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THE SCATTERING OF X-RAYS AND ELECTRON DISTRIBUTION IN THE ATOMS OF CRYSTALS

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Abstract

Critical examination of the method of obtaining the atomic structure-factor and of the Fourier analysis method of determining electron distributions in crystals.—Theories of the Compton effect suggest that modified scattering of x-rays may take place at the expense of regular reflection, and consequently that the atomic structure-factor, which is determined from experimental measurements of the intensity of regular reflection and upon which is based our most direct means of determining electron distribution in atoms, may not represent all of the electrons in the atom. It is therefore necessary to consider critically the determinations of electron distribution in the atoms of crystals which have previously been made. The classical theory, when applied in the form of Darwin's equation to the measured intensities of regular reflection, gives values of the atomic structure factor for Li, C, O, F, Na, Al, Cl, Ca, Fe, which are in accord with our ideas concerning atomic structure. It is shown (this was previously an assumption) that the coefficients of the Fourier's series which is used in determining the electron distribution are all positive in the experimental cases heretofore dealt with. The application of the Fourier analysis to a model argon atom indicates that the accuracy of the analysis depends predominantly upon the accuracy of measurement of the intensities of reflection within angular limits which are easily subject to experimental investigation. Electron distributions obtained from Fourier analysis of the experimentally determined atomic structure-factor curves for several different atoms or ions contain almost exactly the amounts of electricity which we believe from other considerations to exist in the crystals, within radii in good agreement with those calculated from interatomic distances determined by ordinary crystal analysis. Modification of the calculated F values of model atoms to take into account the Compton effect results in F curves which give, upon Fourier analysis, unreasonable distributions of diffracting power. The Fourier analysis can give reasonable distributions of electron density only if the F curves are approximately correct. Since the experimental F curves do give reasonable distributions, it is concluded that any modification which is caused by the Compton effect in the intensity of regular reflection of x-rays is negligible.

Introduction

THE use of atomic structure-factor curves obtained from measurements on the intensity of reflection of x-rays by crystals is our most direct means of determining the electron distribution in atoms. Until recently it was generally conceded that the atomic F curves calculated from experimental intensity measurements with the aid of Darwin's equation[1] represent the variation of scattering power of atoms in which all the electrons are scattering equally effectively. To the contentions that some of the more tightly bound electrons might not scatter as efficiently as the ones with less binding energy, while some of the more loosely bound electrons might be spending a part of their time scattering radiation of modified wave-length

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[1] Darwin, Phil. Mag. **43**, 800 (1922).

and hence would also fail to scatter unmodified radiation with full efficiency, answer was made that the experimental F curves give electron distributions which are in accord with what we expect from other considerations and, if corrected by a considerable amount, would give unreasonable electron distributions. Before such an answer can be considered satisfactory, it is necessary to establish the validity of the method of determining electron distribution, and to show that modification of the true F curve of an atom as suggested by the quantum theory of scattering has a considerable effect upon the electron distribution determined by the Fourier analysis. The author proposes to treat these two problems in the following manner: first, to consider critically the method of obtaining the "atomic structure-factor" from experimental measurements of the intensity of "regular reflection"; second, to investigate further the Fourier analysis method of determining the electron distribution in the atoms of crystals; third, to apply the Fourier analysis to F curves from model atoms before and after the F values are modified to take into account the Compton effect.

It is important to bear in mind the fact that the quantum theories of x-ray scattering,[2] which strongly imply the existence of some influence of the modified scattering process upon that of regular reflection, have been created in the effort to explain the existence and relative intensities of the modified and unmodified scattered radiation at various angles of scattering; and the only test of these theories lies in the measurements of the relative intensities of the modified and unmodified scattered radiation. Experiments on intensity and directional distribution of scattered radiation have not been performed with sufficient accuracy to decide between the classical and the quantum theory. Had it not been for the work on scattering of γ-rays and of x-rays of very short wave-length, Compton's observation of a wave-length shift and the resulting cloud expansion experiments, we should still have no occasion to demand other than a classical theory of scattering. In fact the phenomenon of regular reflection is so well taken care of by the classical theory that one hesitates to admit quantum scattering into the same picture.

