

X-RAY SCATTERING BY ATOMS

1.1 CLASSICAL SCATTERING BY A FREE ELECTRON

When an x-ray beam falls on an atom, two processes may occur: (1) the beam may be absorbed with an ejection of electrons from the atom, or (2) the beam may be scattered. We shall first consider the scattering process in terms of classical theory. The primary beam is an electromagnetic wave with electric vector varying sinusoidally with time and directed perpendicular to the direction of propagation of the beam. This electric field exerts forces on the electrons of the atom producing accelerations of the electrons. Following classical electromagnetic theory, an accelerated charge radiates. This radiation, which spreads out in all directions from the atom, has the same frequency as the primary beam, and it is called scattered radiation.

We shall first consider the scattering from a single free electron following classical theory. One might suppose that this is a waste of time, since we know that x-ray scattering does not follow classical theory. Experimentally we observe both an unmodified scattering with the same wavelength as the primary beam, and a Compton modified scattering with a longer wavelength. Classical theory predicts only the unmodified scattering. However, there are several reasons why the intensity of classical scattering is extremely important for much of what we shall do. (1) The correct wave mechanical treatment of scattering shows that the sum of the intensities of unmodified and modified scattering from each individual electron in the atom is closely equal to the classical intensity per electron. (2) The quantitative unit in which it is convenient to express the scattered intensity from a sample is the electron unit. An intensity in electron units I_{eu} is the intensity from a sample divided by the classical intensity from a single electron. (3) The polarization of both the unmodified and the modified scattering is given correctly by the classical treatment.

Let us consider a single free electron at the origin of Fig. 1.1, with an unpolarized primary beam directed along the X -axis. We are interested in the intensity of scattered radiation at a point P which is at a distance R from the electron at an angle ϕ with the X -axis. We choose the other axes so that the point P is in the XY -plane. Since the primary beam is unpolarized, the electric vector takes with equal probability all orientations in the YZ -plane.

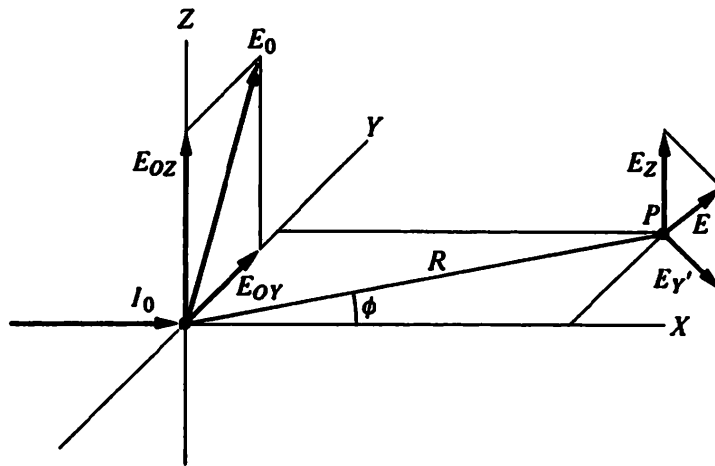


Fig. 1.1 Classical scattering of an unpolarized primary beam by a single free electron at the origin.

We can choose one direction E_0 and later average over all directions. Since it is a vector, E_0 can be resolved into components E_{0Y} and E_{0Z} . If ν is the frequency of the primary beam, the instantaneous values of the electric fields are

$$\epsilon_{0Y} = E_{0Y} \sin 2\pi\nu t, \quad \epsilon_{0Z} = E_{0Z} \sin 2\pi\nu t.$$

Considering first the component ϵ_{0Y} , a force is exerted on the electron which produces a Y -component of acceleration

$$a_{Y'} = \frac{f_{Y'}}{m} = \frac{eE_{0Y}}{m} \sin 2\pi\nu t,$$

where e and m are the charge and mass of the electron.

From electromagnetic theory an accelerated charge radiates. Figure 1.2 illustrates a charge q with an acceleration \mathbf{a} , and at distance R , the electric field ϵ which results from the acceleration. In terms of cgs units, which for x-ray scattering are the simplest, the electric field is given by

$$\epsilon = \frac{qa \sin \alpha}{c^2 R}, \quad (1.1)$$

where c is the velocity of light. The electric field is in the plane of R and α , and its magnitude depends upon the component $a \sin \alpha$. This leads to a very

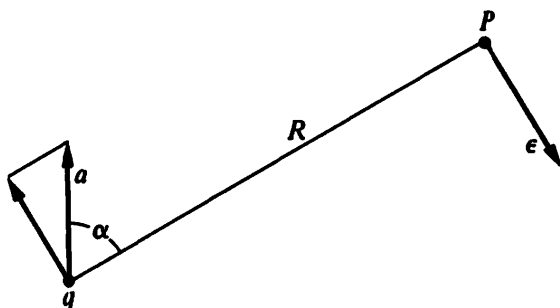


Fig. 1.2 Illustration of the electric field ϵ , produced by a charge q with acceleration a , according to classical electromagnetic theory.

simple and useful rule in considering problems of scattering and polarization. With the eye placed at the point of observation P , the component of acceleration $a \sin \alpha$, which is seen, determines the electric field produced.

