The Scattering of X-rays by Gases and Crystals

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It is shown that, in exact agreement with the wave mechanical result worked out by Wentzel and Waller and Hartree, the Raman-Compton-Jauncey formula for the scattering of x-rays by an atom deduced on the basis of classical electrodynamics may be written

$$I_\phi = I_e\left\{F^2 + Z - \sum_{r=1}^{z} E_r^2\right\}, \qquad \text{(A)}$$

where I_ϕ is the intensity scattered in a direction ϕ with the primary beam, I_e is the scattering from a single isolated electron as calculated by Thomson, Z is the atomic number, E_r is the average amplitude of the waves scattered by the r-th electron in the atom and F is the true atomic structure factor as given by $F=\Sigma_1^z E_r$. This shows that the coherent scattering is proportional to F^2 and that the introduction of the average atomic structure factor F' by Jauncey is unnecessary. On the basis of Eq. (*A*), theoretical formulas for the scattering of x-rays by gases and crystals are redeveloped and the results turn out to explain all the disagreement between theories proposed by Jauncey and the writer.

IN DISCUSSING the scattering of x-rays by polyatomic gases, Jauncey[1] has recently pointed out that the theoretical formula deduced by the writer[2] is not exactly in agreement with that obtained by himself. Since the writer regards the atoms in a polyatomic system (a molecule or a crystal) as the scattering units, this disagreement should also occur when the scattering of x-rays by crystals is dealt with. The purpose of the present note is to discuss this matter in detail.

Taking account of the modification introduced by Jauncey,[3] the Raman-Compton[4] formula for the scattering of x-rays by an atom may be written

$$I_\phi = I_e\{F'^2 + Z - F'^2/Z\}, \qquad (1)$$

where I_ϕ is the intensity scattered at an angle ϕ to a distance R, I_e is the scattering from a single isolated electron as calculated by J. J. Thomson, Z is the atomic number and F' is the average atomic structure factor. According to Jauncey,[3] the relation between the average atomic structure factor F' and the true atomic structure factor F is expressed by

$$F'^2 = F^2 - \left(Z\sum_{r=1}^{Z} F_r^2 - F^2\right)\Big/(Z-1), \qquad (2)$$

[1] G. E. M. Jauncey, Phys. Rev. **39**, 561 (1932).
[2] Y. H. Woo, Phys. Rev. **39**, 555 (1932).
[3] G. E. M. Jauncey, Phys. Rev. **37**, 1193 (1931).
[4] C. V. Raman, Indian J. Phys. **3**, 357 (1928). A. H. Compton, Phys. Rev. **35**, 925 (1930).

where E_r is the average amplitude of the waves scattered by the r-th electron in the atom and where the true atomic structure factor F is given by

$$F = \sum_{r=1}^{Z} E_r. \tag{3}$$

In view of the similarity between Eq. (1) and the formula originally derived by Raman and Compton,[4] the part $I_e F'^2$ was taken[5] by analogy to represent the coherent scattering and the other terms to represent the incoherent scattering. However, there exists no physical or mathematical reason for justifying this separation. On substituting the value of F' given by (2) into Eq. (1), we find as a result of straightforward calculation

$$I_\phi = I_e \left\{ F^2 + Z - \sum_{r=1}^{Z} E_r^2 \right\}. \tag{4}$$

This is exactly the same expression as that obtained by Wentzel[6] and independently by Waller and Hartree[7] on the basis of wave mechanics. This shows that the coherent part of the total intensity is proportional to F^2 and that the introduction of the average atomic structure factor F' by Jauncey is unnecessary. When corrected for the change of wave-length, Eq. (4) becomes

$$I_\phi = I_e F^2 + I_e \frac{Z - \sum_{1}^{Z} E_r^2}{[1 + \gamma(1 - \cos\phi)]^3}, \tag{5}$$

where $\gamma = h/mc\lambda$ and h, m, c and λ have their usual significance.

Recently Herzog[8] has actually compared Eq. (5) with experiments reported by Wollan[9] on absolute measurements of the scattering of Mo K_α rays by helium, neon and argon gases. The agreement seems to be quite satisfactory.

