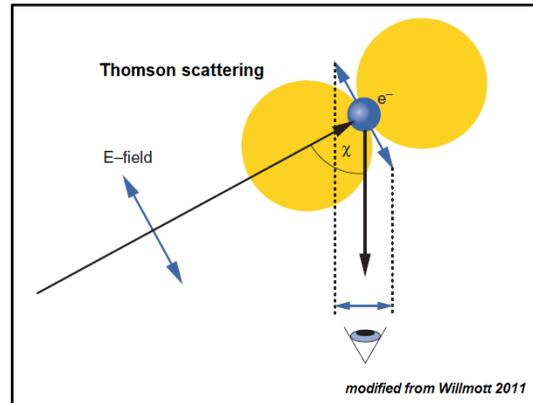


# Notes on x-ray physics

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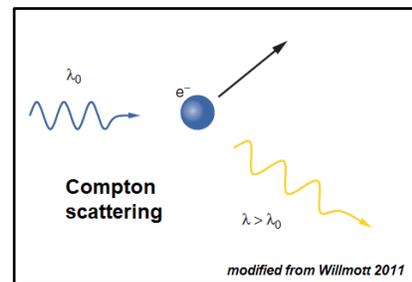
## Thomson scattering and Compton scattering

- Electrons are the main type of particle that can scatter x-rays. Elastic or Thomson scattering occurs when a non-relativistic electron is accelerated by the electrical component of an incoming electromagnetic field from an x-ray. The accelerated electron then reradiates light at the same frequency. Since the frequency of the input light and output light are the same, this is an elastic process.
- The intensity of the re-emitted radiation at an observer's location depends on the angle  $\chi$  between the incident light and the observer. Because of the sinusoidal wave character of light, the scattered intensity at the observer's location is given by the proportionality equation below.



$$I_{\text{ob}} \propto \cos^2 \chi$$

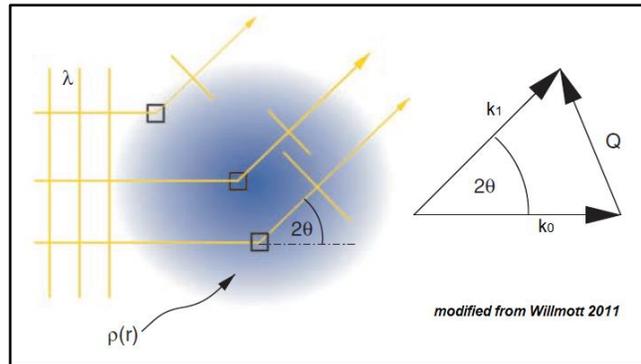
- Light that encounters the electron is scattered if it is incident on the region defined by the electron's classical radius. This region is called the Thomson scattering length  $r_0$ . For a free electron,  $r_0 = 2.82 \times 10^{-5} \text{ \AA}$ .
- Compton scattering occurs when an electron scatters a photon and the scattered photon has a lower energy than the incident photon (an inelastic process). For Compton scattering, a fraction of the incident photon's energy is transferred to the electron.
- The amount of energy lost via Compton scattering where the incident photon has energy  $E_0 = hc/\lambda_0$  and the scattered photon has energy  $E_1 = hc/\lambda_1$  is described by the following equation. Here,  $\psi$  represents the angle between the paths of the incident photon and the scattered photon.



$$\frac{E_0}{E_1} = \frac{\lambda_0}{\lambda_1} = 1 + \frac{h}{mc} \frac{2\pi}{\lambda_0} (1 - \cos \psi)$$

## Scattering from atoms

- X-rays are scattered throughout the volumes of atomic electron clouds. For x-rays that scattered in the same direction as the incident x-rays, the strength of scattering is proportional to the atom's Z-number. In the case of an ionic atom, this value is adjusted to equal the atom's number of electrons. Note that this assumes free electron movement within the cloud.



