \nu t] \sum_H \mathbf{H}'_H \exp [-2\pi i \boldsymbol{\beta}_H . \mathbf{r}] + \exp [2\pi i \nu t] \\ &\quad \times \sum_H \mathbf{H}'^p_H \exp [-2\pi i \boldsymbol{\beta}_H . \mathbf{r}] [\exp (i\varphi_p) + \exp (-i\varphi_p)] .\end{aligned} \tag{16}$$

Note that φ_p contains both time and position coordinates.

In order that coherence conditions may be satisfied, each frequency component has to be dealt with separately. Choosing only the components involving the frequency ν in $\mathbf{D}'$, $\mathbf{H}'$ and $(1-\psi')\mathbf{D}'$, we get

$$\mathbf{D}' = \exp [2\pi i \nu t] \sum_H \mathbf{D}'_H \exp [-2\pi i \boldsymbol{\beta}_H . \mathbf{r}] \tag{17}$$

$$\mathbf{H}' = \exp [2\pi i \nu t] \sum_H \mathbf{H}'_H \exp [-2\pi i \boldsymbol{\beta}_H . \mathbf{r}] . \tag{18}$$

$$\begin{aligned}(1-\psi')\mathbf{D}' &= \exp [2\pi i \nu t] [\sum_H \mathbf{D}'_H \exp [-2\pi i \boldsymbol{\beta}_H . \mathbf{r}] \\ &\quad - \sum_M \sum_L \psi'_M \mathbf{D}'_L \exp [-2\pi i (\boldsymbol{\beta}_L + \mathbf{B}_M) . \mathbf{r}]]\end{aligned} \tag{19a}$$

(we neglect quantities of still smaller order in $\psi' D'$).

Since $\boldsymbol{\beta}_L + \mathbf{B}_M = \boldsymbol{\beta}_{L+M}$, and as the sums extend to infinity, we may put $L+M=H$ and sum over H instead of over M, when (19*a*) takes the form

$$\begin{aligned}(1-\psi')\mathbf{D}' &= \exp [2\pi i \nu t] [\sum_H \mathbf{D}'_H \exp [-2\pi i \boldsymbol{\beta}_H . \mathbf{r}] \\ &\quad - \sum_H \sum_L \psi'_{H-L} \mathbf{D}'_L \exp [-2\pi i \boldsymbol{\beta}_H . \mathbf{r}]] .\end{aligned} \tag{19b}$$

Putting the equations (17), (18) and (19*b*) in (12*a*) and (12*b*) the dispersion relations are at once obtained as

$$\sum_L [\psi'_{H-L} (\boldsymbol{\beta}_H . \mathbf{D}'_L) \boldsymbol{\beta}_H - \psi'_{H-L} \beta^2_H \mathbf{D}'_L] = (k^2_0 - \beta^2_H) \mathbf{D}'_H \tag{20}$$

upon which is to be based the study of interference phenomena. Here $k_0 = \nu/c$ where c is the velocity of light.

4. Intensity of reflection from a perfect crystal traversed by an acoustic wave

In order to see clearly the effect of atomic oscillations on the intensity of X-ray reflection, consider the simple case of a finite bounded crystal of thickness t_0, having plane boundaries. Assume that only one reciprocal lattice point $\mathbf{B}_H$ lies near the surface of the sphere of reflection. We shall consider specifically an internal reflection (the 'Laue' case). Employing arguments similar to those used by Zachariasen (1945) in deriving *his* equations 3·107 to 3·130, we arrive at the result that

$$I'_H / I'^e_0 = |x'_1 x'_2 (c'_1 - c'_2) / (x'_2 - x'_1)|^2 \tag{21}$$

instead of equation 3·130 of Zachariasen. I'_H and I'^e_0 are the intensities of the diffracted and incident beams, x'_1, x'_2 are the amplitude ratios given by

$$\left.\begin{array}{l} x'_1 \\ x'_2 \end{array}\right\} = [-z \pm (q' + z^2)^{\frac{1}{2}}]/\psi'_{\bar{H}} . \tag{22}$$

$$c_1' = \exp\left[-2\pi i (k_0 \delta_{01}'/\gamma_0) t_0\right],\ c_2' = \exp\left[-2\pi i (k_0 \delta_{02}'/\gamma_0) t_0\right] \tag{23}$$

with the following abbreviations

$$\left.\begin{matrix}\delta_{01}'\\ \delta_{02}'\end{matrix}\right\} = \tfrac{1}{2}\left[\psi_0 - z \pm (q' + z^2)^{\frac{1}{2}}\right]. \tag{24}$$

$$z = \tfrac{1}{2}(1-b)\psi_0 + \tfrac{1}{2} b \alpha_H,\ q' = b \psi_H' \psi_{\bar{H}}' \tag{25}$$

$$b = \gamma_0/\gamma_H \tag{26}$$

(ratio of the direction cosines of the incident and diffracted beams)

$$\alpha_H = (1/k_0^2)(B_H^2 + 2\mathbf{k}_0^e . \mathbf{B}_H) \tag{27}$$

$$\mathbf{k}_0^e = \mathbf{u}_0^e/\lambda_0$$

$\mathbf{u}_0^e$ = propagation direction of incident wave outside the crystal, λ_0 = wave length of X-rays in vacuum. After some manipulation equation (21) can be reduced to the form

$$I_H'/I_0'^e = b^2 |\psi_H'|^2 \exp\left[-\mu_0 t\right] \times \left[\sin^2(av') + \sinh^2(aw')\right]/|q' + z^2|, \tag{28}$$

where μ_0 = linear absorption coefficient and

$$v' + iw' = (q' + z^2)^{\frac{1}{2}},\ a = \pi k_0 t_0/\gamma_0,\ t = \tfrac{1}{2}(1/\gamma_0 + 1/\gamma_H) t_0 . \tag{29}$$

