Photon Transport

SNU/NUKE/EHK

Photon Interactions

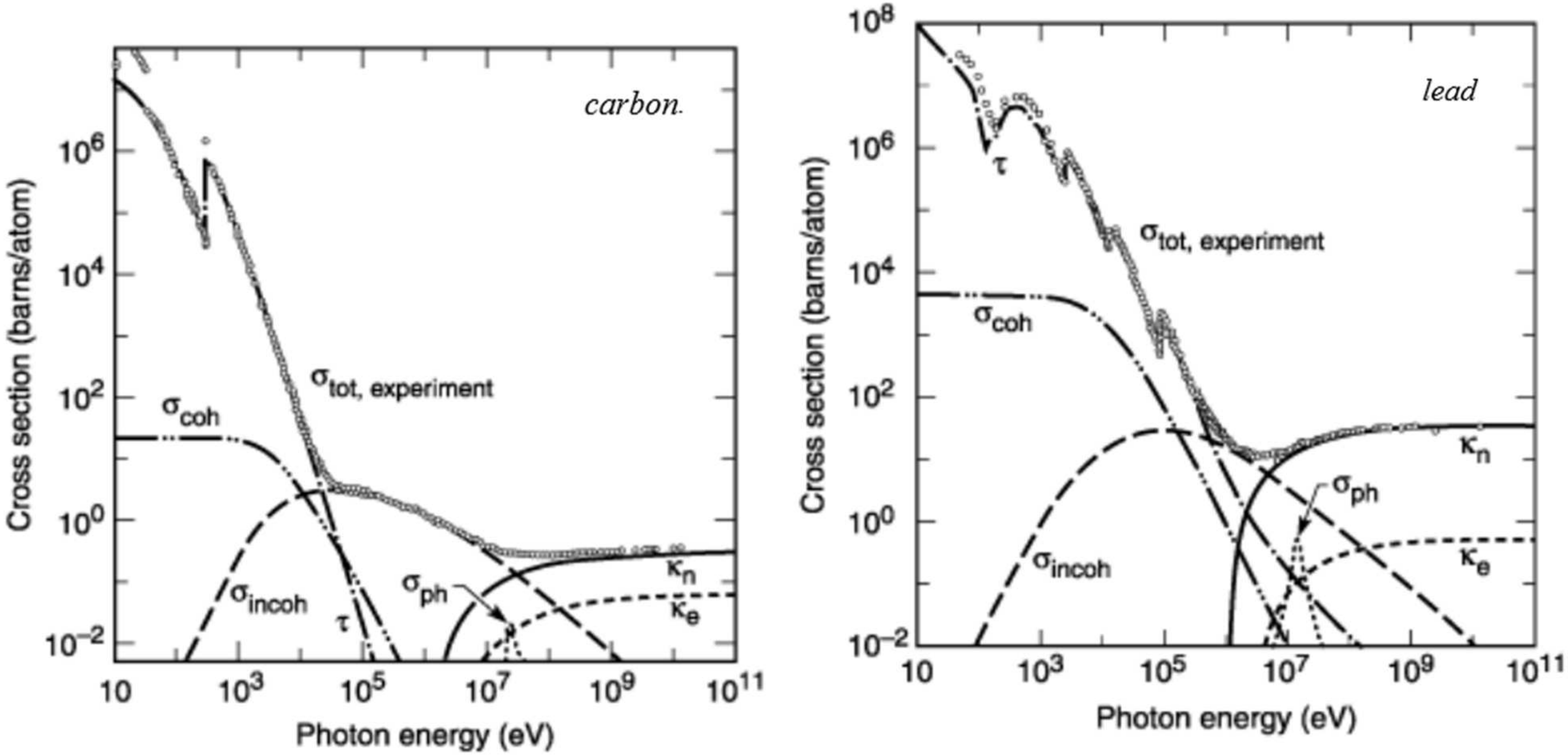
- The movements of a photon through a medium consists of a series of straight flight paths interrupted by interactions between the photon and one of the constituent nuclei or electrons.
- A collision may
  - change the energy and the traveling direction of the photon (scattering), or
  - cause the incorporation of the photon into any atom (absorption), which may lead to the production of secondary particles.

Photon Interactions

- The movements of a photon through a medium consists of a series of straight flight paths interrupted by interactions between the photon and one of the constituent nuclei or electrons.
- A collision may
  - change the energy and the traveling direction of the photon (scattering), or
  - cause the incorporation of the photon into any atom (absorption), which may lead to the production of secondary particles..

Interaction Modes of Photons

- Interaction with atoms or molecules
  - Rayleigh scattering with no energy loss
- interaction with orbital electrons
  - photoelectric absorption
  - Compton scattering
- interaction with nuclei
  - pair production (E>1.02 MeV)
  - nuclear reaction (E>>1.02 MeV)



Total photon cross section σ_{tot} as a function of energy, showing the contributions of different processes: τ, atomic photo-effect (electron ejection, photon absorption); σ_{coh}, coherent scattering (Rayleigh scattering—atom neither ionized nor excited); σ_{incoh}, incoherent scattering (Comp- ton scattering off an electron); K_n, pair production, nuclear field; K_e, pair production, electron field; σ_{ph}, photonuclear absorption (nuclear absorption, usually followed by emission of a neutron or other particle). (Figure courtesy of J. H. Hubbell.)