By means of Eq. (1.1), we can now express the instantaneous value of the electric field due to the acceleration $a_{1'}$:

$$\epsilon_{1'} = \frac{e^2 E_{0Y'}}{mc^2 R} \sin 2\pi\nu t \cos \phi.$$

Expressed in terms of an amplitude, $\epsilon_{1'} = E_{1'} \sin 2\pi\nu t$ where the amplitude is given by

$$E_{1'} = \frac{e^2 E_{0Y'}}{mc^2 R} \cos \phi.$$

Similar reasoning applied to the initial amplitude E_{0Z} leads to

$$E_Z = \frac{e^2 E_{0Z}}{mc^2 R}.$$

The resultant amplitude E at the point of observation is then given by

$$E^2 = E_Z^2 + E_{1'}^2 = \frac{e^4}{m^2 c^4 R^2} (E_{0Z}^2 + E_{0Y'}^2 \cos^2 \phi).$$

We now let E_0 take with equal probability all orientations in the YZ -plane and consider the appropriate averages

$$\langle E_{0Y'}^2 \rangle + \langle E_{0Z}^2 \rangle = \langle E_0^2 \rangle.$$

Since the Y - and Z -axes are equivalent,

$$\langle E_{0Y'}^2 \rangle = \langle E_{0Z}^2 \rangle = \frac{1}{2} \langle E_0^2 \rangle$$

and

$$\langle E^2 \rangle = \langle E_0^2 \rangle \frac{e^4}{m^2 c^4 R^2} \left(\frac{1 + \cos^2 \phi}{2} \right). \quad (1.2)$$

The observable quantity is the intensity I , where by intensity we shall always mean energy per unit area per unit time. In cgs units, the intensity is given by

$$I = \frac{c}{8\pi} \langle E^2 \rangle,$$

where E is the amplitude or maximum value of a sinusoidally varying field. Multiplying both sides of Eq. (1.2) by $c/8\pi$, we obtain

$$I = I_0 \frac{e^4}{m^2 c^4 R^2} \left(\frac{1 + \cos^2 \phi}{2} \right). \quad (1.3)$$

Equation (1.3) gives the intensity of classical scattering by a single free electron, and it is often called the Thomson scattering equation. The factor $(1 + \cos^2 \phi)/2$ is called the polarization factor for an unpolarized primary beam. If the primary beam is not unpolarized, the polarization factor takes a different form. The numerical value involved in Eq. (1.3) is important. Since we are using cgs units, R is in cms, and

$$\frac{e^4}{m^2 c^4} = \frac{(4.802 \times 10^{-10})^4}{(9.107 \times 10^{-28})^2 (2.998 \times 10^{10})^4} = 7.94 \times 10^{-26} \text{ cm}^2.$$

At a few centimeters from a single electron, the ratio I/I_0 is therefore of the order 10^{-26} , and one might think that the intensity of scattered x-rays would be far too small to measure. However when we recall that in even 1 milligram of matter the number of electrons is approximately 10^{20} , we see that the intensity of scattered radiation from a sample of matter is not necessarily too small to measure.

1.2 POLARIZATION BY SCATTERING

For x-rays there are no Nicol prisms or polaroid sheets to produce polarization. However, scattering at any angle will produce partial polarization, and scattering at 90° produces complete linear polarization. An example of a polarizer and analyzer is given by Fig. 1.3. An unpolarized x-ray beam directed along the X -axis falls on a scatterer such as a block of carbon at O .

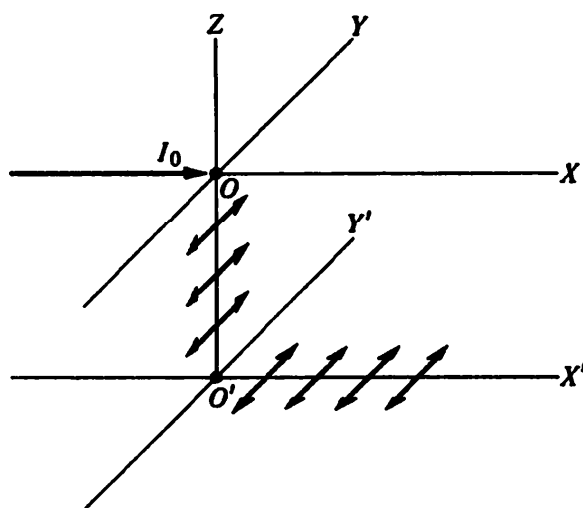


Fig. 1.3 A double scattering experiment which illustrates the production of a polarized beam by scattering at 90° , and the analysis of the polarized beam by a second scattering at 90° .