- By contrast, x-rays that are scattered at some angle  $2\theta$  relative to the incident x-rays exhibit lower scattering magnitudes. Each of the x-rays scattered at angle  $2\theta$  will possess different magnitudes and phases depending on where they were scattered from within the atomic cloud. As a result, the scattering amplitude for the x-rays at angle  $2\theta$  will be a vector sum of these waves with distinct magnitudes and phases.
- A wavevector  $\mathbf{k}$  is a vector with magnitude  $2\pi/\lambda$  that points in the direction of a wave's propagation. The difference between the wavevector of the incident wave  $\mathbf{k}_0$  and the wavevector of the scattered wave  $\mathbf{k}_1$  is equal to a scattering vector  $\mathbf{Q}$  (that is,  $\mathbf{Q} = \mathbf{k}_0 - \mathbf{k}_1$ ). The magnitude of  $\mathbf{Q}$  is given by the following equation.

$$\|\mathbf{Q}\| = \frac{4\pi}{\lambda} \sin \theta$$

- The atomic scattering factor  $f$  describes the total scattering amplitude for an atom as a function of  $\sin(\theta)/\lambda$ . By assuming that the atom is spherically symmetric,  $f$  will depend only on the magnitude of  $\mathbf{Q}$  and not on its orientation relative to the atom. Values for  $f$  can be found in the International Tables for Crystallography or computed using nine known coefficients  $a_{1,2,3,4}$ ,  $b_{1,2,3,4}$ , and  $c$  (which can also be looked up) and the following expression. The coefficients vary depending on the atom and ionic state. The units of  $f$  are the scattering amplitude that would be produced by a single electron.

$$f = \sum_{i=1}^4 \left( a_i \exp\left(\frac{-b_i \sin^2 \theta}{\lambda^2}\right) \right) + c$$

- If the incident x-ray has an energy that is much less than that of an atom's bound electrons, the response of the electrons will be damped due to their association with the atom. (This no longer assumes free electron movement within the cloud). As a result,  $f$  will be decreased by some value  $f_a$ . The value  $f_a$  increases when the

incoming x-ray's energy is close to the energy level of the electron and decreases when the incoming x-ray's energy is far above the energy levels of the electrons.

- When the incident x-ray's energy is close to an electron's energy level (called an absorption edge), the x-ray is partially absorbed. With this process of partial absorption, some of the radiation is still directly scattered and another part of the radiation is re-emitted after a delay. This re-emitted radiation interferes with the directly scattered radiation. To mathematically describe the effect of the re-emitted radiation's phase shift and interference,  $f$  is adjusted by a second term  $f_b$  (which is an imaginary value). Far from absorption edges,  $f_b$  has a much weaker effect (it decays by  $E^{-2}$ ). The total atomic scattering factor is then given by the following complex-valued equation.

$$f_{\text{total}} = f - f_a + if_b$$

### Refraction, reflection, and absorption

- A material's index of refraction can be expressed as a complex quantity  $n_c = n_{\text{Re}} + in_{\text{Im}}$ . The real part represents the rate at which the wave propagates through the material and the imaginary part describes the degree of attenuation that the wave experiences as it passes through the material.
- The reason that a material can possess a complex refractive index involves the complex plane wave equation. The wavenumber  $k = 2\pi/\lambda_0$  is the spatial frequency in wavelengths per unit distance and it is a constant within the complex plane wave equation ( $\lambda_0$  is the wave's vacuum wavelength). The complex wavenumber  $k_c = kn_c$  is the wavenumber multiplied by the complex refractive index. As such, the complex refractive index can be related to the complex wavenumber via  $k_c = 2\pi n_c/\lambda_0$  where  $\lambda_0$  is the vacuum wavelength of the wave. After inserting  $2\pi(n_{\text{Re}} + in_{\text{Im}})/\lambda_0$  into the complex plane wave equation, a decaying exponential can be simplified out as a coefficient for the rest of the equation. The decaying exponential represents the attenuation of the wave in the material. Once this simplification is performed, the equation's complex wavenumber is converted to a real-valued wavenumber.