Pair Production in Nucleus Field

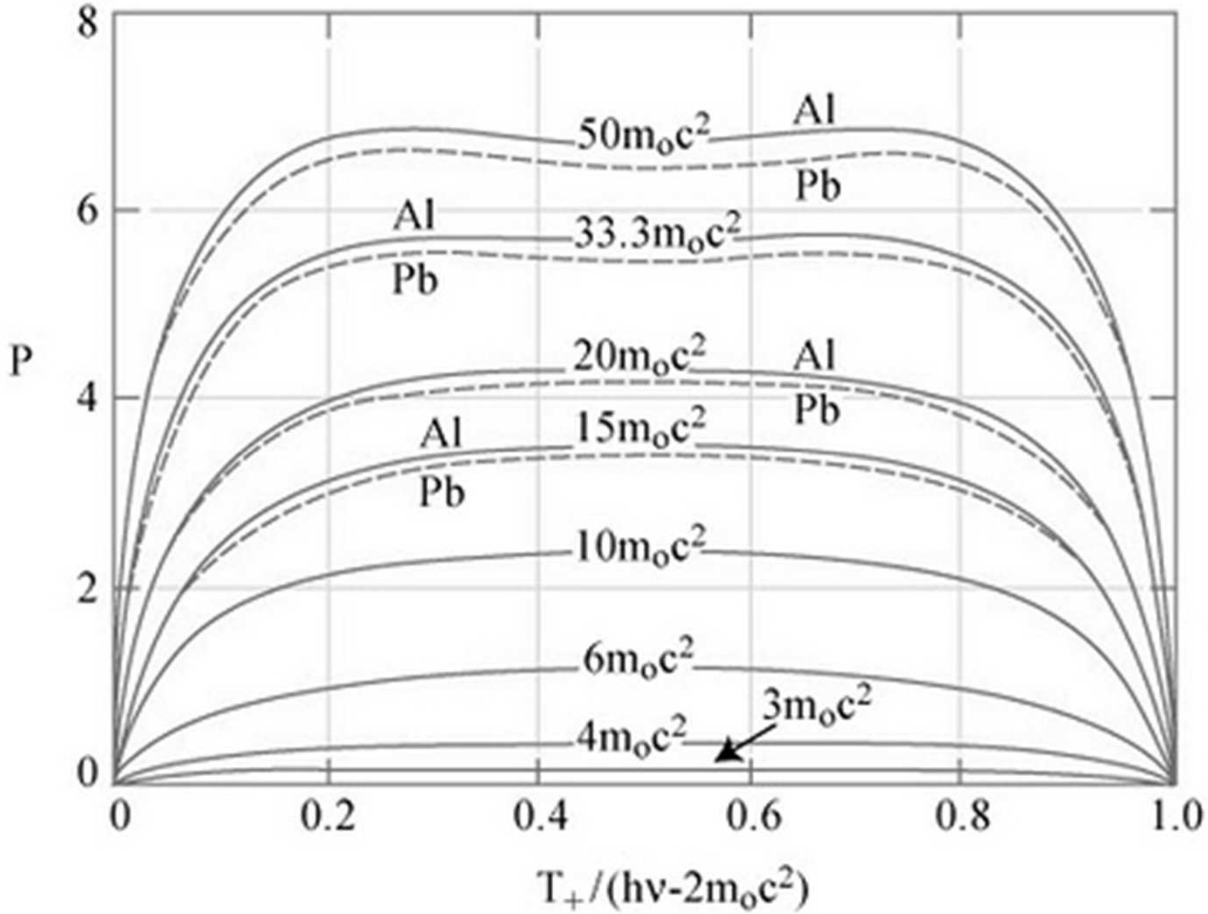
$$\gamma + \text{nucleus} \rightarrow e^+ + e^- + \text{nucleus}$$

- ✓ The high-energy limit of the pair production cross section per nucleus takes the form:

$$\lim_{\alpha \to \infty} \sigma_{\rm pp}(\alpha) = \sigma_0^{\rm pp} Z^2 \left(\ln(2\alpha) - \frac{109}{42} \right)$$

where $\alpha = E_\gamma / m_e c^2$ and $\sigma_o^{pp} = 1.80 \times 10^{-27}$ cm^2/nucleus. Note that the cross section grows logarithmically with incoming photon energy.

- ✓ Note that the rest-mass energy of the electron-positron pair must be created and so this interaction has a threshold at $E_\gamma = 2m_e c^2$. The cross section is exactly zero below this energy.
- ✓ The kinetic energy distribution of the electrons and positrons is remarkably "flat" except near the kinematic extremes of $K_\pm = 0$ and $K_\mp = E_\gamma / m_e c^2$.