The electrons in the block are accelerated in all directions in the YZ -plane. To determine the nature of the scattered radiation from O to O' , we use the rule which was discussed in connection with Eq. (1.1). Placing the eye at O' and looking back toward the scatterer at O , we see only the Y -component of the electron accelerations. Hence the scattered radiation from O to O' will be linearly polarized with electric field in the Y -direction. The scattering at 90° has produced a polarized beam.

To analyze the polarization, imagine a second scatterer at O' . The electrons at O' will be accelerated only in the Y' -direction. With the eye placed at X' , we see the full component of the Y' -acceleration, and hence there will be a scattered beam along the X' -axis, which is polarized with electric field in the Y' -direction. Placing the eye at Y' , we see no component of the Y' -acceleration of the electrons and hence the intensity of scattering along the Y' -axis is zero. A recorder pivoted at O' and moving in the $X'Y'$ -plane, would record a maximum at X' and zero at Y' . The second scattering at 90° plays the role of an analyzer.

Since the Bragg reflections from a crystal are nothing but sharp maxima in the scattered radiation, any Bragg reflection at approximately $2\theta = 90^\circ$ is a linearly polarized beam. Scattering is often done with blocks of low atomic number such as carbon. In this case an appreciable fraction of the scattered intensity is due to the Compton modified component. However, the polarization of both the unmodified and the Compton modified scattering follows exactly the same rules that have been developed here for classical scattering.

1.3 SCATTERING FROM SEVERAL CENTERS, COMPLEX REPRESENTATION

Our next problem is to formulate a simple procedure for handling the scattering from several centers. In Fig. 1.4 we have a plane parallel beam directed toward the right. Scattering takes place from several centers, 1, 2, 3, n , and we are interested in the intensity of scattering at a point of observation P .

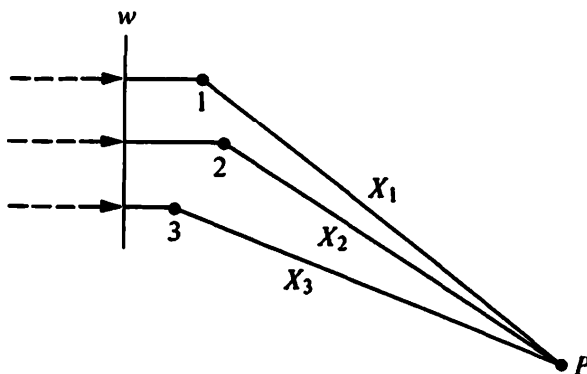


Fig. 1.4 Scattering of a plane parallel primary beam by several scattering centers. The lengths X_n are the total distances from a wave front W in the primary beam to the point of observation P .

The relative phases at P are determined by the path lengths X_1, X_2, X_3, X_n from a wave front W in the primary beam to the point P . The instantaneous value of the electric field at P , in each of the scattered waves, is given by the usual expression for a traveling wave:

$$\epsilon_n = E_n \cos \left(2\pi\nu t - \frac{2\pi X_n}{\lambda} \right), \quad (1.4)$$

where ν is the frequency, λ the wavelength, and the amplitudes E_1, E_2, E_n are, in general, different from one another. Expanded, the equations are written

$$\epsilon_n = E_n \cos 2\pi\nu t \cos 2\pi X_n/\lambda + E_n \sin 2\pi\nu t \sin 2\pi X_n/\lambda.$$

The resultant instantaneous field at P is given by the sum

$$\epsilon = \sum \epsilon_n = \cos 2\pi\nu t \sum E_n \cos \frac{2\pi X_n}{\lambda} + \sin 2\pi\nu t \sum E_n \sin \frac{2\pi X_n}{\lambda}.$$

Let

$$\begin{aligned} \sum E_n \cos \frac{2\pi X_n}{\lambda} &= E \cos \phi, \\ \sum E_n \sin \frac{2\pi X_n}{\lambda} &= E \sin \phi. \end{aligned} \tag{1.5}$$

With these abbreviations, the instantaneous field at P is given by

$$\epsilon = E(\cos 2\pi\nu t \cos \phi + \sin 2\pi\nu t \sin \phi) = E \cos (2\pi\nu t - \phi).$$

Hence the quantity E , which was introduced in Eqs. (1.5), is the amplitude of the resultant field at P . But the only quantity that we can observe at P is the intensity, and in cgs units this is given by

$$I = \frac{cE^2}{8\pi}.$$

Hence it is only E^2 that is of interest to us, and from Eqs. (1.5) this is given by

$$E^2 = \left(\sum E_n \cos \frac{2\pi X_n}{\lambda} \right)^2 + \left(\sum E_n \sin \frac{2\pi X_n}{\lambda} \right)^2. \tag{1.6}$$