$$\begin{aligned} E(x, t) &= \text{Re}[E_0 \exp(i(k_c x - \omega t))] = \text{Re} \left[ E_0 \exp \left( i \left( \left( \frac{2\pi(n_{\text{Re}} + in_{\text{Im}})}{\lambda_0} \right) x - \omega t \right) \right) \right] \\ &= \exp \left( -\frac{2\pi n_{\text{Im}} x}{\lambda_0} \right) \text{Re}[E_0 \exp(i(kx - \omega t))] \end{aligned}$$

- For x-rays, a material's complex refractive index for wavelength  $\lambda$  is related to the atomic scattering factors of atoms in the material using the following equation.  $N_j$  represents the number of atoms of type  $j$  per unit volume and  $f_j(0)$  is the atomic scattering factor in the forward direction (angle of zero) for atoms of type  $j$ . Recall that  $r_0$  is the Thomson scattering length.

$$n_c = 1 - \frac{r_0}{2\pi} \lambda^2 \sum_j N_j f_j(0)$$

- The refractive index is a function of the wavelength. For most optical situations, as the absorption maximum of a material is approached from lower frequencies, the refractive index increases. But when the radiation's frequency is high enough that it passes the absorption maximum, the refractive index decreases to a value of less than one.
- The refractive index is defined by  $n = c/v$ , where  $v$  is the wave's phase velocity. Phase velocity is the rate at which a wave's phase propagates (i.e. how rapidly one of the wave's peaks moves through space). Rearranging the equation,  $v = c/n$  is obtained. When the refractive index is less than one, the phase velocity is greater than the speed of light. However, this does not violate relativity because the group velocity (not the phase velocity) carries the wave's energy and information. For comparison, group velocity is the rate at which a change in amplitude of an oscillation propagates.
- Anomalous dispersion occurs when the radiation's frequency is high enough that the refractive index of a material is less than one. As a result, x-rays entering a material from vacuum are refracted away from the normal of the refracting surface. This is in contrast to the typical case where the radiation would be refracted toward the normal of the refracting surface. In addition, the refracted wave is phase shifted by  $\pi$  radians.
- The complex refractive index is often expressed using the equation below. Here,  $\delta$  is called the refractive index decrement and  $\beta$  is called the absorption index. Note that  $n_{Re} = 1 - \delta$  and  $n_{Im} = \beta$  (as a comparison to the previously used notation). Recall that  $n_{Im} = \beta$  describes the degree of a wave's attenuation as it moves through a material.

$$n_c = 1 - \delta + i\beta$$

- The refractive index decrement can be approximately computed using the average density of electrons  $\rho$ , the Thomson scattering length  $r_0$ , and the wavenumber  $k = 2\pi/\lambda_0$ . Note that this approximation is better for x-rays that are far from an absorption edge.

$$\delta \approx \frac{2\pi\rho r_0}{k^2}$$

- With most materials, the resulting real part of the index of refraction is only slightly less than one when dealing with x-rays. For example, a typical electron density of one electron per cubic Angstrom yields a  $\delta$  value of about  $5 \times 10^{-6}$ .
- Snell's law applies to the index of refraction for x-rays and is given as follows.

$$\frac{\cos(\theta_{\text{incident}})}{\cos(\theta_{\text{refracted}})} = n_{Re}$$

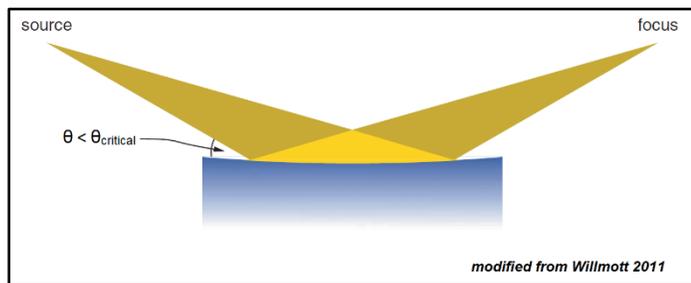
- Because the index of refraction for x-rays is slightly less than one, total external reflection can occur when x-rays are incident on a surface at angles less than the critical angle  $\theta_{\text{critical}}$ . This stands in contrast with the total internal reflection that commonly occurs with visible light.