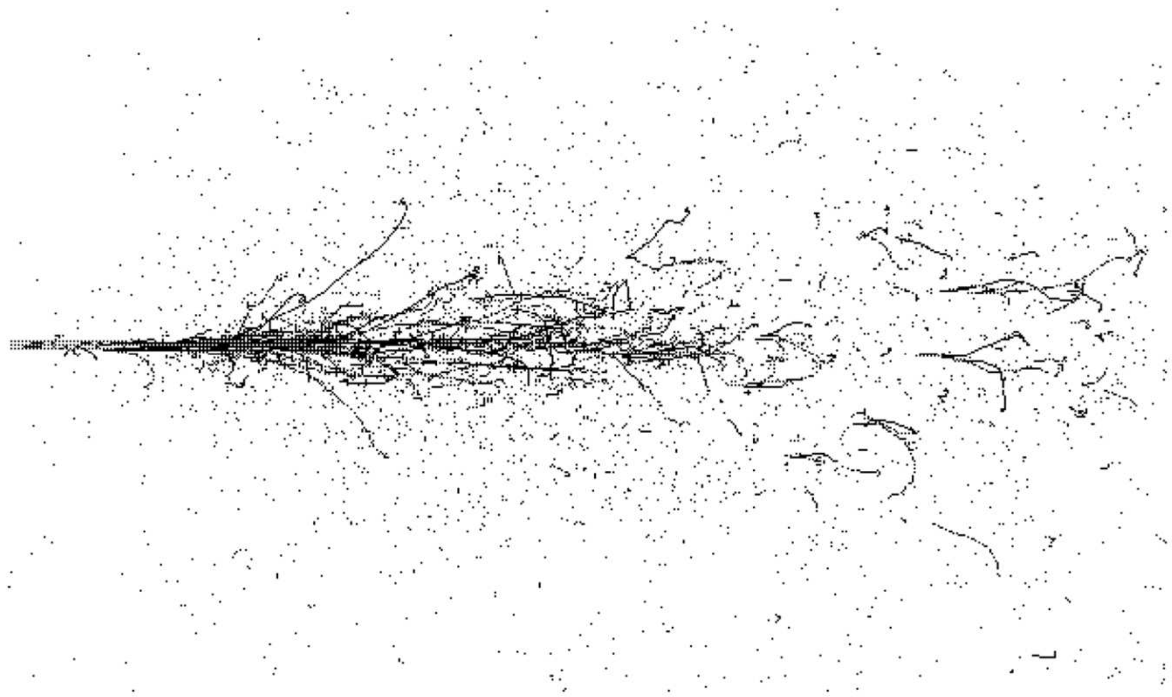


8
6
4
2
0
P
Al
Pb
50m₀c²
33.3m₀c²
20m₀c²
15m₀c²
10m₀c²
6m₀c²
4m₀c²
3m₀c²
0
0.2
0.4
0.6
0.8
1.0
T₊/(hν-2m₀c²)

Pair Production in Electron Field (cont.)

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

- ✓ Occasionally it is one of the electrons in the atomic cloud surrounding the nucleus that interacts with the incoming photon and provides the necessary third body for momentum and energy conservation. This interaction channel is suppressed by a factor of 1/Z relative to the nucleus-participating channel.
- ✓ In this case, the atomic electron is ejected with two electrons and one positron emitted. ("triplet" production)
- ✓ It is common to include the effects of triplet production by "scaling up" the two-body reaction channel and ignoring the 3-body kinematics. This is a good approximation for all but the low-Z atoms.



- A simulation of the cascade resulting from five 1.0 GeV electrons incident from the left on a target.
- The electrons produce photons which produce electron–positron pairs and so on until the energy of the particles falls below the cascade region.
- Electron and positron tracks are shown with black lines. Photon tracks are not shown explaining why some electrons and positrons appear to be "disconnected".

Compton Scattering

$\gamma + \text{Atom} \rightarrow \gamma + e^- + \text{Ion}^+$

- ✓ The Compton interaction is an inelastic "bounce" of a photon from an electron in the atomic shell of a nucleus and also known as "incoherent" scattering in recognition of the fact that the recoil photon is reduced in energy.
- ✓ At high energies, the Compton interaction approaches asymptotically:

$$\lim_{\alpha\rightarrow\infty} \sigma_{\text{inc}}(\alpha) = \sigma_0^{\text{inc}} \frac{Z}{\alpha}$$

where $\sigma_o^{inc} = 3.33 \times 10^{-25}$ cm^2/nucleus and $\alpha = E_\gamma / m_e c^2$.

– The cross section is proportional to Z (i.e. the number of electrons) and falls off as $1/E_\gamma$.

Compton Scattering (cont.)

$$\lim_{\alpha \to \infty} \sigma_{\text{inc}}(\alpha) = \sigma_0^{\text{inc}} \frac{Z}{\alpha}$$

- The cross section per unit mass is nearly a constant independent of material.
- Unlike the pair production cross section, the Compton cross section decreases with increased energy.
- The energy-weighted cross section is nearly a constant independent of energy.

Compton Scattering (cont.)