To obtain the intensity, we need only the quantity E^2 given by Eq. (1.6). We shall now develop the method of the complex exponential, which is much simpler to use in diffraction problems, and which can be justified by showing that it leads to the same value of E^2 . In terms of $i = \sqrt{-1}$, we write Eq. (1.4) in the complex exponential form

$$\epsilon_n = E_n e^{i[2\pi\nu t - (2\pi X_n/\lambda)]}.$$

Since $e^{-ix} = \cos x - i \sin x$, we can write

$$\epsilon_n = e^{i2\pi\nu t} \left(E_n \cos \frac{2\pi X_n}{\lambda} - i E_n \sin \frac{2\pi X_n}{\lambda} \right).$$

Forming the sum,

$$\epsilon = \sum \epsilon_n = e^{i2\pi\nu t} \left(\sum E_n \cos \frac{2\pi X_n}{\lambda} - i \sum E_n \sin \frac{2\pi X_n}{\lambda} \right).$$

We next write the complex conjugate ϵ^* , which for any complex quantity is obtained by replacing i by $-i$:

$$\epsilon^* = e^{-i2\pi\nu t} \left(\sum E_n \cos \frac{2\pi X_n}{\lambda} + i \sum E_n \sin \frac{2\pi X_n}{\lambda} \right).$$

The product $\epsilon\epsilon^*$ is then given by

$$\epsilon\epsilon^* = \left(\sum E_n \cos \frac{2\pi X_n}{\lambda} \right)^2 + \left(\sum E_n \sin \frac{2\pi X_n}{\lambda} \right)^2. \quad (1.7)$$

Comparing Eqs. (1.6) and (1.7), we see that

$$\epsilon\epsilon^* = E^2. \quad (1.8)$$

Hence by proper use of the complex exponential, we arrive at the quantity E^2 , and this is all that we need to obtain the intensity I .

We shall use the complex exponential representation since it generally simplifies the mathematical manipulations. What we have just proved can be formulated as a set of rules. For each scatterer write in complex form the instantaneous value of the electric field at the point of observation. Sum these values, and form the complex conjugate of the sum. The product of the sum and its complex conjugate is then equal to E^2 the square of the amplitude. The intensity at the point of observation is given by $I = cE^2/8\pi$.

1.4 SCATTERING BY AN ATOM

We first consider the classical scattering from a group of electrons confined to a small volume such as the volume of an atom. The conditions are shown by Fig. 1.5. The primary beam, of amplitude E_0 polarized so that E_0 is normal to the plane of the paper, has a direction represented by the unit vector s_0 . The electrons are clustered about point O , the position of each represented by a vector r_n . We consider scattering at a point of observation P , at a large distance R from the electrons, in a direction given by a unit vector s .

In terms of a wave front through O , the instantaneous value of the field in the primary beam acting on electron n is given by

$$\epsilon_0 = E_0 \cos \left(2\pi\nu t - \frac{2\pi X_1}{\lambda} \right).$$

To represent the magnitude and phase of the scattered beam at P due to electron n , we can multiply by the classical factor for an electron and

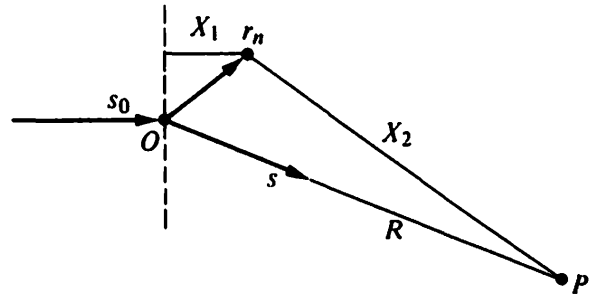


Fig. 1.5 Scattering by a group of electrons at positions r_n . The unit vectors s_0 and s give the direction of the primary beam and the direction to the point of observation P .

consider the total path as $X_1 + X_2$:

$$\epsilon_n = \frac{E_0 e^2}{mc^2 X_2} \cos \left[2\pi\nu t - \frac{2\pi}{\lambda} (X_1 + X_2) \right].$$

This neglects a 180° jump in phase in the scattering, but this is of no importance to the present problem since it is the same for all the electrons. Considering that the source and the point of observation are both at distances very large compared to the length $|\mathbf{r}_n|$, we can make the usual plane wave approximations. In the denominator $X_2 \rightarrow R$, and in the cosine

$$X_1 + X_2 \rightarrow \mathbf{r}_n \cdot \mathbf{s}_0 + R - \mathbf{r}_n \cdot \mathbf{s} = R - (\mathbf{s} - \mathbf{s}_0) \cdot \mathbf{r}_n.$$

