Departamento
de Física

Interactions of photons with Matter

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Radiation

Ionizing

Directly ionizing

- Electrons
- Protons
- Neutrons
- α particles

Indirectly ionizing

EM WAVES with $\lambda < 100nm$

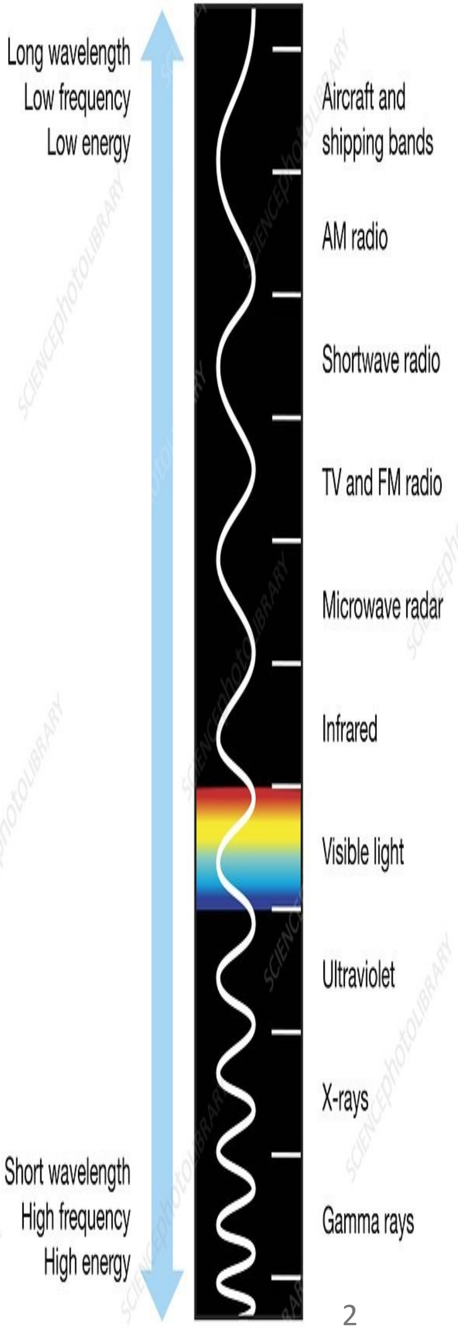
- **X rays** ($0.01\ nm < \lambda < 10\ nm$)
- **γ rays** ($\lambda < 0.01\ nm$)

Non-ionizing

EM WAVES

$\lambda \geq 100nm$

- UV
- Visible
- Infrared
- Microwaves
- Radio waves

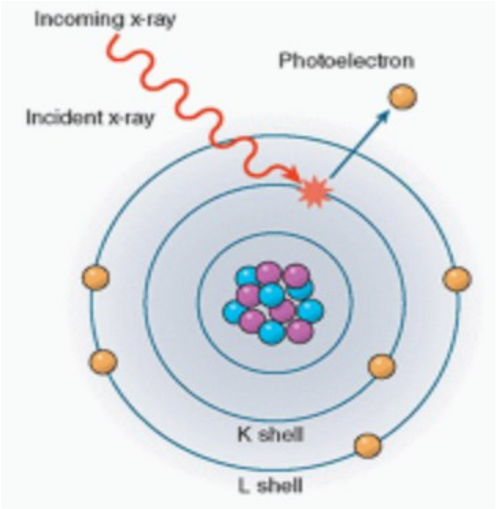


Talk Content

1. Photoelectric effec
2. Compton effect
3. Rayleigh Scattering
4. Pair Production
5. Inroduction to XPCI

$\gamma + A \longrightarrow A^+ + e^-$

Photoelectric effect



For a hydrogen-like atom in the ground state: $\psi_{100}(r) = \left(\frac{Z^3}{\pi a^3}\right)^{1/2} e^{-Zr/a}$

The final sate is a free electron: $\psi_f(k) = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{r}}$

Assuming polarization along the z-axis:

$$\langle f|H_I|i\rangle = M_{fi} = -\frac{eE_0}{(2\pi)^{3/2}}\left(\frac{Z^3}{\pi a^3}\right)^{1/2} \int z\, e^{-i\vec{k}\cdot\vec{r}} e^{-Zr/a} d^3r$$

Kinetic energy of the ejected electron:

$$\hbar\omega - I_Z = \frac{\hbar^2 k^2}{2m} \quad ; \quad I_Z = \frac{13.6\ eV\ Z^2}{n^2}$$

Transition rate for photoelectric absorption:

$$W_{fi} = \frac{2\pi}{\hbar}\left|\left\langle \psi_f(k)\middle| -\frac{e}{m}\vec{A}\cdot\vec{p}\middle|\psi_{nlm}\right\rangle\right|^2 \rho(E_f)$$

For atomic dimensions: $ka \ll 1 \ \Rightarrow\ e^{i\vec{k}\cdot\vec{r}} \approx 1$

$\Longrightarrow \vec{A} \approx \hat{\epsilon} A_0 e^{-i\omega t}$ dipole approximation

$$W_{fi} = \frac{2\pi}{\hbar}\left|\left\langle \psi_f(k)\middle| -e\vec{E}\cdot\vec{r}\middle|\psi_{nlm}\right\rangle\right|^2 \rho(E_f)$$

Solving the integral and performing angular averaging:

$$\left\langle \left|M_{fi}\right|^2 \right\rangle = \frac{2^9}{3} e^2 E_0^2 \left(\frac{Z}{a}\right)^5 \frac{k^2}{[k^2 + (Z/a)^2]^6}$$

The number of states in a shell of radius k and thickness dk

$$dN = 2\frac{V}{(2\pi)^3} 4k^2 dk = \frac{V}{\pi^2} k^2 dk; \quad \text{with } E = \frac{\hbar^2 k^2}{2m} \Longrightarrow \rho(E) = \frac{dN}{dE} = \frac{V}{\pi^2}\frac{m}{\hbar^2} k$$

$$W_{fi} = \frac{2^{10}}{3\pi}\frac{m\, e^2 E_0^2}{\hbar^3}\left(\frac{Z}{a}\right)^5 \frac{k^3}{[k^2 + (Z/a)^2]^6}$$

This is the plane wave aproximation

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Photoelectric absortion cross section

$$\sigma_{ph} = \frac{Transition\ rate}{Flux} = \frac{W_{fi}}{\Phi_\gamma}$$

where $\Phi_\gamma = \frac{I}{\hbar\omega} = \frac{\varepsilon_0 c E_0^2}{2\hbar\omega}$

$$\sigma_{ph} = \frac{2^{11}}{3\pi}\frac{m\,e^2\omega}{\varepsilon_0 c\,\hbar^2}\left(\frac{Z}{a}\right)^5 \frac{k^3}{[k^2+(Z/a)^2]^6}$$

This equation allows to calculate the high energy limit :