✓ At low energies, the Compton cross section becomes a constant with energy. That is,

$$\lim_{\alpha \to 0} \sigma_{\text{inc}}(\alpha) = 2\sigma_0^{\text{inc}} Z$$

– This is the classical limit and it corresponds to Thomson scattering, which describes the scattering of light from "free" (unbound) electrons.

– In almost all applications, the electrons are bound to atoms and this binding has a profound effect on the cross section at low energies.

– However, above about 100 keV one can consider these bound electrons as "free", and ignore atomic binding effects, which is a good approximation for most materials.

Compton Scattering (cont.)

- The differential cross section of photons scattered from a single free electron is taken from the Klein-Nishina formula.

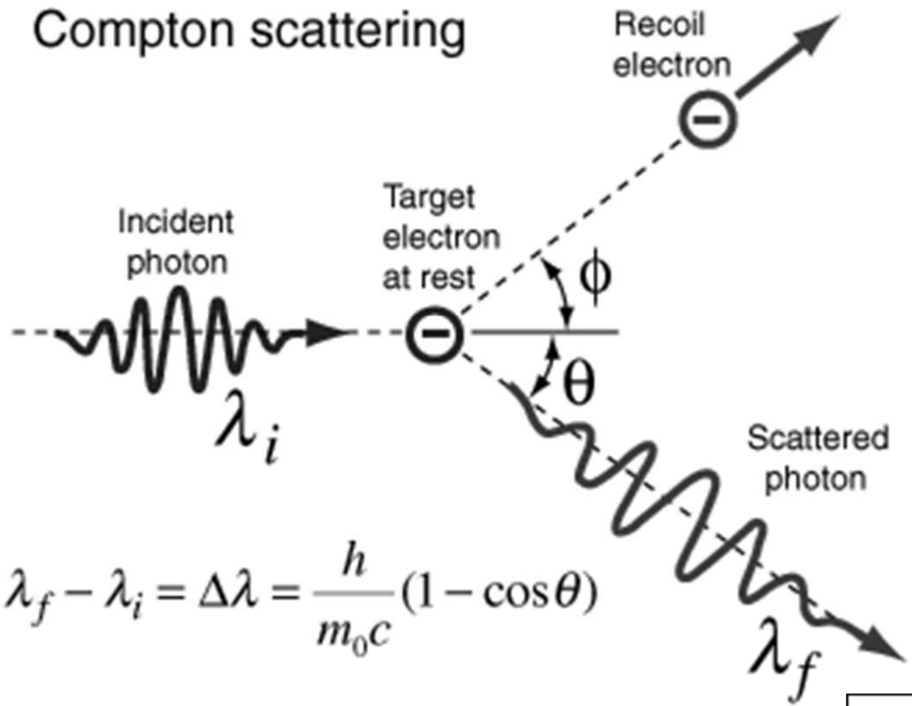
$$\frac{d\sigma}{d\Omega} = \alpha^2 r_c^2 P(E_\gamma,\theta)^2[P(E_\gamma,\theta) + P(E_\gamma,\theta)^{-1} - 1 + \cos^2(\theta)]/2$$

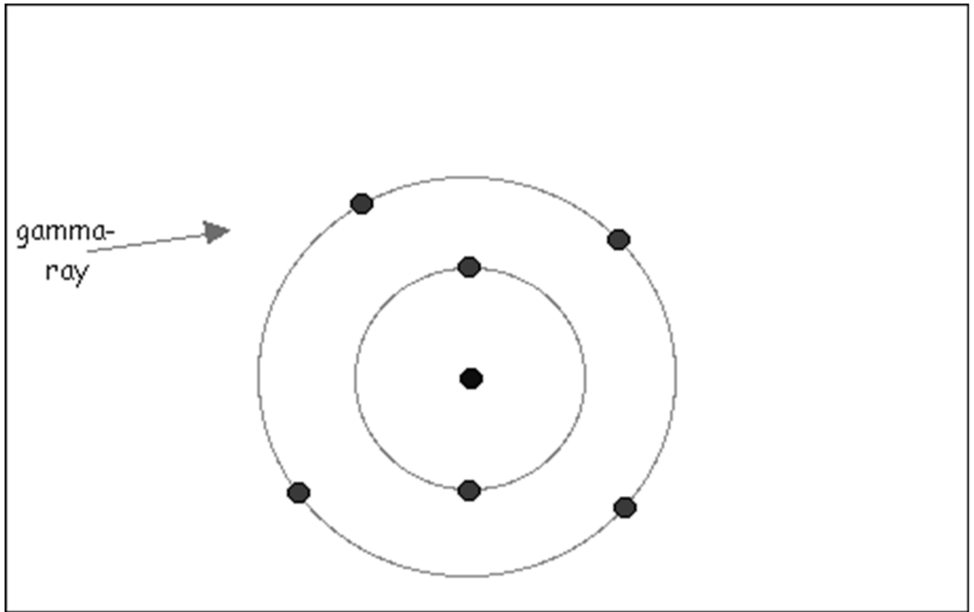
where $d\sigma/d\Omega$ is a differential cross section, $d\Omega$ is an infinitesimal solid angle element, α is the fine structure constant (~1/137.04), θ is the scattering angle; $r_c = \hbar/m_e c$ is the "reduced" Compton wave length of the electron (~0.38616 pm); m_e is the mass of an electron (~511keV/c^2); and $P(E_\gamma,\theta)$ is the ratio of photon energy after and before the collision:

$$E_\gamma' / E_\gamma = P(E_\gamma,\theta) = \frac{1}{1 + (E_\gamma/m_e c^2)(1-\cos\theta)}$$