$$\theta_{\text{critical}} = \arccos(n_{\text{Re}})$$

- The critical angle can be approximated with a high level of accuracy using the following equation (derived from the Taylor expansion of the cosine function). With typical values of  $\delta$  on the order of  $10^{-5}$ ,  $\theta_{\text{critical}}$  is often equal to just a few milliradians (or a few tenths of a degree). These small angles relative to the surface are called grazing angles.

$$\theta_{\text{critical}} \approx \sqrt{2\delta}$$

- Because grazing incident angles facilitate x-ray reflection, special curved mirrors can be used to focus x-rays. The curvature of these mirrors must be small enough that the steepest incident angle is less than  $\theta_{\text{critical}}$ . It should be noted that, even when undergoing total external reflection, x-rays do penetrate the reflecting material to a depth of a few nanometers via an evanescent wave.



- The absorption index  $\beta$  is related to the value  $f_b$  using the following equation where  $r_0$  is the Thomson scattering length. Recall that  $f_b$  represents the effects of scattering from absorption and remission of x-rays with energies that are close to the absorption edges of a material.

$$\beta = \frac{r_0 \lambda^2 f_b}{2\pi}$$

- Using the process explained earlier for computing the decaying exponential  $\exp(-2\pi n_{\text{Im}}x/\lambda_0)$  that represents the attenuation of a wave's amplitude as it travels through a material, the decay of a wave's intensity as it travels through a material can also be found. Recall that  $\lambda_0$  is the wavelength in a vacuum. Because intensity is proportional to the square of the amplitude, the equation below describes the exponential decay of a wave's intensity in a material. (This decaying exponential function is multiplied by the equation of the wave). Here,  $\mu$  is called the absorption coefficient and is defined as the reciprocal of the thickness of a material required to decrease a wave's intensity by a factor of  $1/e$ . The absorption coefficient is a rough indication of a material's electron density and electron binding energy.

$$\frac{I}{I_0} = \exp\left(-\frac{4\pi\beta x}{\lambda_0}\right) = \exp(-\mu x)$$

- The correspondences between the atomic configurations associated with an x-ray absorption edge and the commonly used name for said absorption edge are given in the following table. The subscripts used with the configurations represent the total angular momenta.

Edge	Configuration	Edge	Configuration
K	1s	N <sub>1</sub>	4s
L <sub>1</sub>	2s	N <sub>2</sub>	4p <sub>1/2</sub>
L <sub>2</sub>	2p <sub>1/2</sub>	N <sub>3</sub>	4p <sub>3/2</sub>
L <sub>3</sub>	2p <sub>3/2</sub>	N <sub>4</sub>	4d <sub>3/2</sub>
M <sub>1</sub>	3s	N <sub>5</sub>	4d <sub>5/2</sub>
M <sub>2</sub>	3p <sub>1/2</sub>	N <sub>6</sub>	4f <sub>5/2</sub>
M <sub>3</sub>	3p <sub>3/2</sub>	N <sub>7</sub>	4f <sub>7/2</sub>
M <sub>4</sub>	3d <sub>3/2</sub>	O <sub>1</sub>	5s
M <sub>5</sub>	3d <sub>5/2</sub>	O <sub>2</sub>	5p <sub>1/2</sub>