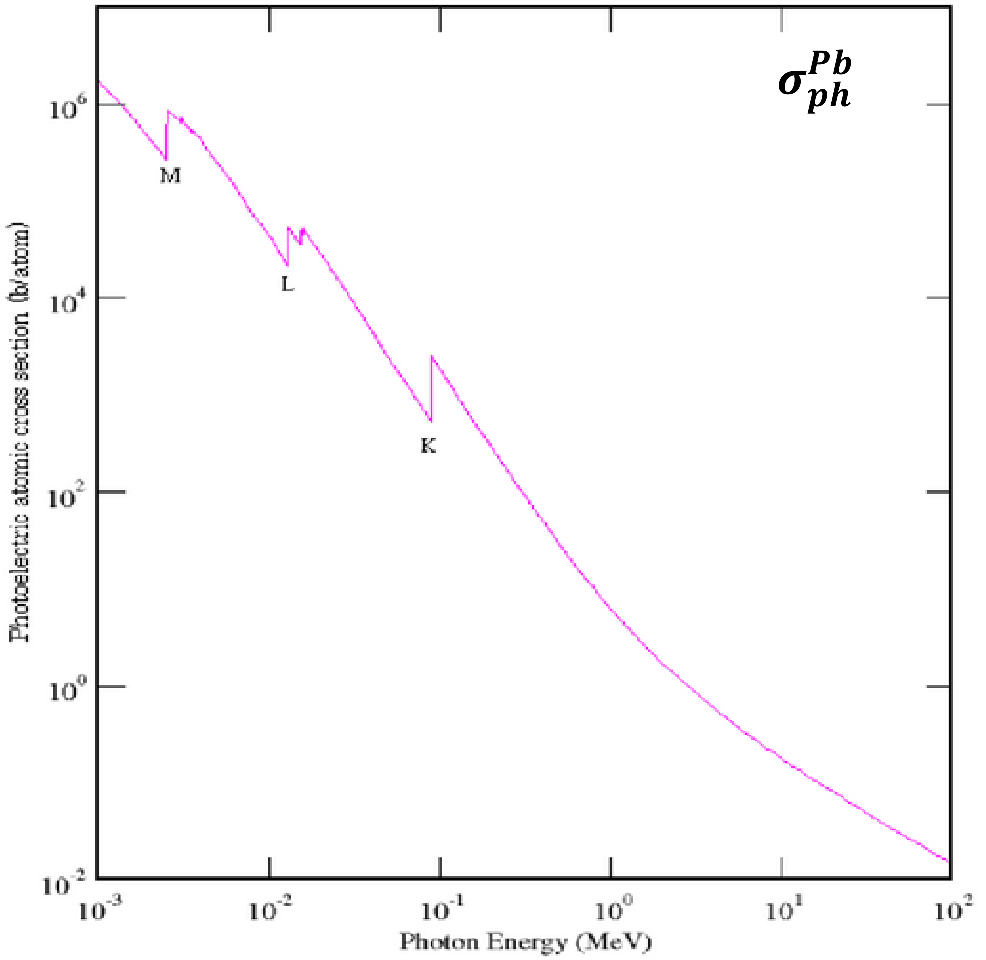
$$\hbar\omega \gg I_Z \Longrightarrow \sigma_{ph} \approx C\frac{Z^5}{E_\gamma^{7/2}}$$

The low energy limit ($\hbar\omega \approx I_Z$) requires to modify ψ for the ejected electron: The electron is not free, it is influenced by the Coulomb potential:

$$\sigma_{ph} = \frac{2^9\pi^2\alpha a^2}{3Z^2}\left(\frac{I_Z}{\hbar\omega}\right)^4 \frac{e^{-4\xi cot^{-1}\xi}}{1-e^{-2\pi\xi}}\ ;\ \xi = \sqrt{\frac{I_Z}{\hbar\omega}}$$

Stobbe formula

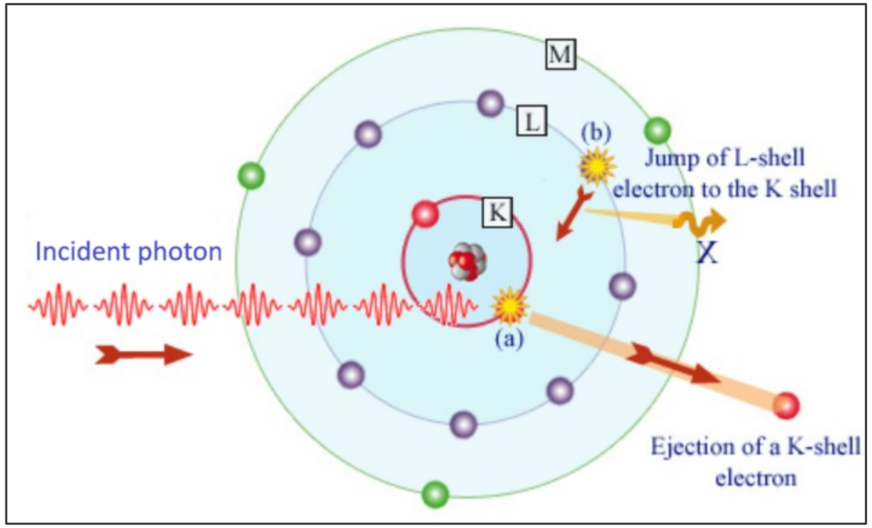
In the limit $\hbar\omega \approx I_Z$: $\sigma_{ph} \approx 6.3\times10^{-22}Z^{-2}$



1. Quantun Mechanics, special chapters, W. Greiner, Springer 1998
2. Quantum Electrodynamics, W. Greiner, J. Reinhart, Springer, 2009
3. Relativistic Quantum mechics and field, theory, F. Gross, J. Wiley&sons, 1993

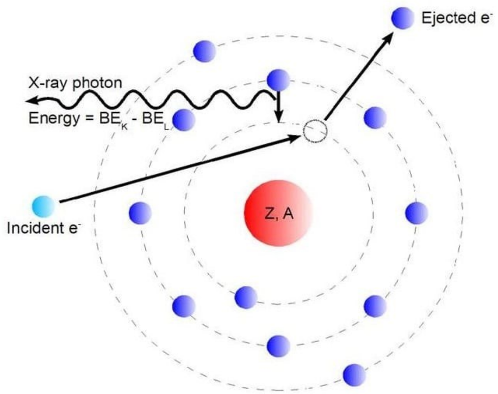
Characteristic X-ray emission

An X-ray photon is emitted when a higher shell electron ocupies a vacancy from an ejected electron due to ionization



https://radioactivity.eu.com/articles/phenomenon/photoelectric_effect

Characteristic X-rays



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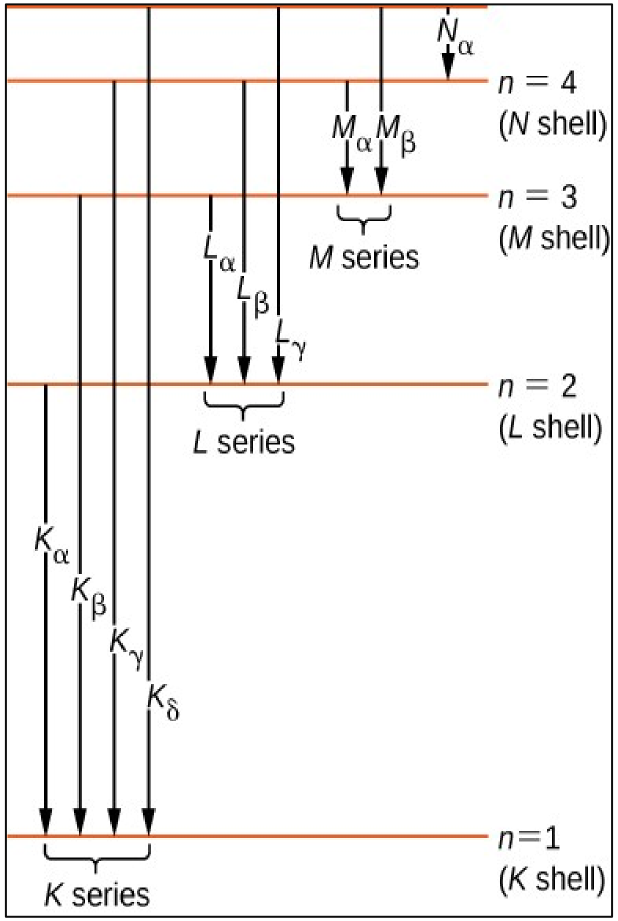
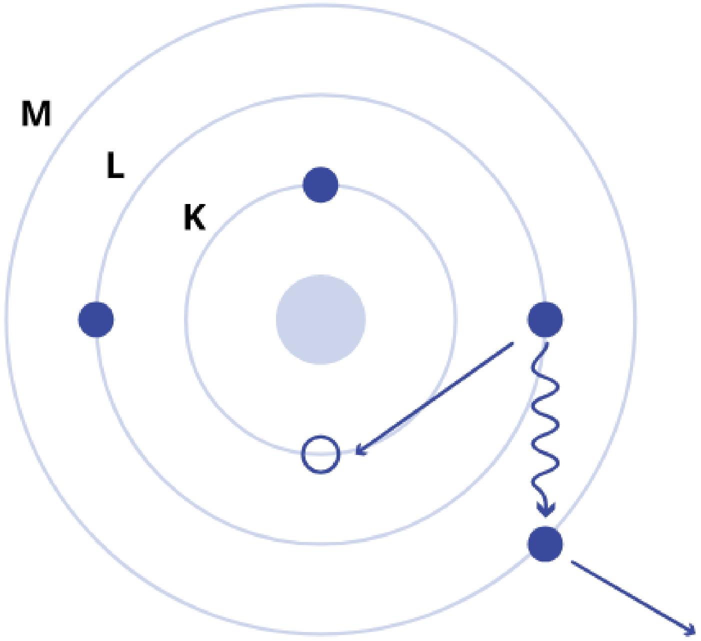
https://oncologymedicalphysics.com/kilovoltage-x-ray-generation/