- The final energy of the scattered photon, E_γ', depends only on the scattering angle and the original photon energy:

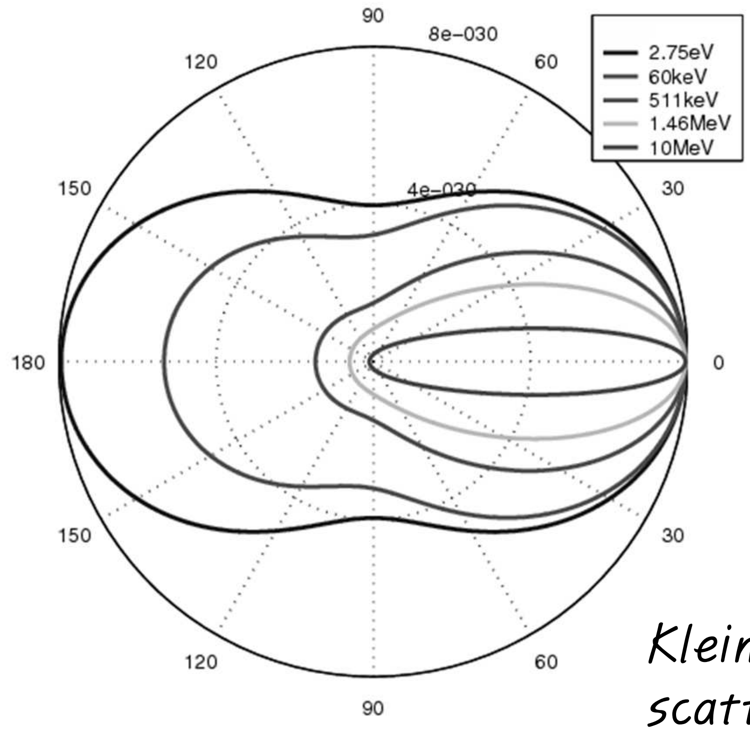
$$E'_\gamma(E_\gamma, \theta) = E_\gamma \cdot P(E_\gamma,\theta)$$


Compton scattering
Recoil electron
Incident photon
Target electron at rest
ϕ
θ
λ_i
Scattered photon
λ_f
$$\lambda_f - \lambda_i = \Delta\lambda = \frac{h}{m_0 c}(1 - \cos\theta)$$


gamma-ray

Compton Scattering (cont.)

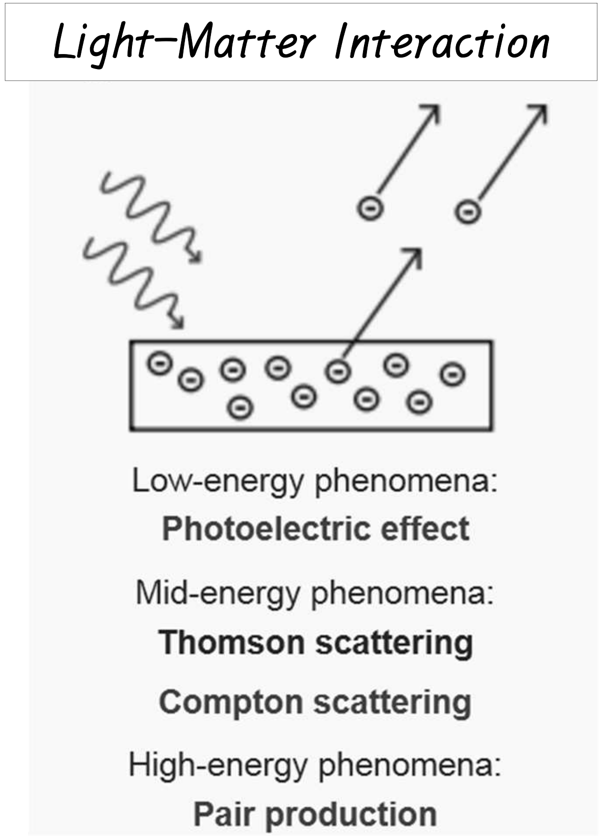
- Before the formula derived by Oskar Klein and Yoshio Nishina, J.J. Thomson derived the cross section of photons scattered by a free electron.
- Note that If $E_\gamma \ll m_e c^2$, $P(E_\gamma, \theta) \rightarrow 1$ ($E'_\gamma \sim E_\gamma$) and the Klein-Nishina formula is reduced to Thomson expression..