### X-ray fluorescence and Auger emission

- Materials fluoresce after bombardment with x-rays or high-energy electrons. If electrons are used, the emitted light consists of Bremsstrahlung radiation (which comes from the deceleration of the electrons) and fluorescence lines. The Bremsstrahlung radiation includes a broad spectrum of wavelengths and has low intensity while the fluorescence lines are sharp peaks and exhibit high intensity. If x-rays are used to bombard a material, there is no Bremsstrahlung radiation, but fluorescence lines occur.
- Different materials exhibit different characteristic fluorescence lines. These x-ray fluorescence lines are caused by outer-shell electrons relaxing to fill the holes left after the ejection of photoelectrons. However, not all electronic transitions are allowed, only those which follow the selection rules for electric dipoles. These selection rules are given below. J is the total angular momentum and can be computed from the sum of the Azimuthal quantum number L (which determines the type of atomic orbital) and the spin quantum number S (which determines the direction of an electron's spin).

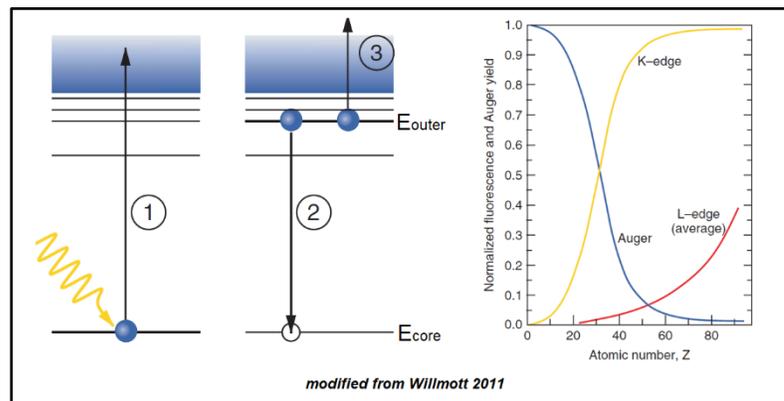
$$\Delta L = \pm 1, \quad \Delta S = 0, \quad \Delta J = 0, \pm 1$$

- The nomenclature for x-ray fluorescence lines is based on the shell to which an electron relaxes. If an excited electron relaxes to the 1s shell state, then the fluorescence line is part of the K series. For an excited electron that relaxes to the 2s or 2p state, the fluorescence line is part of the L series. The M series includes relaxations to 3s, 3p, and 3d. The N series includes relaxations to 5s, 5p, 5d, and 5f. As such, the Azimuthal quantum number determines if the fluorescence line

falls into the K, L, M, or N series (there are some series beyond these as well which follow the same pattern). The transition within each series that exhibits the smallest energy difference is labeled with  $\alpha$  (i.e.  $K\alpha$ ), the transition with the next smallest energy difference is labeled with  $\beta$ , and so on. It should be noted that the fluorescence lines are further split by the effects of electron spin and angular momentum and so are labeled with suffixes of 1, 2, etc.

- Auger emission is the process where a photoelectron is ejected, an outer shell electron relaxes to fill the hole, and the released energy causes ejection another electron instead of emitting a photon. The energies of emitted Auger electrons are independent of the energies of the incident photons.
- The excess energy released by the relaxation of the outer shell electron is equal to  $|E_{\text{core}} - E_{\text{outer}}|$ . In order for the last electron ejection to occur, the electron must have a binding energy that is less than the excess released energy from the relaxation. The kinetic energy of the ejected Auger electron is  $|E_{\text{core}} - E_{\text{outer}} - E_{\text{binding}}|$ . Note that  $E_{\text{binding}}$  is the binding energy of the Auger electron in the ionized atom (which is different from the binding energy in the neutral form of the atom).
- Auger emission and x-ray fluorescence are competitive with each other.

Fluorescence is stronger for heavier atoms (higher Z-number) since they exhibit larger energy differences between adjacent shells as well as binding electrons more tightly. For the same reasons, Auger emission is stronger from atoms with lower Z-numbers.



**Reference:** Willmott, P. (2011). *An Introduction to Synchrotron Radiation: Techniques and Applications*. Wiley.