Expressed in terms of the complex exponential, the sum of the instantaneous fields at P is given by

$$\epsilon = \frac{E_0 e^2}{mc^2 R} e^{2\pi i[\nu t - (R/\lambda)]} \sum_n e^{(2\pi i/\lambda)(\mathbf{s} - \mathbf{s}_0) \cdot \mathbf{r}_n}. \quad (1.9)$$

However, electrons do not scatter in the manner predicted by classical theory. From both theory and experiment we know that there are two kinds of scattering: (a) unmodified scattering (same wavelength) and (b) Compton modified scattering (longer wavelength). In scattering from a crystal, it is the unmodified scattering which gives rise to the Bragg reflections. The modified scattering from the different electrons is completely incoherent because of the change in wavelength, and accordingly it produces only a diffuse background. A correct treatment of x-ray scattering involves wave mechanical methods which we are not in position to consider here. However, the results of the wave mechanical treatment can be expressed as simple rules which allow us to calculate the unmodified and modified scattering from an atom.

To calculate the unmodified scattering from an atom, we consider that each electron is spread out into a diffuse cloud of negative charge, characterized by a charge density ρ expressed in electron units. The quantity ρdV is the ratio of the charge in volume dV to the charge of one electron, so that for each electron $\int \rho dV = 1$. The wave mechanical treatment then says that the amplitude of unmodified scattering from the element ρdV is equal to ρdV times the amplitude of classical scattering from a single electron. To get the total amplitude of unmodified scattering from one electron, we must integrate over the volume occupied by the electron, and in doing this make proper allowance for the phase of the contribution from each element ρdV .

The instantaneous value of electric field for the unmodified scattering, due to one of the electrons in an atom, is then given directly by Eq. (1.9), by considering that instead of electrons at positions \mathbf{r}_n we have charge

elements ρdV at positions \mathbf{r} , and by replacing the sum by an integral:

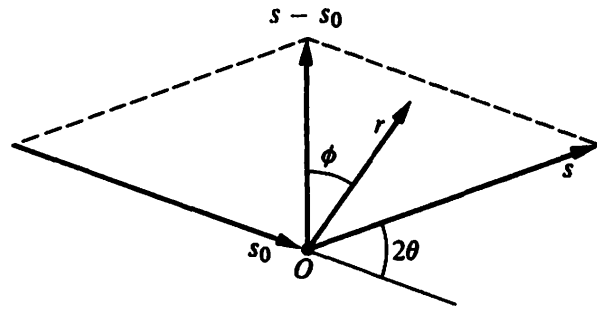
$$\epsilon_e = \frac{E_0 e^2}{mc^2 R} e^{2\pi i [vt - (R/\lambda)]} \int e^{(2\pi i/\lambda)(\mathbf{s}-\mathbf{s}_0)\cdot\mathbf{r}} \rho dV. \quad (1.10)$$

The quantity represented by the integral is called f_e , the scattering factor per electron

$$f_e = \int e^{(2\pi i/\lambda)(\mathbf{s}-\mathbf{s}_0)\cdot\mathbf{r}} \rho dV. \quad (1.11)$$

Evidently f_e is the ratio of the amplitude of unmodified scattering from one electron to the amplitude scattered by an electron according to classical theory. Stated in another way, f_e is the amplitude of unmodified scattering per electron, expressed in electron units.

Fig. 1.6 Relation between the $\mathbf{s} - \mathbf{s}_0$ vector and the vector \mathbf{r} for an atom centered at O .



Of course it is not true that the charge distribution has spherical symmetry for each electron in the atom. However for closed groups of inner electrons, spherical symmetry exists, and we can work with the combined charge distribution for the electrons of a closed group. By assuming spherical symmetry for the charge distribution $\rho = \rho(r)$, and taking the origin at the center of the atom, we obtain a simple expression for f_e . In terms of the quantities represented by Fig. 1.6, $(\mathbf{s} - \mathbf{s}_0) \cdot \mathbf{r} = 2 \sin \theta r \cos \phi$, and with the abbreviation

$$k = \frac{4\pi \sin \theta}{\lambda}, \quad (1.12)$$

we can write

$$f_e = \int_{r=0}^{\infty} \int_{\phi=0}^{\pi} e^{ikr \cos \phi} \rho(r) 2\pi r^2 \sin \phi d\phi dr.$$

The integration with respect to ϕ is readily performed, and we obtain

$$f_e = \int_0^{\infty} 4\pi r^2 \rho(r) \frac{\sin kr}{kr} dr. \quad (1.13)$$

For an atom containing several electrons, the amplitude of unmodified scattering per atom is the sum of the amplitudes per electron:

$$f = \sum_n f_{en} = \sum_n \int_0^{\infty} 4\pi r^2 \rho_n(r) \frac{\sin kr}{kr} dr. \quad (1.14)$$

The quantity f plays an important role in x-ray diffraction theory, and it is usually called the atomic scattering factor. Evidently f is the amplitude of unmodified scattering per atom expressed in electron units (amplitude in units of the amplitude from a single electron according to classical theory). To compute f , we need only to know the radial dependence of the electron density in the atom $\sum_n \rho_n(r)$. For any atom, f is a function of $(\sin \theta)/\lambda$, since it is a function of k . Calling Z the number of electrons in the atom,

$$\sum_n \int_0^\infty 4\pi r^2 \rho_n(r) dr = Z,$$

and f approaches Z at small values of $(\sin \theta)/\lambda$.