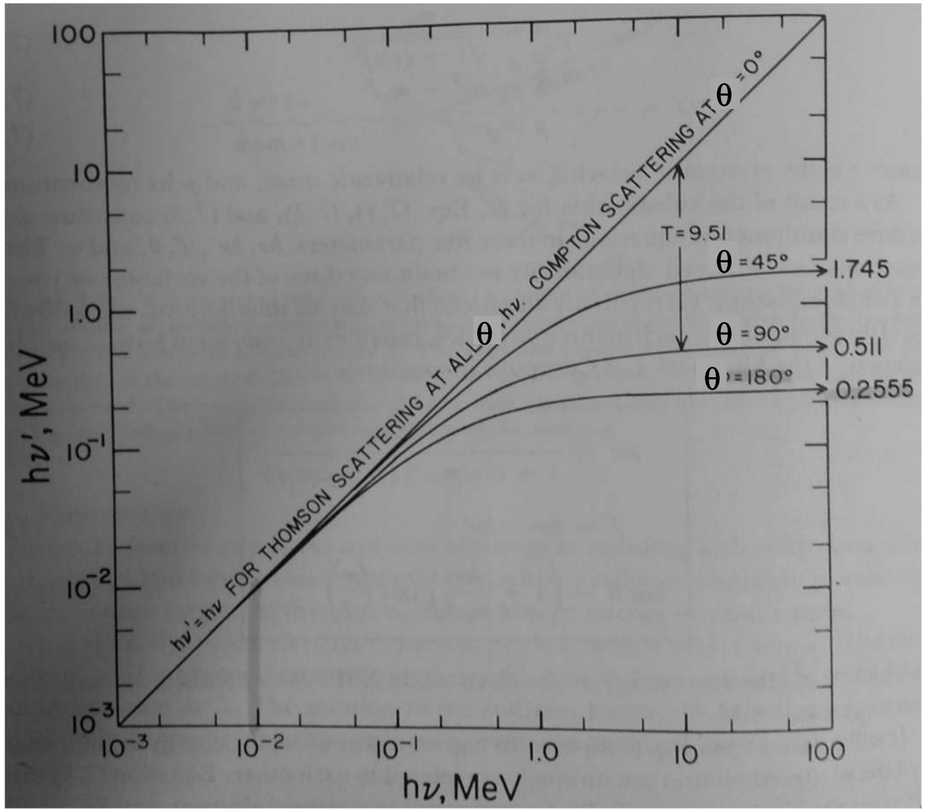
Klein-Nishina distribution of scattering-angle cross sections

(Thomson Scattering)

- ✓ the elastic scattering of electromagnetic radiation by a free charged particle.
- ✓ Just the low-energy limit of Compton scattering: the particle kinetic energy and photon frequency are the same before and after the scattering.
  - This limit is valid as long as the photon energy is much less than the mass energy of the particle: $h\nu \ll m_0c^2$.