REGULAR REFLECTION AND ATOMIC STRUCTURE-FACTOR

Regular reflection has been subjected to a much more severe quantitative examination than any other scattering phenomenon. Darwin's classical theory[1] of the intensity of reflection by an imperfect crystal is upheld by experiments which have been made by a variety of different methods. Bragg, James and Bosanquet[3] and Wasastjerna[4] determined the absolute intensity of reflection from a single crystal of rock-salt, obtaining values, on the basis of Darwin's expression, in close agreement with each other and in accord with our present ideas concerning atomic structure. Bearden[5] made a determination of the absolute intensity of reflection from powdered NaCl,

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[2] Jauncey, Phys. Rev. **29**, 757 (1927).

[3] W. L. Bragg, James and Bosanquet, Phil. Mag. **42**, 1 (1921).

[4] Wasastjerna, Soc. Scient. Fenn. Comm. Phys. Math. **2** No. 15 (1924).

[5] Bearden, Phys. Rev. **29**, 20 (1927).

obtaining a value in close agreement with that of Bragg, James and Bosanquet. His measurements by the powdered crystal method and those of the author[6] have served further to confirm Darwin's treatment of reflection by an imperfect crystal. Darwin's equation has been used by the aforementioned workers and by Claassen[7] and Ponte[8] to obtain atomic structure-factor curves for the following atoms or ions: Li, C, O, F, Na, Al, Cl, Ca, Fe. The F curves are about what are to be expected from our notions concerning the number and distribution of electrons in these atoms. A change of more than about twenty percent in the observed F values at small angles would upset either our ideas concerning atomic structure or our faith in the Darwin equation. *The experimental work on the intensity of regular reflection does not require us to adopt a quantum theory.* Only the fact that a quantum theory is necessary to explain other scattering phenomena leads us to inquire whether the same theory can be disregarded in the case of regular reflection.

Nevertheless, it must be borne in mind that errors in Darwin's expression for the intensity of x-ray reflection, or in the experimental determination of this intensity, will work entirely at the expense of the F curves. For Darwin has attempted to take into account every factor outside of the atom, and has inserted an "atomic structure-factor" in his expression to take care of what goes on inside of the atom. As we have seen, it is highly improbable that there can be any unconsidered factor operating at small angles of reflection; but one cannot be certain from mere inspection of the F curves that some factor is not operative which, negligible at small angles, increases in importance with increasing angle.*

It is the existence of just such a factor that the quantum theory of scattering suggests. Concerning the validity of Darwin's theory, the quantum theory can have nothing more to say than to indicate the possible omission of some important factor in the scattering process. On the classical theory, all the electrons of an atom scatter radiation of the same wave-length, the variation of the F curve with angle of reflection being due to the fact that the electrons are not concentrated at the midplanes of atomic layers in the crystal. The quantum theory requires that a part of the electrons scatter radiation of modified wave-length during a part of the time, being unable to contribute to the F curve during this part of the time. That is, following Jauncey,[2] the regular reflection is due only to scattering from the u electrons; the s electrons are engaged in scattering modified radiation. The s electrons are those most loosely bound and would contribute not a great deal to the F curve, but their number increases as the angle of scattering increases, and

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[6] Havighurst, Phys. Rev. **28,** 869, 882 (1926).

[7] Claassen, Proc. Phys. Soc. London **38,** 482 (1926).

[8] Ponte, Phil. Mag. **3,** 195 (1927).

* In this connection it should be mentioned that objection has been raised by Bishop, Phys. Rev. **28,** 625 (1926), and Kirkpatrick, Phys. Rev. **29,** 632 (1927), to intensity calculations which are based upon the assumption that the incident radiation was completely unpolarized. If Bishop's interpretation of his experiments, that the characteristic radiation from a Mo tube is as much as 15 percent polarized, is accepted, the polarization factor of Darwin's equation would be altered so as to increase the author's F values at large angles 5–10 percent.

their potential contribution to the F curve at large angles, where the observed values of F are small, might be relatively great. It appears possible, then, that the experimental F curves are in considerable error, especially at large angles. Williams[9] and Jauncey[2] have attempted to calculate the approximate amount of this error.

The assumption is made in the work of Williams and Jauncey that modification takes place equally probably at the expense of regularly reflected and diffusely scattered unmodified radiation. That is, that the number of s electrons, for scattering at any particular angle, is the same in an atom which is scattering independently as in an atom which is scattering in conjunction with other atoms. Although this assumption seems justified, Williams suggests the possibility of an effective increase of mass of the scattering electrons when their atoms are scattering in conjunction which would, at the reflecting angle, transform all s electrons into u electrons. It is easy to suppose that regular reflection results from a process quite independent of that of modified scattering, and the author inclines to such a possibility as the best solution of the problems raised in this discussion.