The simple treatment of the atomic scattering factor, which we have given here, is based on two assumptions: (a) the x-ray wavelength is much smaller than any of the absorption edge wavelengths in the atom, and (b) the electron distribution in the atom has spherical symmetry. If the first condition is not satisfied, a dispersion correction is necessary. The correction can be expressed in the form

$$f = f_0 + \Delta f' + i \Delta f'', \quad (1.15)$$

where f is the corrected scattering factor, f_0 is the value found in the tables, and $\Delta f'$, $\Delta f''$ are the real and imaginary parts of the dispersion correction. The imaginary part $\Delta f''$ represents a small shift in phase of the scattered radiation. The angular dependence of $\Delta f'$ and $\Delta f''$ is much smaller than that of f_0 . An example in which the second condition is not satisfied is given by the diamond crystal. The lack of complete spherical symmetry in the electron distribution in carbon allows weak Bragg reflections from diamond which could not exist if the distributions had complete spherical symmetry.

To compute the intensity of modified scattering from an atom, we use another result from the wave mechanical treatment. For each electron considered individually, the intensity of unmodified scattering plus the intensity of modified scattering is equal to the intensity of classical scattering per electron. Written in terms of an unpolarized primary beam, and calling i_e the intensity of modified scattering per electron expressed in electron units:

$$\begin{aligned} I_0 \frac{e^4}{m^2 c^4 R^2} \left(\frac{1 + \cos^2 2\theta}{2} \right) f_e^2 + I_0 \frac{e^4}{m^2 c^4 R^2} \left(\frac{1 + \cos^2 2\theta}{2} \right) i_e \\ = I_0 \frac{e^4}{m^2 c^4 R^2} \left(\frac{1 + \cos^2 2\theta}{2} \right) \end{aligned}$$

and hence $i_e = 1 - f_e^2$. Since the modified scattering from the different electrons is incoherent, the intensity of modified scattering per atom is the sum of the intensities of modified scattering from the electrons:

$$i(M) = \sum_n i_{en} = Z - \sum_{n=1}^Z f_{en}^2. \quad (1.16)$$

To illustrate the use of Eqs. (1.14) and (1.16), let us suppose that the electron density for each of the three electrons in neutral Li can be represented by a hydrogen-like expression of the form

$$\rho = \frac{e^{-(2r/a)}}{\pi a^3},$$

where for each K electron $a_K = 0.20 \text{ \AA}$ and for the L electron $a_L = 1.60 \text{ \AA}$. The expression is already normalized so that

$$\int_0^\infty 4\pi r^2 \frac{e^{-(2r/a)}}{\pi a^3} dr = 1.$$

From Eq. (1.13),

$$f_e = \int_0^\infty 4\pi r^2 \frac{e^{-(2r/a)}}{\pi a^3} \frac{\sin kr}{kr} dr = \frac{1}{[1 + (2\pi a \sin \theta/\lambda)^2]^2}$$

and hence

$$f_{eK} = \frac{1}{[1 + (2\pi a_K \sin \theta/\lambda)^2]^2}, \quad f_{eL} = \frac{1}{[1 + (2\pi a_L \sin \theta/\lambda)^2]^2}.$$

From Eq. (1.14), the atomic scattering factor for Li is given by

$$f_{Li} = 2f_{eK} + f_{eL}.$$

Using Eq. (1.16), the intensity of modified scattering in electron units is given by

$$i(M) = 3 - 2f_{eK}^2 - f_{eL}^2.$$

Figure 1.7 shows plots of f_{eK} , f_{eL} , f , and $i(M)$ against $(\sin \theta)/\lambda$ for a neutral Li atom, which for purposes of illustration is supposed to have the assumed charge distribution.