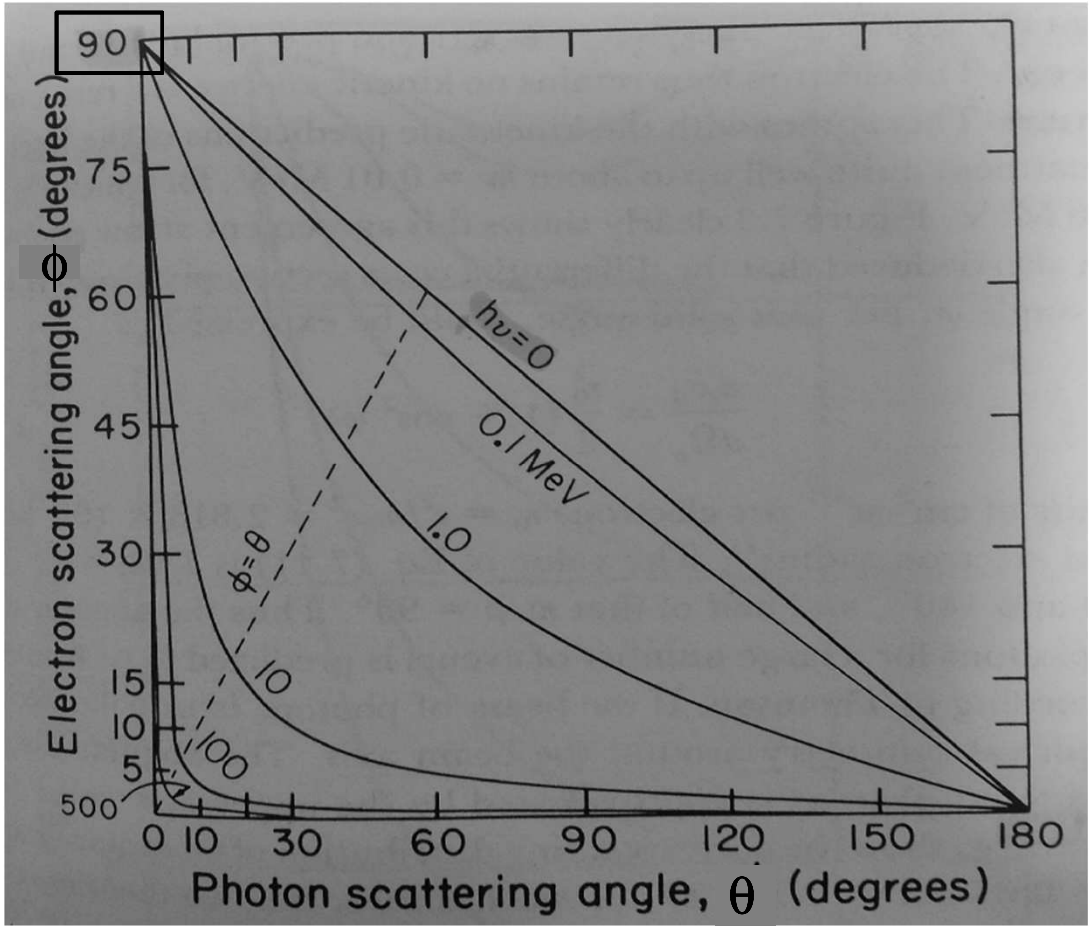
E_γ' vs. E_γ



$$\boxed{E_\gamma'/E_\gamma} = P(E_\gamma, \theta) = \frac{1}{1 + (E_\gamma/m_e c^2)(1 - \cos\theta)} \sim 1, \text{ at } E_\gamma \ll m_e c \text{ for all } \theta.$$

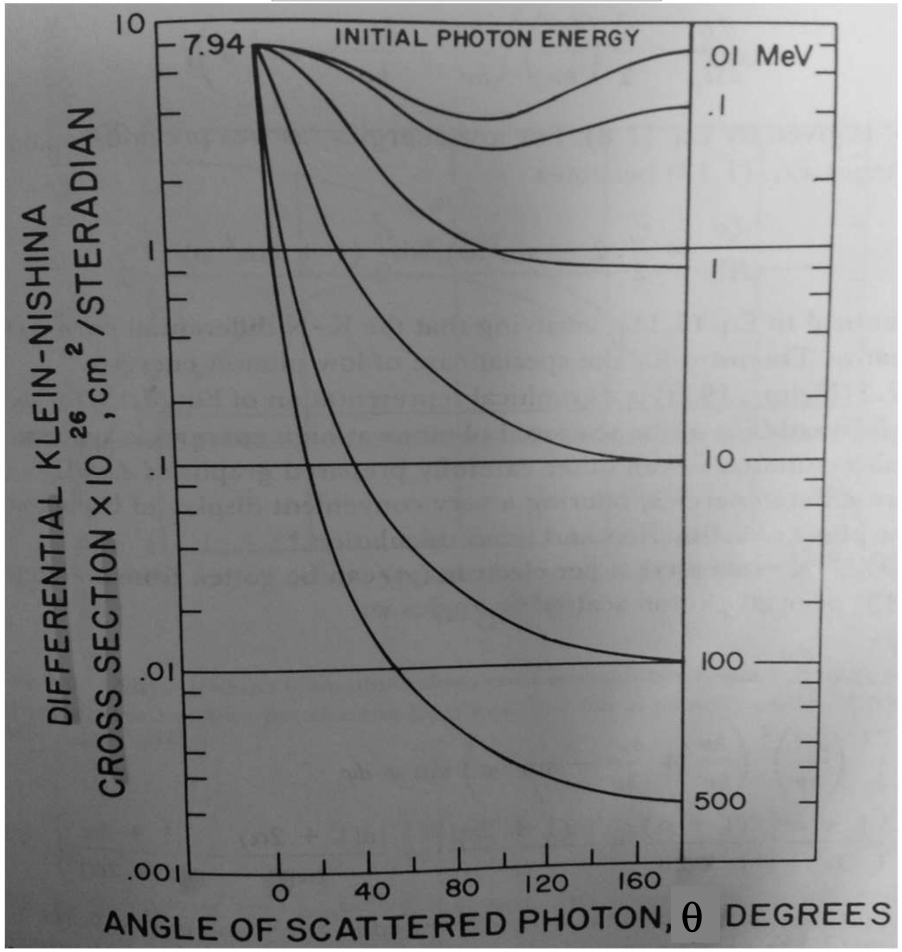
$$= 1, \text{ at all } E_\gamma \text{ for } \theta = 0.$$

$$\boxed{\sim \frac{m_e c^2}{E_\gamma (1 - \cos\theta)}}, \text{ at } E_\gamma \gg m_e c \text{ for } \theta \neq 0$$