If we admit the necessity of applying a correction for the Compton effect to experimental F curves, we find the direct determination of such a correction impossible. The only data on which to base the correction are the relative intensities of modified and unmodified scattered radiation at various angles, and for the use of such data one would need to have a model of the atom in which the positions of the s electrons were designated.

Williams[9] and Jauncey[2] have attempted to calculate the effect of modified scattering upon the F curve calculated by Hartree's method[10] for a model atom. Their procedure is to determine the potential F contributions from the s electrons at various angles of scattering, and to correct Hartree's curve by these amounts. They obtain modified F curves which are more nearly in accord with experimental ones than are the original Hartree curves. It must be remembered that whatever "agreement of theory with experiment" they obtain depends entirely upon the assumed correctness of Hartree's atomic models, which are based upon the Stoner scheme and empirical screening constants for the different electronic orbits. Atomic F curves from the model atoms of Pauling,[11] obtained on the basis of Schrödinger's mechanics and empirical screening constants, are different from those of Hartree, the differences being chiefly due to the fact that Pauling's electron distributions are continuous. This continuousness of electron distribution would give a smoothness to the calculated F curves which Hartree's curves lack, and would bring them more nearly in accord with experimental curves. Corrections to such curves for the influence of modified scattering would be different from those to Hartree's curves.

We are thus left in a predicament if we recognize the necessity of correcting the experimental F curves. An experimental correction for modified

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[9] Williams, Phil. Mag. **2,** 657 (1926).

[10] Hartree, Phil. Mag. **50,** 289 (1925).

[11] Pauling, Proc. Roy. Soc. **A114,** 181 (1927); J. Amer. Chem. Soc. **49,** 765 (1927).

scattering is impossible, and the empirical corrections vary with the atomic model adopted.

Fourier Analysis and Electron Distribution

If we admit that the experimental F curves may be in appreciable error because of the effect of modified scattering, we should criticize the electron distributions obtained therefrom. Before making such a criticism, it is advisable to consider somewhat closely the limitations of the Fourier analysis method of determining electron distribution.

Fourier analysis. Following Duane,[12] we may write the general term of the Fourier's series representing the volume density $\rho(xyz)$ of the diffracting power at a point in the unit cell of a crystal as

$$A_{n_1n_2n_3} \sin\left(2\pi n_1 x/a_1-\delta_{n_1}\right) \sin\left(2\pi n_2 y/a_2-\delta_{n_2}\right) \sin\left(2\pi n_3 z/a_3-\delta_{n_3}\right) \qquad (1)$$

$A_{n_1n_2n_3}$ is proportional to the structure factor for diffraction from the $n_1n_2n_3$ plane, where $n_1n_2n_3$ are the Miller indices of the different crystal planes multiplied by the order of diffraction; a_1, a_2, a_3 are the lengths of sides of the unit cell, and the δ's are phase constants. It was stated by Duane, and reiterated by the author[13] that in order to obtain a unique distribution of diffracting power from the series, it is necessary to make two assumptions, as follows: 1. The distribution of diffracting power conforms to the symmetry of the crystal. This symmetry fixes the values of the δ's. 2. All the coefficients of the Fourier series have positive values at the center of the heaviest atom of the unit cell.

While there seems to be no objection to the first of these assumptions, the second is by no means necessarily valid. The actual A values in the series are square roots of measured intensities, so that the sign of any A is quite undetermined. Further consideration of the significance of these A values, however, leads us to understand why the second assumption was valid for all of the previous applications of the Fourier analysis. The A values of (1) are really F values, being taken from the experimental F curves. The question, then, is whether the F values ever have negative signs. At small angles, the F values are undoubtedly positive, and it is not until the F^2 curve touches zero that there can be any possibility of negative F values. Since our experimental F^2 curves do not reach to zero and are simply extrapolated to that point, the F values must be all positive. If an experimental F^2 curve were obtained which touched zero and then rose again, it would be a question whether the F curve had crossed zero and become negative, or had touched zero and risen again to positive values. The F curve from a model sodium atom discussed in a previous paper,[13] without including the effect of thermal vibration, does cross zero, and some of the A's in the Fourier's series representing electron density are negative.