https://www.careers360.com/physics/characteristic-x-rays-topic-pge

Auger electrons

Secondary electrons can be emitted from an atom during relaxation



Auger electron emission

https://www.ossila.com/pages/auger-electrons

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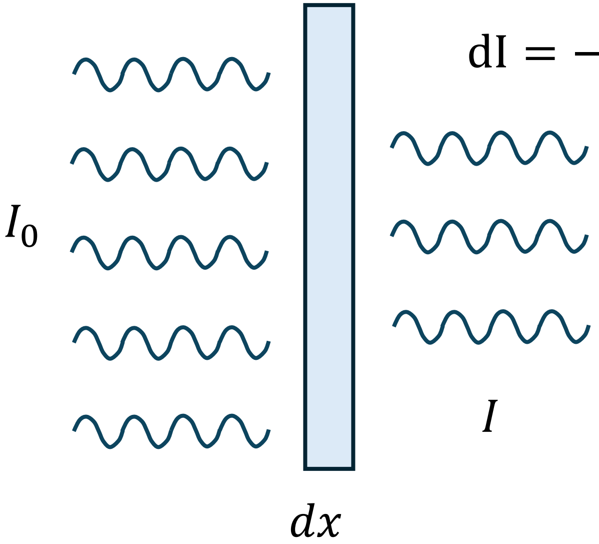
Linear attenuation coefficient



$$dI = -\mu I dx \Longrightarrow I = I_0 e^{-\mu x} \text{ (Beer-Lambert law)}$$

$$\mu = n\sigma \, ; \quad [\mu] = cm^{-1}$$

Mass attenuation coefficient:

$$\mu = \frac{\mu}{\rho} ; \quad [\mu_{ph}] = cm^2 g^{-1}$$

$$\mu = \mu_{ph} + \mu_C + \mu_{pair} + \mu_R$$

Some data bases for attenutaion coefficients:

NIST-XCOM: https://physics.nist.gov/PhysRefData/Xcom/html/xcom1.html

HENKE: https://henke.lbl.gov/optical_constants/

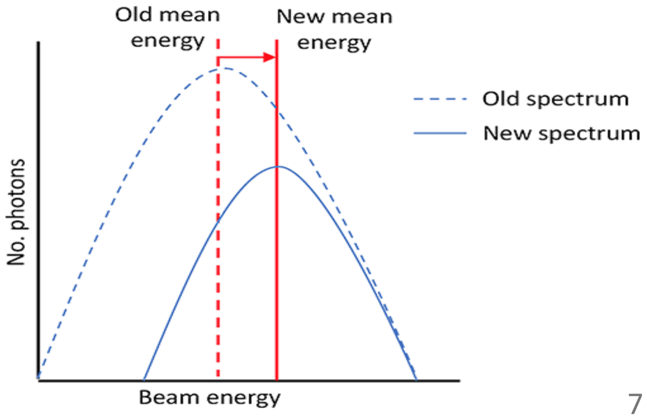
Half value layer

Thickness needed to reduce incident beam intensity by half:

$$I = \frac{I_0}{2} = I_0 e^{-\mu x_{1/2}} \Longrightarrow x_{1/2} = \frac{\ln(2)}{\mu}$$

Beam hardening

A polychromatic X-ray beam becomes more energetic ("harder") as it passes through an object



K-edge subtraction imaging

The abrupt increase in the photoelectric x-section at the K-shell is useful for X-ray imaging

Take 2 images at energies below and a bove a K-edge:

$$E_1 < E_K \quad ; \quad E_2 > E_K$$

For normal tissue: $\mu(E_2) \approx \mu(E_1)$

For a contrast agent: $\mu(E_2) \gg \mu(E_1)$

Image 1: $I_1 = I_0 exp(-\mu_B(E_1)x_B - \mu_C(E_1)x_C)$

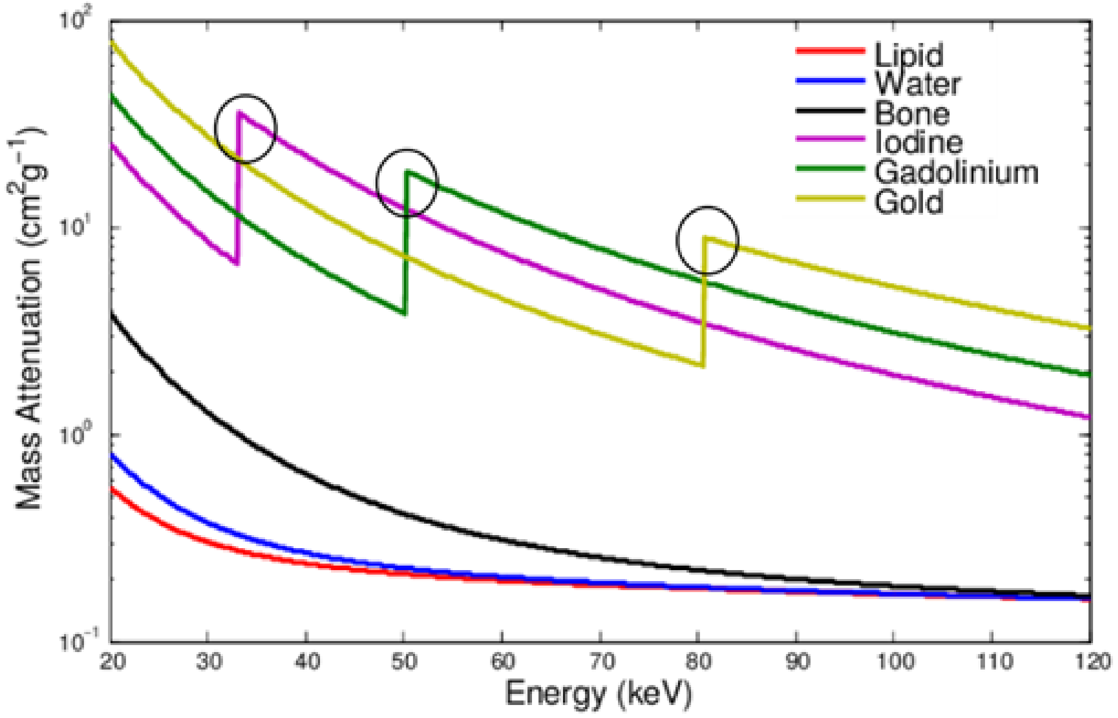
Image 2: $I_2 = I_0 exp(-\mu_B(E_2)x_B - \mu_C(E_2)x_C)$

Take logarithms and subtract:

$$ln(I_0/I_1) = \mu_B(E_1)x_B + \mu_C(E_1)x_C$$

$$- \; ln(I_0/I_2) = \mu_B(E_2)x_B + \mu_C(E_2)x_C$$

$$x_C \approx \frac{ln(I_0/I_1) - ln(I_0/I_2)}{\mu_C(E_1) - \mu_C(E_2)}$$



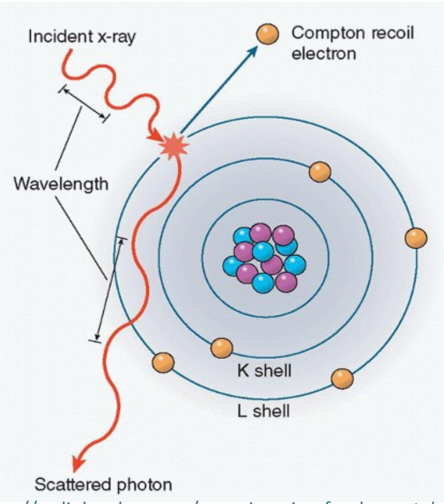
https://www.spectralphotoncountingct.com/en/page/contrast-agents-k-edge-imaging

A common technique in Angiography, Cancer imaging, contrast-enhanced mammography, material id, etc.

