LETTERS TO THE EDITORS

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Diffuse Reflexion of X-Rays

I WISH to add some remarks concerning the theory of the new effect described by G. D. Preston in his article published under the above title in NATURE of April 19, p. 467. A critical study of the suggestions brought forward by Sir C. V. Raman and Sir William Bragg showed that they cannot be accepted as possible explanations, and some photographs kindly sent to me by Mrs. Lonsdale convinced me that the effect ought to be a consequence of Debye's well-known theory of the influence of thermal vibrations on the scattering of X-rays. As the literature on this subject, although extended, is not satisfactory, I have (in collaboration with Miss K. Sarginson) reconsidered the problem assuming that the scattering power of each single atom is known, and only the influence of the atomic vibrations is to be determined.

Apart from the effect on the intensity of the Laue spots (treated by Debye, Waller and others), there exists a background scattering given by an expression which is not an average over the vibrations (as specific heat is) but depends explicitly on their amplitudes and frequencies. The expressions are rather complicated. In order to simplify them we have assumed that the vectorial waves of atomic vibrations can be approximately replaced by scalar waves. Even then the formula is too complicated to be written down here. It gives a definite intensity distribution of the scattered light for any direction of the incident beam relative to the crystal. It depends, apart from the universal constants, h, k, c, on the wave-length λ of the X-rays and some properties of the atoms and the lattice: the lattice constant, the atomic weight and the function $\omega(\mathbf{q})$ representing the elastic frequencies as a function of the wave vector $\mathbf{q}$. In fact, the intensity is in this approximation a monotonically decreasing function of this $\omega(\mathbf{q})$; therefore the maxima of intensity coincide with the minima of $\omega(\mathbf{q})$.

This result explains most of the features which have been discussed in connexion with the extra spots. The first point is the fact that each extra spot is associated with a Laue spot which it passes when the crystal is rotated, with rapidly changing intensity (increasing for approach to the Laue spot). Indeed, the Laue spots are given by the absolute minima $\omega(2\pi\ ) = 0$ ($\mathbf{h} = (h_1\ h_2\ h_3)$ three integers), which occur only for definite relative positions of crystal and incident ray. If the crystal is rotated the wave vector $\mathbf{q}$, as argument of $\omega(\mathbf{q})$, has to satisfy the relation

$$\mathbf{q} = \mathbf{K}' - \mathbf{K},$$

where $\mathbf{K}, \mathbf{K}'$ are the wave vectors of the incident and scattered beam. If $\mathbf{K}$ is given, $\omega(\mathbf{q})$ is a function of $\mathbf{K}'$ which has relative minima: these are the centres of the extra spots. This result, that the position of the spots is closely connected with the vibrational spectrum of the crystal, is very remarkable. It leads immediately to an understanding of the success of Sir William Bragg's formula. I cannot accept Preston's and Bragg's suggestion that there exist little groups of atoms (such as Bragg's cubes) which scatter independently of the rest of the crystal. This explanation is based on the assumption that the interference effects are due to the *geometry* of the lattice. In fact, these new interferences, which depend on temperature, are due to the *dynamics* of the lattice. One has merely to assume that the forces between the atoms are negligible except for first neighbours; then $\omega(\mathbf{q})$ becomes a periodic function in the reciprocal lattice of the very type from which Bragg derives his formula. We obtain precisely Bragg's formula for a body-centred cubic lattice, and very similar ones for other cubic lattices. But we get in addition a reasonable law for the intensity as a function of temperature which cannot be obtained by any purely geometrical explanation.

We have also studied in detail the behaviour of the extra spots in the neighbourhood of a Laue spot h, with the help of a development in powers of $\varphi - \varphi_h$, the angular displacement of the crystal from the position corresponding to a Laue spot. If the direction of the incident beam is taken as x-axis, and the crystal is rotated about the y-axis, we obtain for the direction cosines ξ, η, ζ ($\xi^2 + \eta^2 + \zeta^2 = 1$) of the scattered beam

$$\begin{cases} \eta - \eta_h = \eta_h \xi_h (\varphi - \varphi_h) \\ \xi - \xi_h = (\zeta_h^2 + \xi_h - 1)(\varphi - \varphi_h), \end{cases}$$

where ξ_h, η_h, ζ_h is the direction vector of the Laue spot. These formulæ are purely geometrical and give no information about the physical mechanism. The same holds for the formula giving the angle χ between the extra ray and the Laue ray, for which one obtains

$$\chi = 2 \sin^2 \frac{\theta_h}{2} (\varphi - \varphi_h)$$

where θ_h is the deflexion angle of the Laue spot, which has been derived by several authors (Faxen, Raman, Jauncey, Preston, Lonsdale) on different assumptions.

The physical assumptions of the theory can be tested only by a discussion of the expression obtained for the intensity distribution. We have determined the shape of the spot, that is, the lines of equal intensity; they are ellipses the minor axes of which coincide with the meridian passing through the Laue spot. We have further calculated the maximum and the total intensity of the extra spot; these depend on the neighbouring Laue spot, on the temperature, the wave-length of the X-rays, and the constants of the crystal, chiefly the maximum frequency ω_m of the elastic spectrum, or the corresponding temperature $\theta' = h\omega_m/k$. All results are in qualitative agreement with the observations.

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