Model argon atom. Electron distributions calculated by Compton,[14] Bearden,[5] and the author[13] for Na and Cl from very similar experimental

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[12] Duane, Proc. Nat. Acad. Sci. **11,** 489 (1925).

[13] Havighurst, Phys. Rev. **29,** 1 (1927).

[14] A. H. Compton, X-Rays and Electrons, Chap. 5. Van Nostrand and Co., New York, 1926.

data show differences at large distances from the centers of the atoms which make it desirable to investigate the limits of accuracy of the Fourier analysis. Since all experimental F curves must be extrapolated to zero at large angles of reflection, the method of extrapolation may affect the final distribution of electrons given by the analysis. Furthermore, Compton and Bearden extrapolated their F curves to zero value of sin θ, using the number of electrons in the ion which is supposed to exist in the crystal as the final F value. At least one point from this extrapolated curve is used in each of their determinations of radial electron distribution. The author has not made this latter extrapolation because he wished to avoid all assumptions as to the amount of diffracting power associated with a lattice point. In order to determine the effect of errors in various parts of the F curve on the result of the Fourier analysis, the author has made use of a model argon atom with electrons arranged on concentric spherical shells as follows:

2 electrons on a shell of radius 0.03A
8 electrons on a shell o. radius 0.20A
2 electrons on a shell of radius 0.80A
6 electrons on a shell of radius 1.00A

f and F values were calculated in the same way as was done for the model sodium ion in a previous paper,[13] the same temperature factor being used. F and $n\ F_n$ values are plotted in the upper part of Fig. 1 against sin θ for $\lambda = 0.1126$A. It is seen that the discreteness of the electron distribution in the model atom has produced marked changes of slope in the F curve. Probably no actual atom has such a discrete electron distribution, but it is to our advantage to subject the Fourier analysis to an especially rigid examination by the adoption of such an improbable arrangement. The electron distribution obtained by Fourier analysis of the calculated F curve is given as the heavy line curve of the lower part of Fig. 1. Compton's expression[14] for the radial electron density was used:

$$Udr = 4\pi r/D \sum_{1}^{\infty}(2nF_n/D) \sin (2\pi nr/D)dr \tag{2}$$

We want to determine the effect of arbitrary changes in various parts of the F curve upon the electron distribution. The region over which it would be possible for the author to make experimental investigation is included between abscissa values $0.02-0.13$ in the upper figure.

First, let us change the value of F_1, which would be an extrapolated point in the method used by Compton and Bearden. A change of 10 percent in F_1 has so little effect upon the electron distribution that a new curve need not be drawn. Now let us change the values of the F's at large angles by making the extrapolation shown with the dotted line (a) in the $n\ F_n$ curve. The electron distribution becomes that shown by the dotted line (a) of the lower figure. Larger changes in the extrapolation would produce greater changes in the electron distribution, but nothing very important. One can understand this, for with small values of $n\ F_n$ and increasing periodicity, the higher members of the series tend to neutralize each other, and add very little to the total electron density. Of course, if experimental *F* values were confined to rather small angles, or if the *F* curve had not fallen to a fairly low value before extrapolation, the effect of the extrapolated part of the curve would be more important. But the chief characteristics of the radial distribution curve are due to the $n\ F_n$ values which are greatest—that is, to those which may be determined experimentally. Consider the effect of a slight smoothing of the *F* curve, something which might conceivably be done by an experimenter who obtained a curve such as that given in the figure. If the *F* curve is smoothed as shown by the broken line (*b*) and the corresponding broken $n\ F_n$ curve, values of several of the *F*'s are changed by 2–10 percent. The effect of these changes is shown by the broken line (*b*) of the electron distribution curve. The area under this curve is only 16.7 electrons. Evidently, accurate determinations of the *F* values within the ordinary range of investigation are necessary to a correct electron distribution curve, while the extrapolated portion of the curve is of secondary importance.