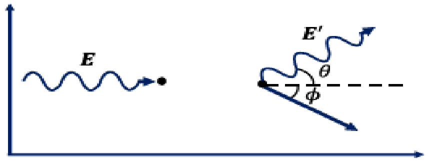
Photon counting detectors with polychromatic sources: Take only one image and divide in energy bins.

Compton scattering

$$\boldsymbol{\gamma + e^- \longrightarrow \gamma' + e^-}$$



https://radiologykey.com/x-ray-imaging-fundamentals/

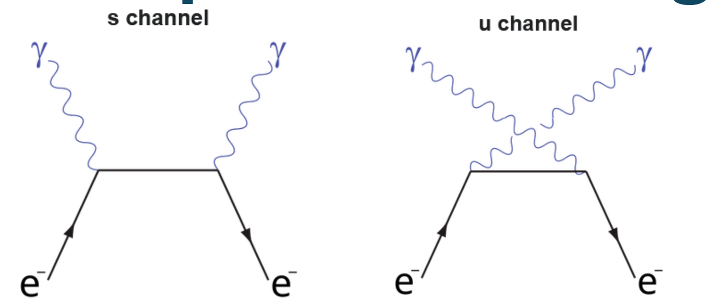


$$p_i^\mu = \left(\frac{E}{c} + mc, p, 0{,}0\right);\ p_e^\mu = \left(\frac{E_e}{c}, \vec{p}_e\right)$$

$$p_{f,\gamma}^\mu = \left(\frac{E'}{c}, p cos\theta, p sen\theta, 0\right)$$

$$p_e^\mu = p_i^\mu - p_{f,\gamma}^\mu \ ;\ p_e^\mu p_{e,\mu} = m^2c^2$$

$$E' = \frac{E}{1 + \frac{E}{mc^2}(1 - cos\theta)}$$



We can get the Compton cross section from Feynman rules (QED):

$$i\mathcal{M}_s = (-ie)^2 \bar{u}(p') \ \not{\epsilon}'^* \frac{i(\not{p} + \not{k} + m)}{(p+k)^2 - m^2} \ \not{\epsilon} u(p)$$

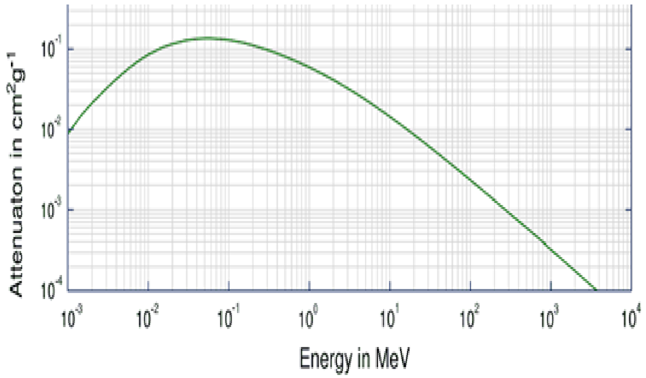
$$i\mathcal{M}_u = (-ie)^2 \bar{u}(p') \ \not{\epsilon} \frac{i(\not{p} - \not{k}' + m)}{(p-k')^2 - m^2} \ \not{\epsilon}'^* u(p).$$

$$\overline{|\mathcal{M}|^2} = \frac{1}{2} \sum_{\text{spins}} |\mathcal{M}|^2.$$

$$\frac{d\sigma}{d\Omega} = \frac{1}{64\pi^2 m_e^2} \left(\frac{E'_\gamma}{E_\gamma}\right)^2 |\mathcal{M}|^2$$

$$\frac{d\sigma}{d\Omega} = \frac{r_e^2}{2} \left(\frac{E'}{E}\right)^2 \left[\frac{E'}{E} + \frac{E}{E'} - \sin^2\theta\right]$$

Klein-Nishina Formula



When $E \ll m_e c^2$: $E \sim E'$,
→ Thompson scattering:

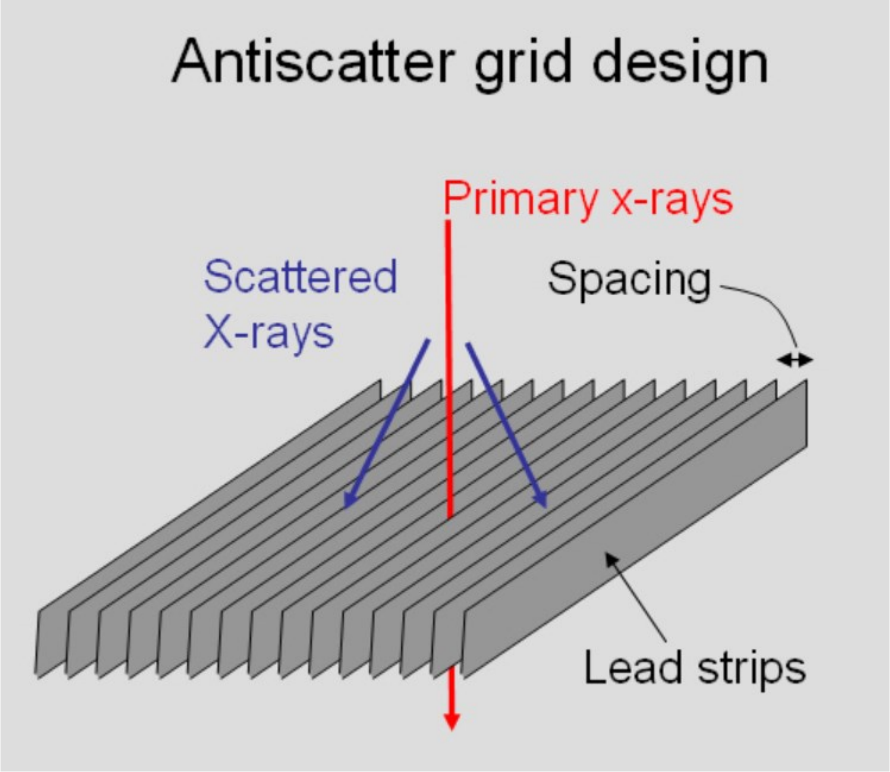
$$\frac{d\sigma}{d\Omega} = \frac{r_e^2}{2}(1 + \cos^2\theta)$$

When $E \gg m_e c^2$:

$$\sigma \sim \frac{\ln(E/m_e c^2)}{E}$$

Compton scattering: effect on imaging

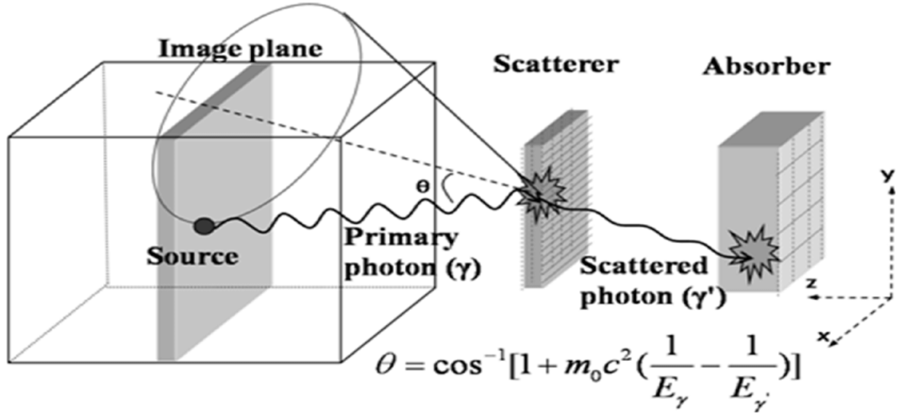
In conventional X-ray imaging: Compton scattering is a source of image degradation. Solution:



https://www.upstate.edu/radiology/education/rsna/radiography/scattergrid.php

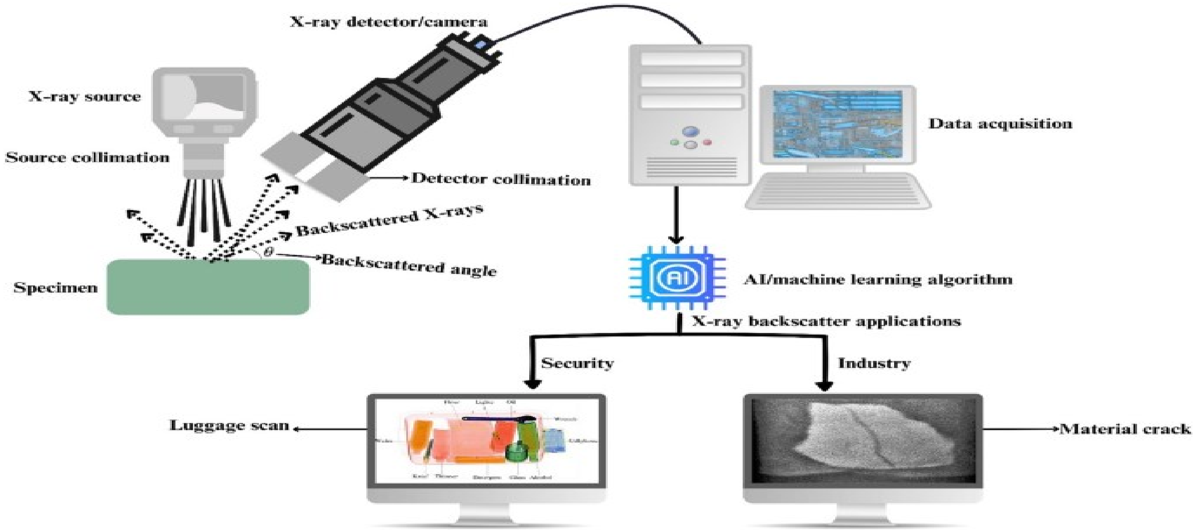
Compton Camera

Reconstruct direction of gamma rays in the energy range where Compton scattering is the dominant effect



https://www.researchgate.net/figure/Principle-of-a-Compton-camera-The-Compton-scattering-angle-is-the-opening-angle-of-the_fig1_224353796

Compton back-scattering imaging



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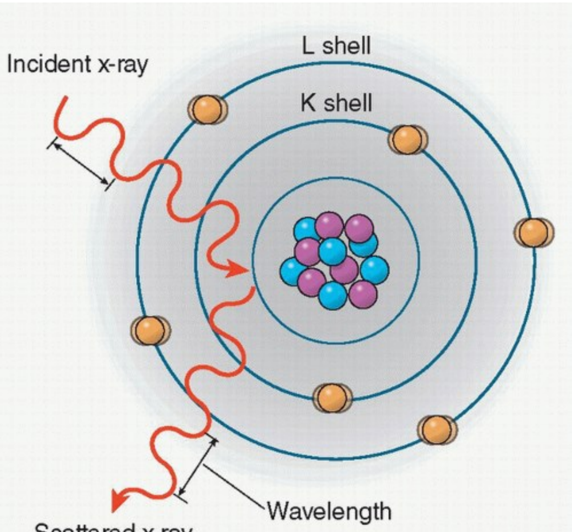
$$\gamma + A \longrightarrow \gamma + A$$

Rayleigh scattering



https://radiologykey.com/x-ray-imaging-fundamentals/

Elastic scattering of photons by particles with sizes smaller than the the photon wavelenght.

If we assume a plane with polarization along the x-axis:

$$\vec{E}(t) = E_0 e^{-i\omega t}\hat{x}$$

The equation of motion for a bound electron:

$$m\ddot{x} + m\omega_0^2 x = -eE_0 e^{-i\omega t}$$

$$\Longrightarrow x = \frac{-eE_0}{m(\omega_0^2 - \omega^2)} e^{-i\omega t}$$

There is an induced dipole moment:

$$p_0 = -ex = \alpha E_0$$

The power radiated from an oscillating dipole is:

$$P = \frac{\omega^4 \alpha^2 E_0^2}{12\pi\varepsilon_0 c^3}$$

The inciden EM wave intensity:

$$I = \frac{1}{2} c\varepsilon_0 E_0^2$$

Then, the Rayleigh cross section can be found as:

$$\boxed{\sigma_R = \frac{P}{I} = \frac{\omega^4 \alpha^2}{6\pi\varepsilon_0^2 c^4}}$$

This equation fails when $\lambda \sim a$

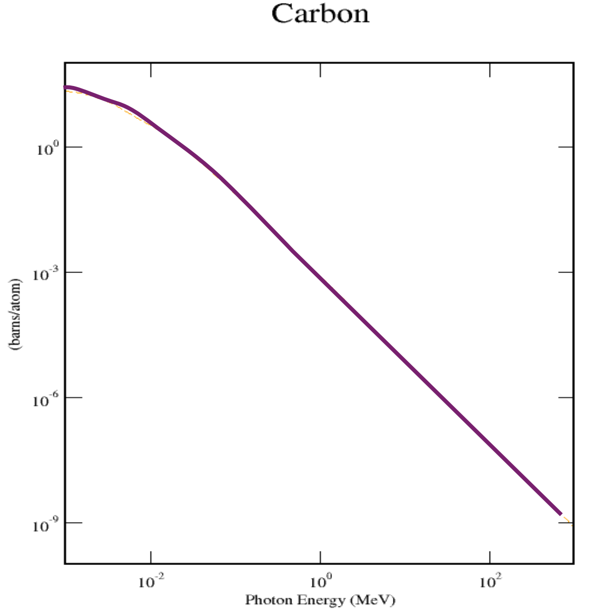
We need to introduce atomic form factor:

$$\frac{d\sigma_R}{d\Omega} = r_e^2 (1 + \cos^2\theta) \frac{|F(q)|^2}{2}$$

For a hidrogen-like charge distribution:

$$F(q) \sim \frac{Z}{(1 + a^2 q^2)^2}$$

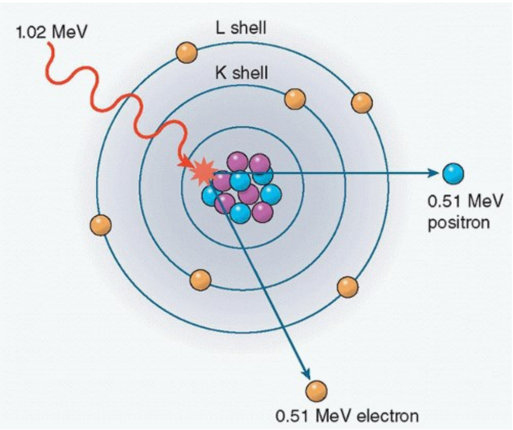
At large energies: $\frac{d\sigma_R}{d\Omega} \sim q^{-8}$

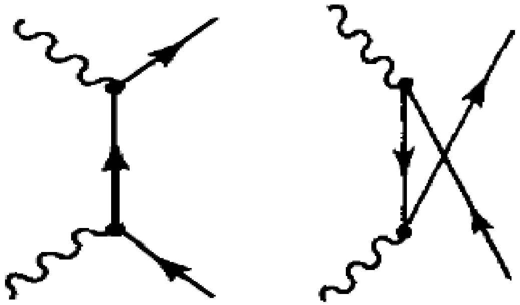


Rayleigh scattering plays an important role in Dark field imaging.