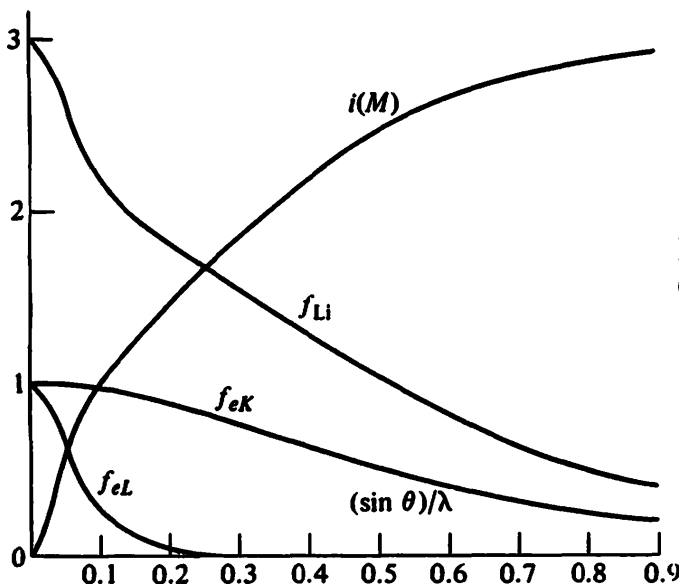


Fig. 1.7 Values of f_{eL} , f_{eK} , f , and $i(M)$ for an assumed charge distribution in neutral Li.

The above treatment is oversimplified. For the modified scattering there is an additional small term coming from cross interaction between the charge densities of different electrons. There is also the Breit Dirac factor $R = (\nu'/\nu)^3$, where ν' is the frequency of the modified scattering and ν is the frequency of the primary beam. The intensity of modified scattering is obtained by multiplying $i(M)$ by the Breit Dirac factor R .

In general it is not necessary to evaluate the various quantities from first principles. Tables of the atomic scattering factor f_0 , the dispersion corrections $\Delta f'$ and $\Delta f''$, and the modified scattering per atom $i(M)$ are given in the International Tables.¹ For K electrons only, the dispersion correction terms $\Delta f'$ and $\Delta f''$ are given in James.² Dispersion corrections for all the electrons have been tabulated by Dauben and Templeton.³ For a thorough treatment of the x-ray scattering by atoms, reference should be made to James.²

REFERENCES

1. *International Tables for X-Ray Crystallography*, Vol. III, 1962.
2. R. W. JAMES: *The Optical Principles of the Diffraction of X-Rays*, G. Bell and Sons Ltd., London, 1948, Chaps. III and IV and p. 608.
3. C. H. DAUBEN and D. H. TEMPLETON: *Acta Cryst.* **8**, 841 (1955).

PROBLEMS

- 1.1 a) An unpolarized primary beam of intensity I_0 is scattered according to classical theory by a single electron. Show that the total scattered power (integral of intensity over area) is given by

$$P = \frac{8\pi}{3} \left(\frac{e^4}{m^2 c^4} \right) I_0.$$

- b) What is the total scattered power if the primary beam has an intensity I_0 and is linearly polarized?

1.2 Assuming classical scattering and incoherency (the intensity from n electrons is n times the intensity from one electron), show that for elements of low atomic number the total scattered power per gram P_{gm} is given by $P_{\text{gm}} = 0.20I_0$.

1.3 A parallel x-ray beam limited by an opening of area 0.50 cm^2 falls upon a 0.10 gm carbon block close to the opening, as shown by Fig. 1.8. The window of the ionization chamber is $2 \times 2 \text{ cm}$, and 5 cm from the carbon block. Assume that for scattering at 90° , the electrons scatter according to classical theory and incoherently (the intensity from n electrons is n times the intensity from one electron). In position A with the block removed, the ionization current is found to be about 2500 times greater than in position B with the block in place. Making reasonable approximations, calculate the number of electrons in the carbon atom.

1.4 A primary beam of wavelength $\lambda = 1.0 \text{ \AA}$, intensity I_0 , small cross-sectional area a_0 , and power $P_0 = I_0 a_0$, falls upon a large flat-faced carbon block. Scattered

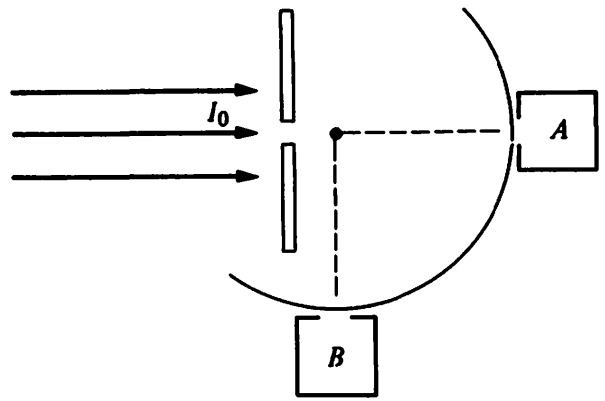


Fig. 1.8 Scattering by a carbon block of an unpolarized primary beam, as considered in Problem 1.3.

radiation is observed at 10 cm from the point of impact. The primary and scattered beams are at 90° to one another, and each makes 45° with the face of the block. Assume that the electrons scatter according to classical theory and incoherently. Making reasonable approximations, what is the value of I/P_0 ? [Hint: Set up the contribution dI from a small volume $a_0 dx$, and allow for absorption. For carbon, and $\lambda = 1.0 \text{ \AA}$, the mass abs. coef. is $\mu_m = 1.37 \text{ cm}^2 \text{ gm}^{-1}$. Answer: $I/P_0 = 4.4 \times 10^{-5} \text{ cm}^{-2}$.]