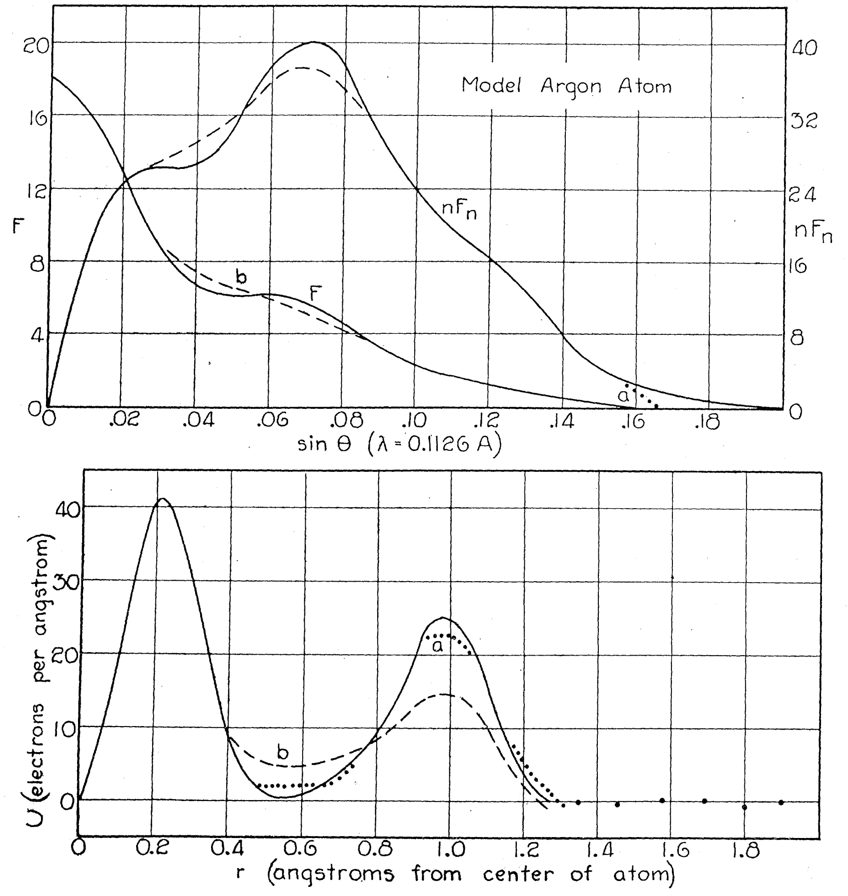

Fig. 1. *F* curve and electron distribution curve for model argon atom.

Do experimental F curves represent all electrons? From the foregoing consideration it is evident that, provided the F curves represent electrons which are scattering radiation equally effectively at all angles, we may place faith in the results of the Fourier analysis.

Does modified scattering influence the F curve of an atom? In the attempt to answer this question we must consider the electron distributions given by Fourier analysis of experimental F curves, and also the distributions resulting when the Fourier analysis is applied to F curves which have been calculated from model atoms with and without allowance for possible modification due to the Compton effect.

Each experimental F curve must give a distribution of diffracting power which is possible—that is, one which has no great negative values and which has a radius within the bounds set by interatomic distances as determined in ordinary crystal analysis. If such a distribution is not given, either the experimental data are wrong or the method is unsound. *Every experimental F curve has given a reasonable distribution of diffracting power.*[13]

From the point of view of Jauncey's theory, we may say that the U curves obtained from Eq. (2) and experimental F values should be false, for they are based upon F curves to which the electrons contribute with varying efficiency at various angles. The Fourier analysis is meant to be applied to F values from an atom in which the number of electrons effective in scattering unmodified x-rays is the same at all angles of scattering. The Fourier analysis assumes this condition to be true, and is unable to cope with the situation presented by Jauncey's theory, where the number of electrons effective in scattering unmodified radiation varies with the angle of scattering. Application of the Fourier analysis to F values from an atom of the latter sort would probably result in an electron distribution which was absurd. The absurdity would not, however, take the form of an unreasonably small area under the U curve, for the number of electrons must equal the value of F at $\sin\theta=0$, and F at $\sin\theta=0$ is unaffected by the Compton effect. The value of F at $\sin\theta=0$ does not enter into expression (2) and no extrapolated or assumed value is necessary; expression (2), however, when integrated, gives the value of F at $\sin\theta=0$, *provided the spacing used in (2) is large enough.* Here lies the absurdity of the electron distributions obtained by Fourier analysis of F curves which have been modified by some influence similar to that of the Compton effect. The spacing necessary to contain all the electrons of an atom is greater than the maximum spacing allowed to that atom by the results of ordinary crystal analysis.