$$\gamma + Z \rightarrow Z + e^- + e^+$$

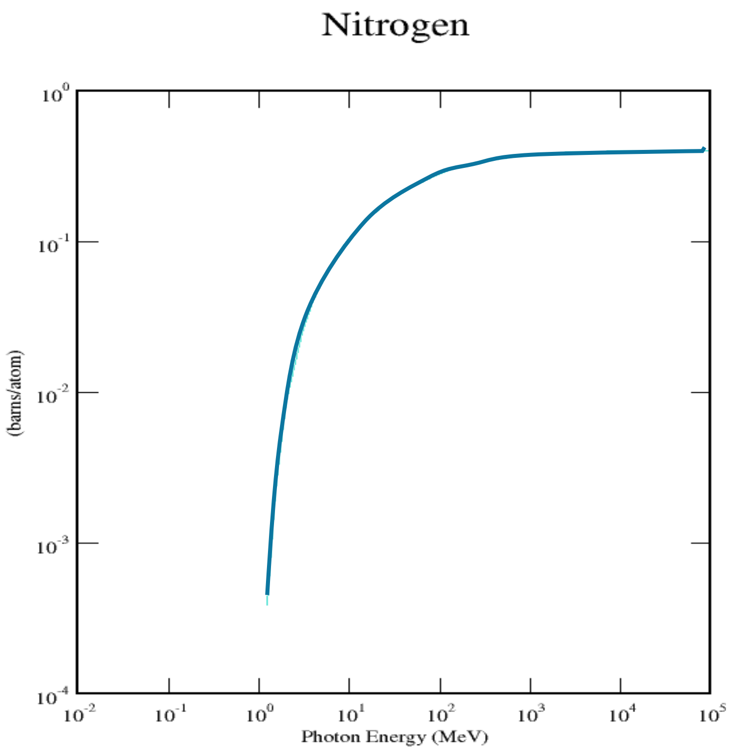
Pair production





$$d\sigma = \frac{1}{4E_\gamma M_N}|\mathcal{M}|^2(2\pi)^4\delta^{(4)}(k + P - p_+ - p_- - P')\, d\Phi_3$$

$$d\Phi_3 = \frac{d^3p_+}{(2\pi)^3 2E_+}\frac{d^3p_-}{(2\pi)^3 2E_-}\frac{d^3P'}{(2\pi)^3 2E'_N}$$



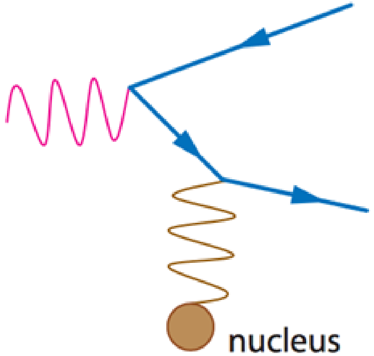
A pesence of a nucleus is needed to absorb mometum.

Threshold energy: $E_\gamma = 2mc^2$

In the limit $E_\gamma \gg m_e c^2$:

$$\sigma_{\gamma\to e^+e^-} = \frac{28}{9}Z^2\alpha r_e^2\left[\ln(183Z^{-1/3}) - f(Z)\right]$$

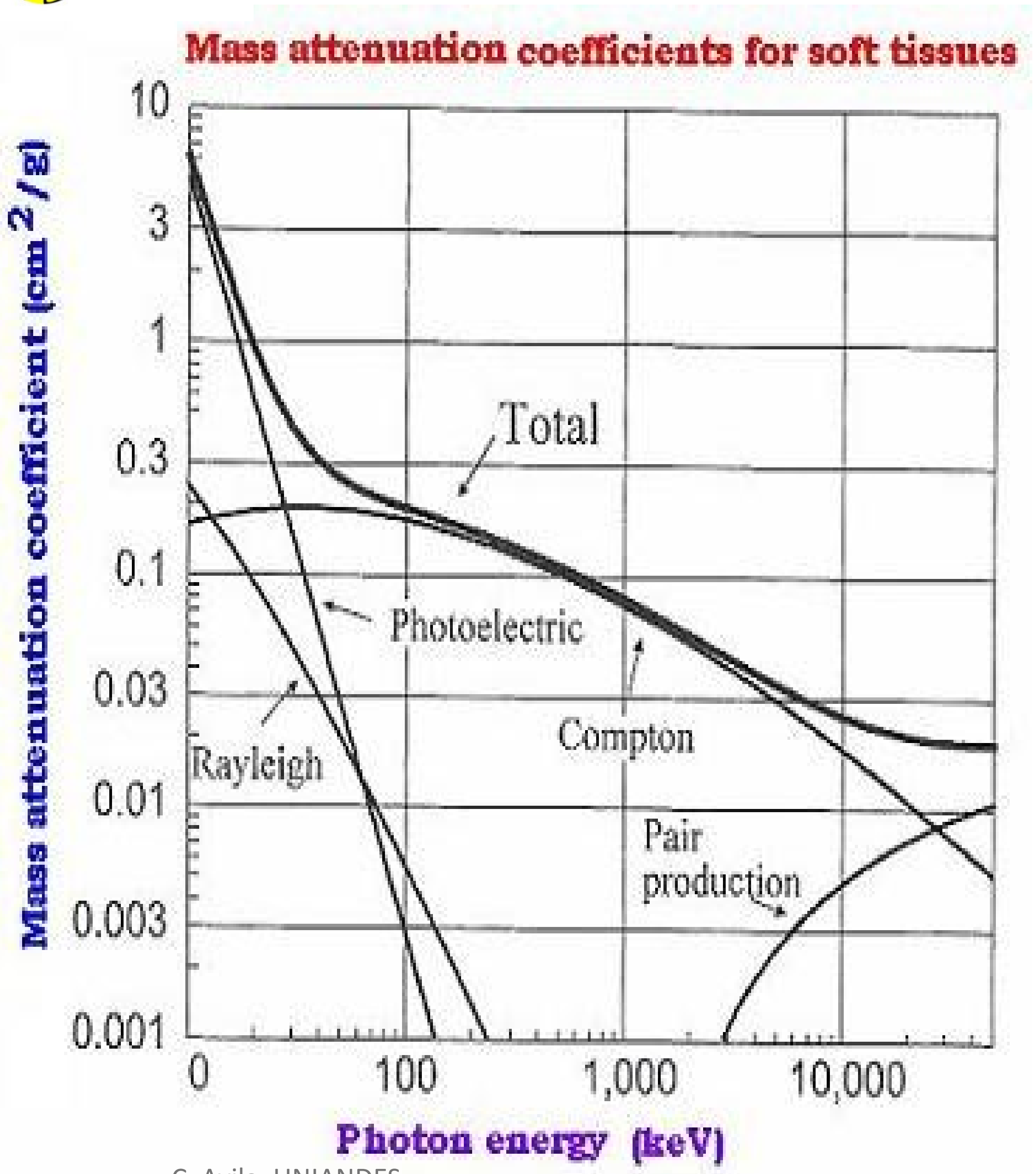
$$f(Z) = (Z\alpha)^2\sum_{n=1}^{\infty}\frac{1}{n(n^2 + (Z\alpha)^2)}$$