On the basis of Eq. (5) and following the arguments presented by the writer in previous papers,[10] the theoretical formulas for the scattering of x-rays by gases and crystals can be easily redeveloped. For the scattering from a simple cubic crystal consisting of atoms of one kind, the diffusely scattered intensity is given by

[5] Cf. G. E. M. Jauncey, Phys. Rev. **38,** 1 (1931); **39,** 561 (1932); Y. H. Woo, Phys. Rev. **39,** 555 (1932).

[6] G. Wentzel, Zeits. f. Physik **43,** 1 and 779 (1927).

[7] I. Waller, Zeits. f. Physik **51,** 213 (1928); Waller and Hartree, Proc. Roy. Soc. **A124,** 119 (1929). The more exact formula obtained by these authors differs from Eq. (4) by including some negative terms arising from consideration of Pauli's principle, but the contribution to the total scattering due to these negative terms is negligible in comparison with that due to the terms included in Eq. (4).

[8] G. Herzog, Zeits. f. Physik **70,** 583 and 590 (1931). Cf. also Y. H. Woo, Sci. Rep. Tsing, Univ. AI, No. 4 (1932).

[9] E. O. Wollan, Phys, Rev. **37,** 862 (1931).

[10] Y. H. Woo, Proc. Nat. Acad. Sci. **17,** 467 (1931); Phys. Rev. **38,** 6 (1931), and **39,** 555 (1932).

$$I_\phi = NI_e\left\{(1 - e^{-2M})F^2 + \frac{Z - \sum_1^Z E_r^2}{[1 + \gamma(1 - \cos\phi)]^3}\right. \cdot \tag{6}$$

For the intensity scattered by a gas molecule containing atoms $I, \cdots i, \cdots n$ arranged at fixed distances from each other, the formula becomes

$$I_{\phi n} = I_e \sum_1^n \sum_1^n F_i F_j \frac{\sin kS_{ij}}{kS_{ij}} + I_e \sum_1^n \frac{Z_i = \sum_1^{Z_i} E_r^2}{[1 + \gamma(1 - \cos\phi)]^3} \cdot \tag{7}$$

In Eq. (6) N is the number of atoms per unit volume of the crystal and e^{-2M} is the temperature factor as calculated by Debye[11] and Waller[12] and in Eq. (7) F_i is the true atomic structure factor for the i-th atom, $k = (4\pi/\lambda)\sin\frac{1}{2}\phi$, s_{ij} is the distance of any atom i from any other atom j. The other quantities have the same meaning as those employed in Eq. (5). When applied to the scattering by a diatomic gas consisting of two like atoms, Eq. (7) gives for the scattering per electron

$$S = \frac{I_{\phi 2}}{2ZI_e} = \left(1 + \frac{\sin kS}{kS}\right)\frac{F^2}{Z} + \frac{1 - \frac{1}{Z}\sum_1^Z E_r^2}{[1 + \gamma(1 - \cos\phi)]^3} \tag{8}$$

where s is the distance between the two atoms in the scattering molecule.

It will be noticed that Eq. (6) agrees with the formula deduced by Jauncey and Harvey[13] provided the latter is properly corrected for the change of wavelength. Also a comparison of Eqs. (7) and (8) with those recently obtained by the writer[14] and Jauncey[15] will clearly show that, if the coherent and incoherent scattering be properly separated, the disagreement pointed out by Jauncey no longer exists. Finally, referring the comparison between theory and experiment recently made by the writer,[14] it can be readily concluded that Eq. (8) is supported by Wollan's measurements[16] on the scattering of Mo K_α radiation by diatomic gases.

[11] P. Debye, Ann. d. Physik **43,** 49 (1914).
[12] I. Waller, Zeits. f. Physik **17,** 389 (1923); *Upsala Dissertation,* (1925).
[13] Jauncey and Harvey, Phys. Rev. **37,** 1203 (1931).
[14] Y. H. Woo, Phys. Rev. **39,** 555 (1932).
[15] G. E. M. Jauncey, Phys. Rev. **39,** 561 (1932).
[16] E. O. Wollan, Phys. Rev. **37,** 862 (1931); Proc. Nat. Acad. Sci. **17,** 475 (1931).