Effect of empirical corrections for Compton effect. It will aid us in properly estimating the force of the foregoing paragraph to find out what change in electron distribution is caused by an approximate modification of an F curve from a model atom for the Compton effect. Jauncey has calculated the modifications to be made in the F curve of a Hartree model Cl^- ion, and gives F values[15] for the modified curve which should be experimentally ob-

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[15] Private communication. The author is indebted to Professor Jauncey for his criticism of this paper.

tained as a result of the effect of modified scattering, assuming, of course, that the atom model used by Hartree is correct. These F values are given in Table I in the column headed F_u. The model atom has its electrons arranged as follows:

$2K$	electrons in circular orbits with radius	0.0335A
$2L_I$	electrons in elliptical orbits with av. r	0.314
$6\ L_{III}$	electrons in circular orbits with radius	0.165
$2\ M_I$	electrons in elliptical orbits with av. r	1.21
$6\ M_{III}$	electrons in elliptical orbits with av. r	1.21

The author has multiplied the original F values of Jauncey by a temperature factor $e^{-.006n^2}$ in order to secure a more rapidly convergent series. The inclusion of such a factor results in a small increase in the radius of each shell and makes each shell rather diffuse in structure, but otherwise has no effect.

TABLE I

F values from model atoms, modified by the Compton effect.

Cl^- model $D_1=7.10A.$ $\lambda=0.710A.$				Argon model $D_1=5.628A.$ $\lambda=0.1126A.$					
n	F_u	n	F_u	n	F_c	F_u	n	F_c	F_u
0	18	15	0.92	0	18	18	15	.31	.35
1	16.80	16	.70	1	16.36	15.55	16	.17	.27
2	13.02	17	.54	2	12.61	11.31	17	.11	.20
3	10.35	18	.41	3	8.83	8.86	18	.08	.15
4	8.42	19	.31	4	6.72	6.98	19	.03	.12
5	6.88	20	.23	5	6.22	5.65	20	−.01	.09
6	5.73	21	.17	6	6.27	4.48	21	−.01	.07
7	4.67	22	.11	7	5.77	3.54	22	.01	.05
8	3.88	23	.08	8	4.63	2.78	23	.02	.04
9	3.24	24	.06	9	3.28	2.12	24	.02	.03
10	2.72	25	.04	10	2.35	1.61	25	.02	.02
11	2.25	26	.03	11	1.79	1.22	26	.01	.01
12	1.85	27	.02	12	1.42	0.89			
13	1.49	28	.01	13	0.99	.65			
14	1.18	29	.01	14	.60	.48			
		30	.00						

Upon application of the Fourier analysis with the F_u values of Cl^- from Table I and a first order spacing of $D=3.55A$, the curve on the right of Fig. 2 is obtained, ending in the dotted line (c). Under this curve is an area of 16.4 electrons. Evidently too small a spacing was used in the analysis. With a first order spacing of 7.10A, the full line curve (b) is obtained, and the area under the curve is 18.7 electrons. Comparison of the curves resulting from this analysis and the model atom from which the F values were obtained shows that a false distribution has been given by the Fourier analysis. There is no trace of the hump of eight electrons which should appear at a radius of ca. 1.2A. One comes to the conclusion that the F values used in the analysis were wrong; but the F values were obtained from the correct values by modification supposed to be due to the Compton effect. If experimental F values for Cl gave a U curve similar to that of Fig. 2, containing too little electricity unless the radius is absurdly large, one might conclude that the experimental F values were suffering from modification due to the Compton effect. However, the experimental F values from Cl, upon Fourier analysis, give a U curve which contains 18 electrons within a radius which is almost exactly the same as that attributed to Cl^- upon the basis of interatomic distances as determined in ordinary crystal analysis. If one is justified in assuming that the Hartree model is a fairly adequate representation of the atom, one is brought to the conclusion that the experimental F curves, which do *not* cause the same peculiarities in their U curves as those that result from calculated F values modified by Compton effect, and which *do* give reasonable distributions of electrons, have not been appreciably influenced by the Compton effect.