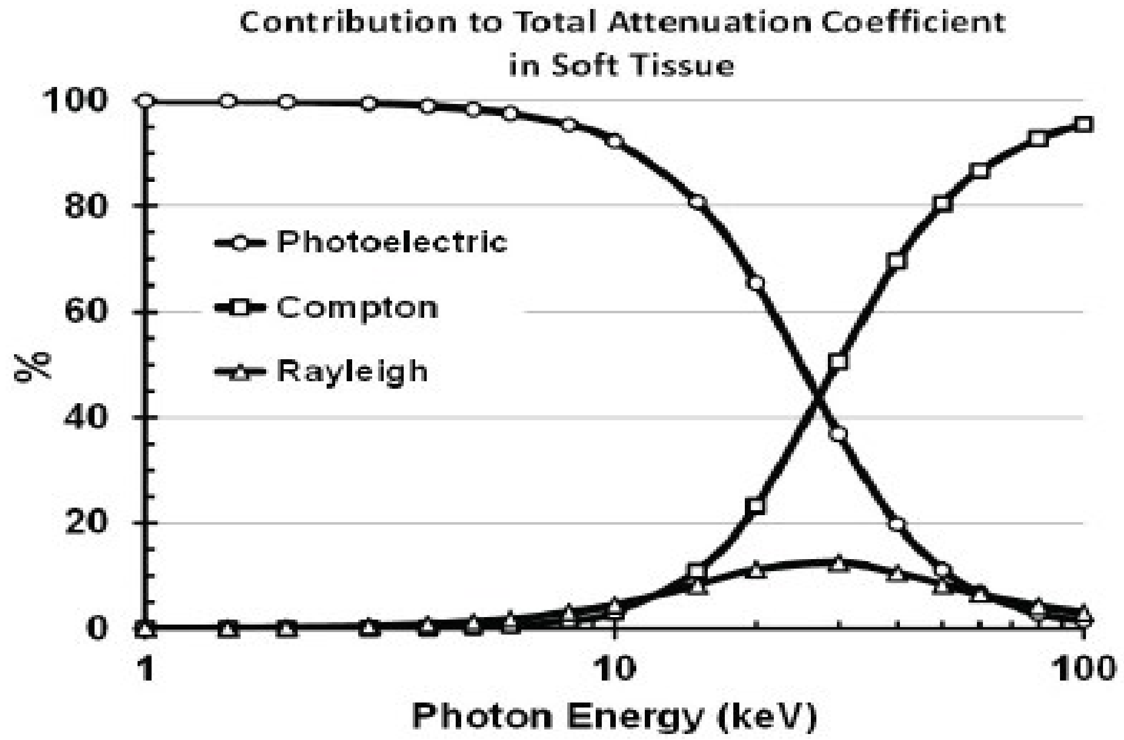


Pair production is negligible in standard x-ray medical imaging.

It is useful in High energy γ ray imaging

$e^- + e^+ \rightarrow \gamma + \gamma$ important in Positron emisión tomography

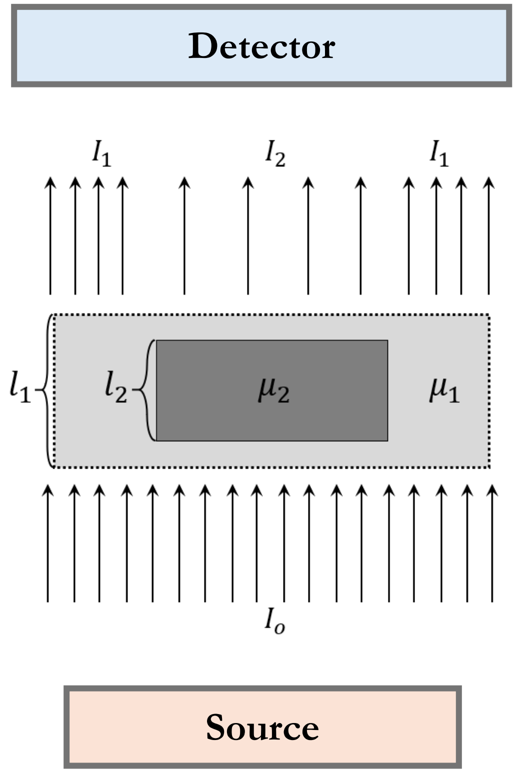


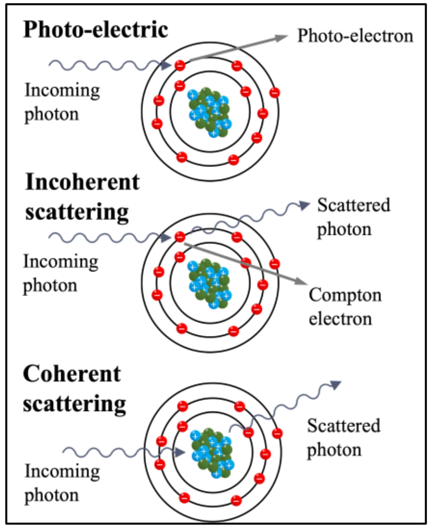


For soft tissue:

- Photoelectric x-section dominates for $E_\gamma < 30\ keV$
- Compton scattering dominates for $30\ keV < E_\gamma < 3\ MeV$
- Pair production is predominant for $E_\gamma > 3\ MeV$

X-RAY ATTENUATION IMAGING BASIC PRINCIPLE





Starting from Beer-Lambert law:

$$I(E,z) = I_o Exp[-\mu(E,z)z]$$

$$\mu = \mu_{photo} + \mu_{incoh-sc} + \mu_{coh-sc}$$

For an object 2 embedded in another object 1:

$$I_2 = I_1 Exp[-\mu_1(l_1 - l_2)] \cdot Exp[-\mu_2 l_2]$$

Contrast can be defined as:

$$C = \frac{I_1 - I_2}{I_1} = 1 - Exp(-l_2(|\Delta\mu|))$$

For polychromatic sources:

$$I(x,y) = \int I_0(x,y) e^{-(\mu_1^\lambda - \mu_2^\lambda)T_0(x,y)} D(\lambda) d\lambda$$

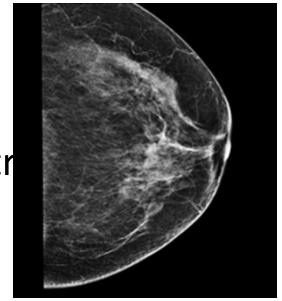
Attenuation imaging produces poor contrast of Object 2 in cases where $\mu_2 \ll \mu_1$ (hollow area of bones) or $\mu_2 \approx \mu_1$ (blood within a blood vessel).

X ray phase contrast imaging (XPCI)

Many biological and human tissues are soft: they have low X- ray absorption → they are difficult to visualize with conventional X ray techniques:

2 specific cases:

- Breast Tissue
- Blood Vessels (withouth a contrast agent)



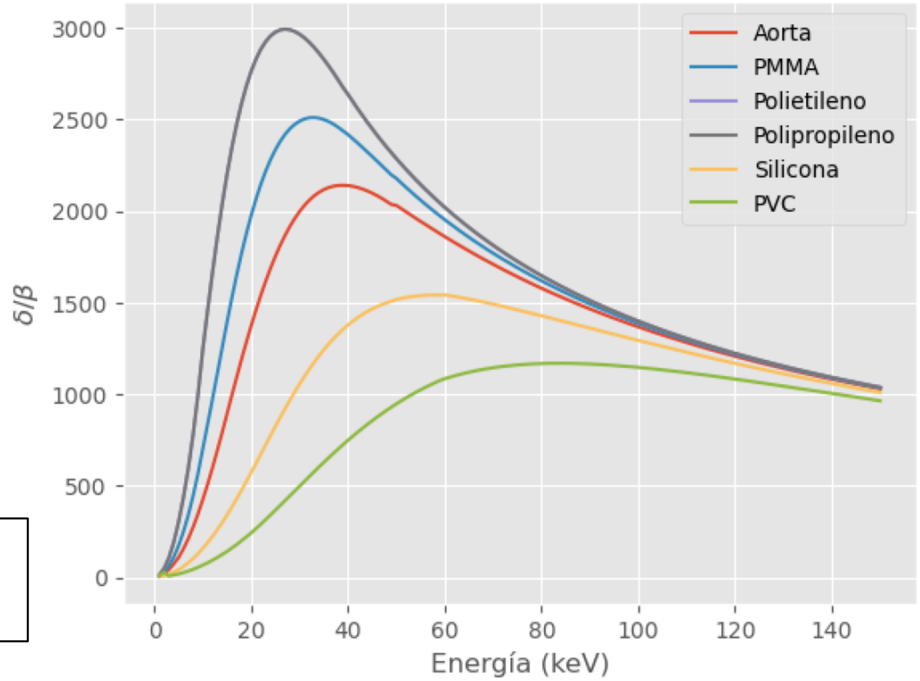
The EM wave propagating through the sample is

$$\psi = \psi_0 exp\left(i\frac{n\omega}{c}z\right)$$

In the x ray energy range the index of refraction can be written as : $n = 1 - \delta + i\beta$

$$\rightarrow \psi = \psi_0 e^{-\beta k_0 z} e^{ikz(1-\delta)}$$

- Phase effects are produced by δ : $\Delta\Phi = -k\int_0^{Z_0} \delta\, dz$
- Attenuation effects are caused by β : $I = |\psi_0|^2 e^{-2k\int_0^{Z_0} \beta\, dz}$