1.5 The unpolarized x-ray beam of Fig. 1.9 is directed in the XZ -plane at an angle 2θ to the X -axis. It is scattered by a carbon block at O . The scattered radiation arriving at O' is partially polarized and we call its intensity I_0 at point O' . This partially polarized beam is scattered classically by an electron at O' . The intensity of the scattering from O' is measured at a point P distance R from O' and at an angle ϕ with the X -axis. Deduce an expression for I in terms of I_0 , R , θ , and ϕ ,

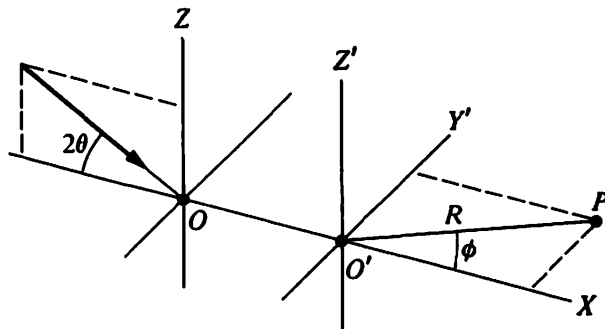
- a) if P is in the XY' -plane;
- b) if P is in the XZ' -plane.

Answer part (b):

$$I = I_0 \frac{e^4}{m^2 c^4 R^2} \left(\frac{1 + \cos^2 2\theta \cos^2 \phi}{1 + \cos^2 2\theta} \right).$$

[Note: The angular factor illustrates the polarization factor for a crystal monochromated beam obtained by using a crystal at O .]

Fig. 1.9 Double scattering of an initially unpolarized beam. The beam scattered by O which falls on an electron at O' is partially polarized. Illustration of Problem 1.5.



1.6 The instantaneous value of the electric field, at the point of observation, due to a number of beams, is

$$\epsilon = \sum_n \epsilon_n = \sum_n E_n e^{i(2\pi\nu t - \phi_n)}.$$

The frequencies ν of the beams are all the same, but the phases ϕ_n are independent of each other and vary randomly with time. This is one example of a set of beams which can be called incoherent with respect to one another. Show that the average intensity is the sum of the individual intensities:

$$\langle I \rangle = \sum_n I_n.$$

1.7 Show that for any atom at very small values of $(\sin \theta)/\lambda$, both the scattering factor f and the intensity of modified scattering $i(M)$ are parabolic functions of $(\sin \theta)/\lambda$, and hence both curves intersect the axis of ordinates with zero slope.

1.8 For the hydrogen atom in the normal state, wave mechanics gives the electron density as

$$\rho = (e^{-2r/a})/\pi a^3, \quad a = 0.53 \text{ \AA}, \quad \int \rho dV = 1.$$

- Derive expressions for f and $i(M)$ as functions of $(\sin \theta)/\lambda$.
- Compute values of f and $i(M)$ for $(\sin \theta)/\lambda = 0.0, 0.2, 0.4$, and compare with the tabulated values.

1.9 Assume that for each of the two electrons in He, the electron density is given by

$$\rho = (e^{-(2r/a)})/\pi a^3, \quad a = 0.32 \text{ \AA}, \quad \int \rho dV = 1.$$

If a beam of $\text{CuK}\alpha$ ($\lambda = 1.54 \text{ \AA}$) falls on a single He atom, at what scattering angle 2θ is the intensity of unmodified scattering equal to that of the modified scattering?

1.10 A beam of $\text{MoK}\alpha$ ($\lambda = 0.71 \text{ \AA}$) falls on a single carbon atom. Using values from the tables, compute the ratio of the total intensity (unmodified plus modified) to that expected if the six electrons scattered according to classical theory and incoherently. Evaluate for $(\sin \theta)/\lambda = 1.1$.

1.11 Assume a model for the carbon atom which is far from reality. Assume that the two K electrons are spread uniformly over the surface of a sphere of radius $r_K = 0.20 \text{ \AA}$ and that the four L electrons are spread uniformly over the surface of a sphere of radius $r_L = 1.50 \text{ \AA}$. Compute and plot f_c as a function of $(\sin \theta)/\lambda$ from 0.0 to 0.6 in steps of 0.1. What incorrect feature in f has been produced by the assumption of spherical shells?