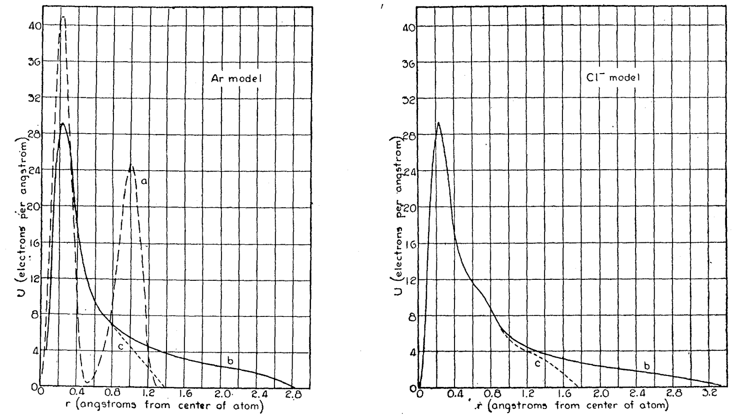

Fig. 2. Electron distributions in model atoms whose F curves have been modified by the Compton effect.

To make the point more clear, let us modify the author's F values for a model argon atom in the manner suggested by Jauncey's theory, and then apply the Fourier analysis to the new set of F values. In Table I under the heading F_c are the author's calculated F values for the model argon atom previously described. The F_u values, which represent F_c modified by the influence of the Compton effect have been calculated by the use of Eq. (3) of Jauncey's paper[2] upon the assumption that $T = V$, where $V = 0.0242/\lambda_s$ if λ_s is expressed in angstrom units. The values of λ_s are as follows[16]:

	K	L_{I}	L_{III}	M_{I}	M_{III}
λ_s	3.865A	22.2	51.7	196.	784.

The broken curve (a) in the left-hand part of Fig. 2 is the same as the full line curve in the lower part of Fig. 1, and represents the electron distribution obtained by a Fourier analysis of the F_c values. The area under this curve is 18 electrons. Application of the Fourier analysis to the argon F_u values of Table I for a spacing of $D = 2.814\text{A}$ gives the dotted line curve (c), which

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[16] K. T. Compton and F. L. Mohler, Bull. Nat. Res. Coun. No. 48 (1924). From $(\nu/R)^{1/2}$ values given on page 109.

coincides with the full line curve during most of its course. Under curve (*c*) the area is 14.1 electrons. When F_u values for a first order spacing of 5.628A are used, the full line curve (*b*) results from the analysis. Under this curve the area is 18.2 electrons. But there is no trace of the hump representing the *M* electrons, and the radius is unreasonably large.

From the standpoint of the Fourier analysis, the consequences of a modification of the *F* values of an atom as suggested by Jauncey's theory are seen to consist of the production of a false electron distribution with an unreasonably large radius. Since the Fourier analysis of experimental *F* values does not give such a patently false electron distribution, the logical conclusion is that the experimental *F* values must not have been affected by the Compton effect in the manner supposed by Jauncey's theory.

CONCLUSION

Although we have seen that the quantum theory of scattering of x-rays, which accounts qualitatively for the Compton effect, suggests the existence of an effect that modifies the atomic-structure factor and which should consequently cause our Fourier analysis determinations of electron distribution to be patently false, yet we find in the electron distribution curves obtained from experimental *F* curves no evidence of falseness which might be attributed to the workings of such an effect. If the Fourier analysis method of determining electron distribution is sound and accurate (this the author believes has been demonstrated), the conclusion is that any modification, caused by the Compton effect, in the intensity of regular reflection of x-rays is very small, and may be neglected.

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Note added November 11, 1927. The recent appearance of articles by Waller [*Nature,* **120,** 155 (1927); *Phil. Mag.* (in press)] and by Wentzel, [*Zeits. f. Physik,* **43,** 779 (1927)], treating the Compton effect on the basis of the Schrödinger theory, serves to illuminate much more clearly the problem of Compton effect and experimental *F* curves. In a paper on "The Intensity of X-ray Reflection" which he presented at the Solvay Conference, W. L. Bragg has made use of the results of Waller and Wentzel in an excellent discussion of the application of Fourier analysis to the determination of electron distribution. Stated briefly, these investigations lead to the conclusion that "the coherent part of the scattered radiation may be directly calculated from the continuous distribution of electricity which is defined by the Schrödinger density distribution in the initial state of the atom." Experimental *F* curves are therefore a measure of the Schrödinger continuous distribution of electricity in the crystal lattice. The results of the author's calculations are to be regarded as confirmatory of Schrödinger's theory in this particular application.