For many soft tissues δ is ~ 3 orders of magnitude greater than β → phase effects could enhance Image constrast

Transport of intensity equation and XPCI

Maxwell equations in vacuum:

$$\nabla^2\psi - \frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} = 0$$

For a monochormatic wave propagating in the z direction:

$$\psi(\vec{r},t) = U(\vec{r})e^{-i\omega t} \Longrightarrow \nabla^2 U + k^2 U = 0$$

With $U = A(x,y,z)e^{ikz}$ and applying the paraxial approximation (: the wave propagates with very small angles with respect to the propation axis):

$$\left|\frac{\partial^2 A}{\partial z^2}\right| \ll \left|2k\frac{\partial A}{\partial z}\right| \Longrightarrow \nabla_\perp^2 A + 2ik\frac{\partial A}{\partial z} = 0$$

The intensity of the wave is:

$I = \psi^*\psi = A^2 \Longrightarrow A = \sqrt{I}e^{i\Phi}$

$$\boxed{\frac{\partial I}{\partial z} + \frac{1}{k}\nabla_\perp \cdot (I\nabla_\perp\Phi)}$$ T.I.E.

T.I.E. : The phase gradient influences the wave intensity!

A finite differences solution of T.I.E.:

$$I(x,y,z+\delta z) \approx I(x,y,z) - \frac{\delta z}{k}\{\vec{\nabla}_\perp I(x,y,z)\cdot\vec{\nabla}_\perp\Phi(x,y) + I(x,y,z)\,\nabla_\perp^2\Phi(x,y)\}$$

The wave intensity depends on the gradiente and laplacian of the phase

Phase-contrast techniques are designed to measure the gradient or the Laplacian of the phase

To account for small angle scattering form sample microstructure a difusión term is added to the T.I.E.:

$$\boxed{\frac{\partial I}{\partial z} = -\frac{1}{k}\nabla_\perp \cdot (I\nabla_\perp\Phi) + \nabla_\perp \cdot (D\nabla_\perp I)}$$

Fokker-Planck equation: allows Dark field imaging

PHASE RETRIEVAL

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One often cited technique in the literature: **Paganin´s method**, which assumes:

1) The sample is uniform
2) The sample is made of a single material
3) The ratio $\gamma = \frac{\delta}{\beta}$ remains constant throug the sample

$$\Phi = -k\int_0^{z_0}\delta\, dz = -\gamma k\int_0^{z_0}\beta dz \qquad \text{since} \quad I(z_0) = I_0 e^{-2k\int_0^{z_0}\beta\, dz}$$

Replacing $I(z_0) = I_0 e^{-2k\int_0^{z_0}\beta\, dz}$ and Φ into the T.I.E.:

$$\frac{1}{\delta z}\left(I(z_0+\delta z) - I(z_0)\right) = -\frac{1}{k}\nabla_T \cdot \left(I_0 e^{-2k\int_0^{z_0}\beta\, dz}\nabla_T\left(-\gamma k\int_0^{z_0}\beta dz\right)\right)$$

$$\Rightarrow \quad \frac{I}{I_0} = e^{-2k\int_0^{z_0}\beta\, dz} - \frac{\gamma\delta z}{2k}\nabla_T^2\left(e^{-2k\int_0^{z_0}\beta\, dz}\right)$$

Taking the Fourier transform and simplifying:

$$\mathcal{F}\left(e^{-2k\int_0^{z_0}\beta\, dz}\right) = \frac{\mathcal{F}\left(\frac{I}{I_0}\right)}{1 + \frac{\gamma\delta z}{2k}\left(k_x^2 + k_y^2\right)}$$

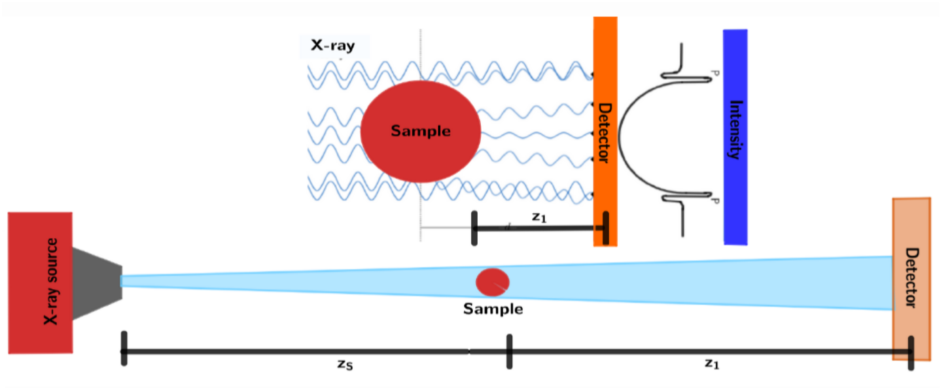
Since $\Phi = \frac{\gamma}{2} ln\left(e^{-2k\int_0^{z_0}\beta\, dz}\right)$ $\Rightarrow$

$$\Phi = \frac{\gamma}{2} ln\left\{\mathcal{F}^{-1}\left[\frac{\mathcal{F}\left(\frac{I}{I_0}\right)}{1 + \frac{\gamma\delta z}{2k}\left(k_x^2 + k_y^2\right)}\right]\right\}$$

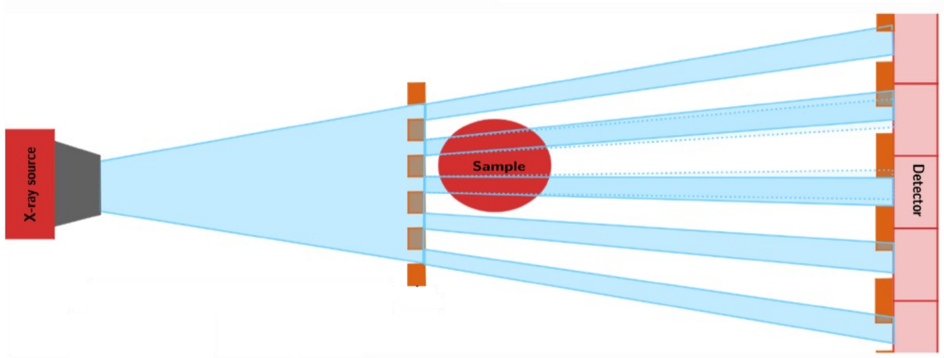
There are more methods to retrieve the pase which depend on the XPCI technique, including the training of NN.

XPCI methods at UNIANDES HEP _LAB

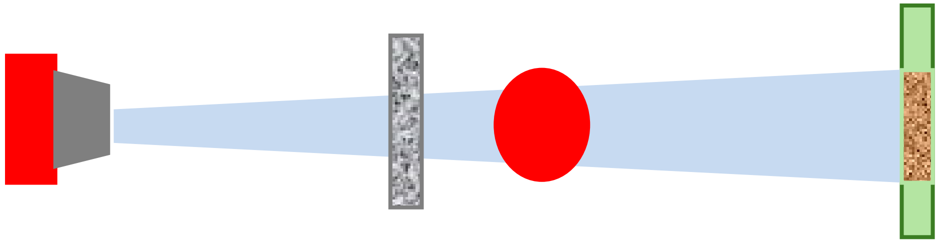
1) Inline - Free propagation



2) Single Mask Edge Illumination



3) Speckle based



CONCLUSIONS

•A detailed understanding of photon–matter interaction cross sections as a function of energy enables the optimal use of different imaging techniques across distinct photon-energy regimes.

•Databases of X-ray interactions with matter are built upon theoretical calculations from quantum electrodynamics (QED) and atomic physics, and are validated against experimental measurements.

•The theoretical foundations of X-ray phase-contrast imaging (XPCI) are the Transport of Intensity Equation (TIE) and the Fokker–Planck equation.