When there is no absorption $\psi_{\bar{H}}' = \psi_H'^*$,

$$\psi_H' \psi_{\bar{H}}' = |\psi_H'|^2,\ \mu_0 = 0,\ w' = 0,$$
$$v' = (b|\psi_H'|^2 + z^2)^{\frac{1}{2}}$$

and in terms of

$$A' = a\sqrt{(|b|)}K|\psi_H'| \tag{30}$$

$$\begin{aligned} y' &= z/[\sqrt{(|b|)}K|\psi_H'|] \\ &= \tfrac{1}{2}(1-b)\psi_0 + \tfrac{1}{2} b\alpha_H/[\sqrt{(|b|)}K|\psi_H'|] \end{aligned} \tag{31}$$

the power ratio takes the simple form

$$\frac{P_H'}{P_0'} = (1/b)(I_H'/I_0'^e) = \sin^2\left[A'(1+y'^2)^{\frac{1}{2}}\right]/(1+y'^2). \tag{32}$$

Here K is the polarization factor, being $|\cos 2\theta|$ for parallel polarization and 1 for normal polarization. The integrated intensity in the y' scale for a thick crystal comes out (just as in the static case) as

$$R_H^{y'} = \int \frac{P_H'}{P_0'} dy' = \pi/2 \tag{33}$$

as P_H'/P_0' in the dynamic case and P_H/P_0 in the static case are of the same form (see Zachariasen's equations 3·140 to 3·152). Hence the integrated intensity in the glancing angle scale for a dynamic crystal is

$$\varrho_H' = R_H^{y'}(d\theta/dy') = \pi|\psi_H'|K/(2\sqrt{(|b|)}\sin 2\theta_B) \tag{34}$$

and for a static crystal, the integrated intensity in the glancing angle scale is

$$\varrho_H = R_H^{y}(d\theta/dy) = \pi|\psi_H|K/(2\sqrt{(|b|)}\sin 2\theta_B). \tag{35}$$

Hence the temperature factor comes out to be

$$\varrho_H'/\varrho_H = |\psi_H'|/|\psi_H| = T_H^p \tag{36}$$

using (11*a*).

Equation (36) holds also for a surface reflection (the 'Bragg' case). Employing similar arguments as for the 'Laue' case, we get

$$I_H'/I_0'^e = |x_1' x_2' (c_1' - c_2')/(c_2' x_2' - c_1' x_1')| \tag{37}$$

from which the integrated intensity for a thick crystal comes out as

$$R_H^{y'} = \pi . \tag{38}$$

Hence the intensity in the glancing angle scale is

$$\varrho_H' = R_H^{y'}(d\theta/dy') = \pi|\psi_H'|K/[\sqrt{(|b|)}\sin 2\theta_B] \tag{39}$$

which at once leads to the expression for the temperature factor as

$$\varrho_H'/\varrho_H = |\psi_H'|/|\psi_H| = T_H^p$$

exactly as for an internal reflection.

5. Temperature factor for a perfect crystal

We may now consider the case of a crystal in thermal vibration. The displacements of the atoms may then be analyzed in terms of a number of waves and the results of the previous section have only to be summed over all p. Instead of equation (2), we have

$$\mathbf{u} = \sum_p \mathbf{a}_p \cos 2\pi(\nu_p t - \mathbf{g}_p . \mathbf{r} - \delta_p) \tag{40}$$

when

$$\exp 2\pi i \mathbf{B}_H . \mathbf{u} = \prod_p \exp\left[i Z_H \cos\varphi_p\right] \tag{41}$$

$$= \prod_p \left[J_0(Z_{Hp}) + 2iJ_1(Z_{Hp})\cos\varphi_p\right] \tag{41a}$$

$$\begin{aligned} &= \prod_p J_0(Z_{Hp}) + 2i\sum_s \left[\prod_p J_0(Z_{Hp})\right] \\ &\quad \times (J_1(Z_{Hs})/J_0(Z_{Hs})\cos\varphi_s \end{aligned}$$

$$= T_H + 2i\sum_s T_H C_H^s \cos\varphi_s \tag{41b}$$

(to a first approximation)

where

$$T_H = \prod_p J_0(Z_{Hp}),\ C_H^s = J_1(Z_{Hs})/J_0(Z_{Hs}). \tag{41c}$$

Putting equations (40) and (41*b*) instead of equations (2) and (10*b*) in equation (9), we have

$$\begin{aligned} \psi' &= \sum_H \psi_H T_H \exp\left[-2\pi i \mathbf{B}_H . \mathbf{r}\right] + i\sum_H\sum_s \psi_H T_H C_H^s \\ &\quad \times \exp\left[-2\pi i \mathbf{B}_H . \mathbf{r}\right]\left[\exp(i\varphi_s) + \exp(-i\varphi_s)\right] \\ &= \sum_H \psi_H' \exp\left[-2\pi i \mathbf{B}_H . \mathbf{r}\right] + \sum_H\sum_s \psi_H'^s \\ &\quad \times \exp\left[-2\pi i \mathbf{B}_H . \mathbf{r}\right]\left[\exp(i\varphi_s) + \exp(-i\varphi_s)\right]. \end{aligned} \tag{42}$$

Proceeding as before we obtain

$$\langle\overline{\varrho_H'/\varrho_H}\rangle = \langle\overline{T_H}\rangle . \tag{43}$$

The bar and ⟨ ⟩ indicate that equation (43) is not only to be averaged over time, but an appropriate statistical weight factor has also to be used for each wave depending on its frequency. Carrying out the averaging, we find (Ramachandran, 1949)

$$\langle \overline{T_H} \rangle = \langle \overline{\prod_p J_0(Z_{Hp})} \rangle = \exp(-M) \qquad (43a)$$

where, with its usual significance,

$$M = (8\pi^2/3)\,(\sin^2\theta/\lambda^2)\overline{u^2}. \qquad (44)$$

Thus we arrive at the result that the integrated intensity of a non-absorbing perfect dynamic crystal is less than the integrated intensity of a non-absorbing perfect static crystal by a factor $\exp(-M)$. It is instructive to see how this reduction is brought about. Taking for example the 'Bragg' case, there is total reflection over a range $-1 < y' < 1$ (just as in the static case where the range of total reflection is $-1 < y < 1$). In the glancing angle scale, the range of total reflection is from

$$(-K|\psi'_H|)/(\sqrt{(|b|)}\sin 2\theta_B) \text{ to } (+K|\psi'_H|)/(\sqrt{(|b|)}\sin 2\theta_B)\,.$$

Thus we see that the effect of thermal oscillation is not to destroy the property of total reflection over a finite range of angles, but only to decrease the range over which the total reflection occurs by a factor $\exp(-M)$ thereby causing the decrease in the value of integrated intensity. Thus the effect of thermal oscillations is to sharpen the reflection curve in the case of perfect crystals. This may not be true however in the case of absorbing crystals. (For a mosaic crystal, we know that the thermal vibration does not affect the sharpness of reflection.) For the 'Laue' case, and perfect crystal, the peak value of P'_H/P'_0 (in the P'_H/P'_0 versus y' curve) is still $\frac{1}{2}$ at $y'=0$ just as in the static case, but the half-width at half-maximum is given by

$$w_{y'} = 1 \quad \text{or} \quad w_\theta = |K\psi'_H|/(\sqrt{(|b|)}\sin 2\theta_B)\,.$$

This again shows that effect of thermal vibration is to sharpen the diffraction pattern of a perfect crystal.

Thus, finally, we get the interesting result that for a perfect non-absorbing crystal the temperature factor correcting the intensity is only $\exp(-M)$ and not $\exp(-2M)$ as in the mosaic crystals. This is because of the fact that while there is a tendency to reduce the intensity by a factor $\exp(-2M)$ when the atoms are oscillating (considered from the kinematical view point), there is an opposing tendency to increase the intensity due to a decrease in primary extinction. These together so balance as to give a reduction of intensity for a perfect non-absorbing crystal only by a factor $\exp(-M)$. Thus we see that the effect of temperature vibration is to change the structure amplitude F of the static crystal to $F\exp(-M)$. Since the integrated intensity of a perfect crystal is proportional to the first power of the structure factor, the temperature factor correcting the intensity comes out to be only $\exp(-M)$. For an ideally mosaic crystal where the intensity is proportional to F^2 the temperature factor becomes $\exp(-2M)$. It is possible also to envisage intermediate types of crystals where the temperature factor may be of the form $\exp(-PM)$ where P may have a value between 1 and 2. This behaviour is analogous to what is obtained in the case of the polarization factor (K for perfect crystal and K^2 for mosaic crystal). This variation of the polarization factor has been made use of for assessing the degree of perfection of crystals (Ramaseshan & Ramachandran, 1954; Chandrasekharan, 1959). It appears, therefore, that the temperature factor also could be used in a similar way to determine the degree of perfection of crystals by measuring the integrated intensity at two different temperatures. The experimental difficulty is however slightly greater in this case and also one cannot be certain that increase of temperature by itself does not lead to an imperfection. In fact, from light scattering studies, such an increase in imperfection has been found to occur in the case of quartz (Humphreys–Owen, 1956).

Although the theory has been developed essentially for X-ray diffraction, it is obvious that the results can be carried over to the diffraction of electrons and neutrons by perfect crystals, as the dynamical theories of these phenomena are quite similar to that of X-ray diffraction.

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