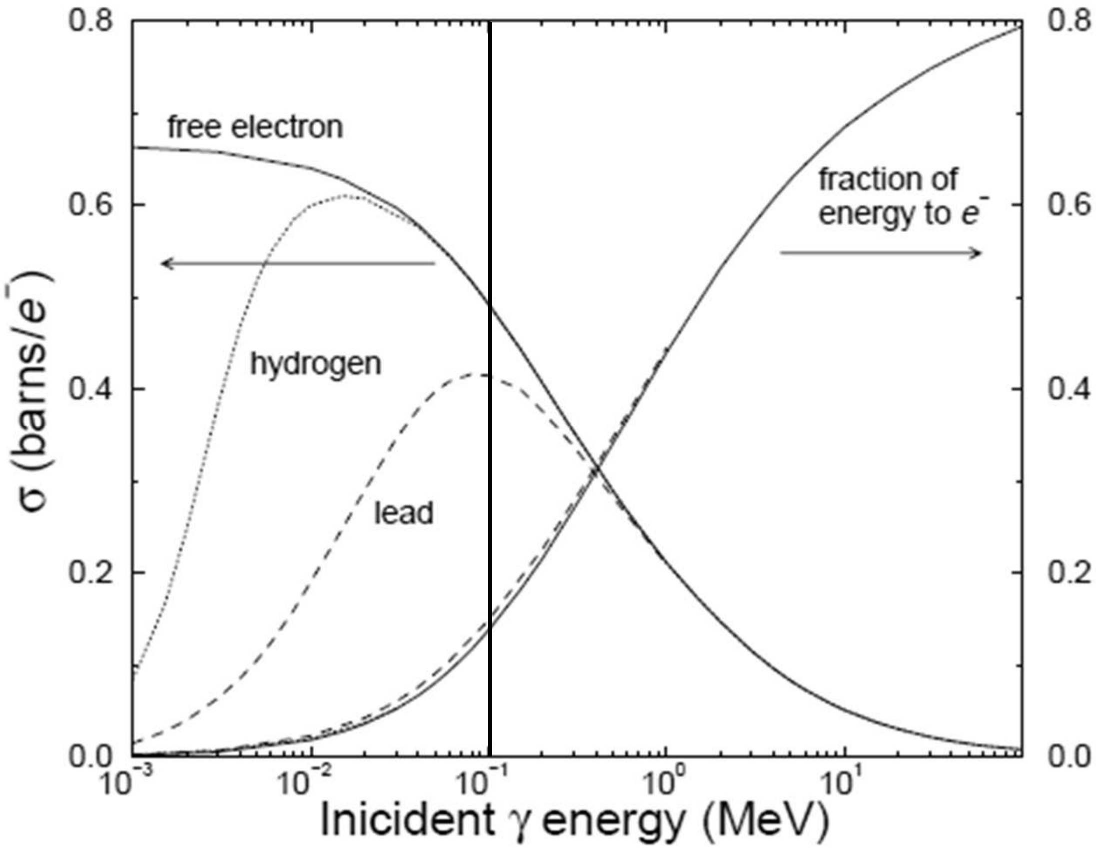
electron scattering angle ϕ vs. photon scattering angle θ

$d\sigma/d\Omega$ *vs.* θ



differential Klein–Nishina cross section $d\sigma/d\Omega$
vs. photon scattering angle θ

effect of electron binding on Compton scattering



for K 1s electron,
88 keV (Pb) & 116 keV (U)

Electron binding energies, in electron volts, for the elements in their natural forms

Element	K 1s	L_1 2s	L_2 $2p_{1/2}$	L_3 $2p_{3/2}$	M_1 3s	M_2 $3p_{1/2}$	M_3 $3p_{3/2}$	M_4 $3d_{3/2}$	M_5 $3d_{5/2}$
1 H	13.6								
Element	**N_4 $4d_{3/2}$**	**N_5 $4d_{5/2}$**	**N_6 $4f_{5/2}$**	**N_7 $4f_{7/2}$**	**O_1 5s**	**O_2 $5p_{1/2}$**	**O_3 $5p_{3/2}$**	**O_4 $5d_{3/2}$**	**O_5 $5d_{5/2}$**
82 Pb	434.3†	412.2†	141.7†	136.9†	147*b	106.4†	83.3†	20.7†	18.1†

Photoelectric Absorption

$\gamma + \text{Atom} \rightarrow e^{-} + \text{Ion}^{+}$

- ✓ The dominant low-energy photon process.
- ✓ The photon gets absorbed by an electron of an atom resulting in escape of the electron from the atom and accompanying small energy photons as the electron cloud of the atom settles into its ground state.
- ✓ The theory concerning this phenomenon is not complete and exceedingly complicated. The cross section formulae are usually in the form of numerical fits and take the form:

$$\sigma_{\text{ph}}(E_\gamma) \propto \frac{Z^m}{E_\gamma^n}$$

where the exponent m on Z ranges from 4 (low energy, below 100 keV) to 4.6 (high energy, above 500 keV) and the exponent n on E_γ ranges from 3 (low energy, below 100 keV) to 1 (high energy, above 500 keV).

Photoelectric Absorption (cont.)

- ✓ The high-energy fall-off is the same as the Compton interaction. However, the high-energy photoelectric cross section is depressed by a factor of about $Z^{3.6}10^{-8}$ relative to the Compton cross section and so is negligible in comparison to the Compton cross section at high energies.

$$\sigma_{\mathrm{ph}}(E_\gamma) \propto \frac{Z^m}{E_\gamma^n} \quad vs. \quad \lim_{\alpha\to\infty} \sigma_{\mathrm{inc}}(\alpha) = \sigma_0^{\mathrm{inc}} \frac{Z}{\alpha} \quad (\alpha = E_\gamma / m_e c^2)$$

($m \sim 4.6$, $n \sim 1$ at high photon energy)

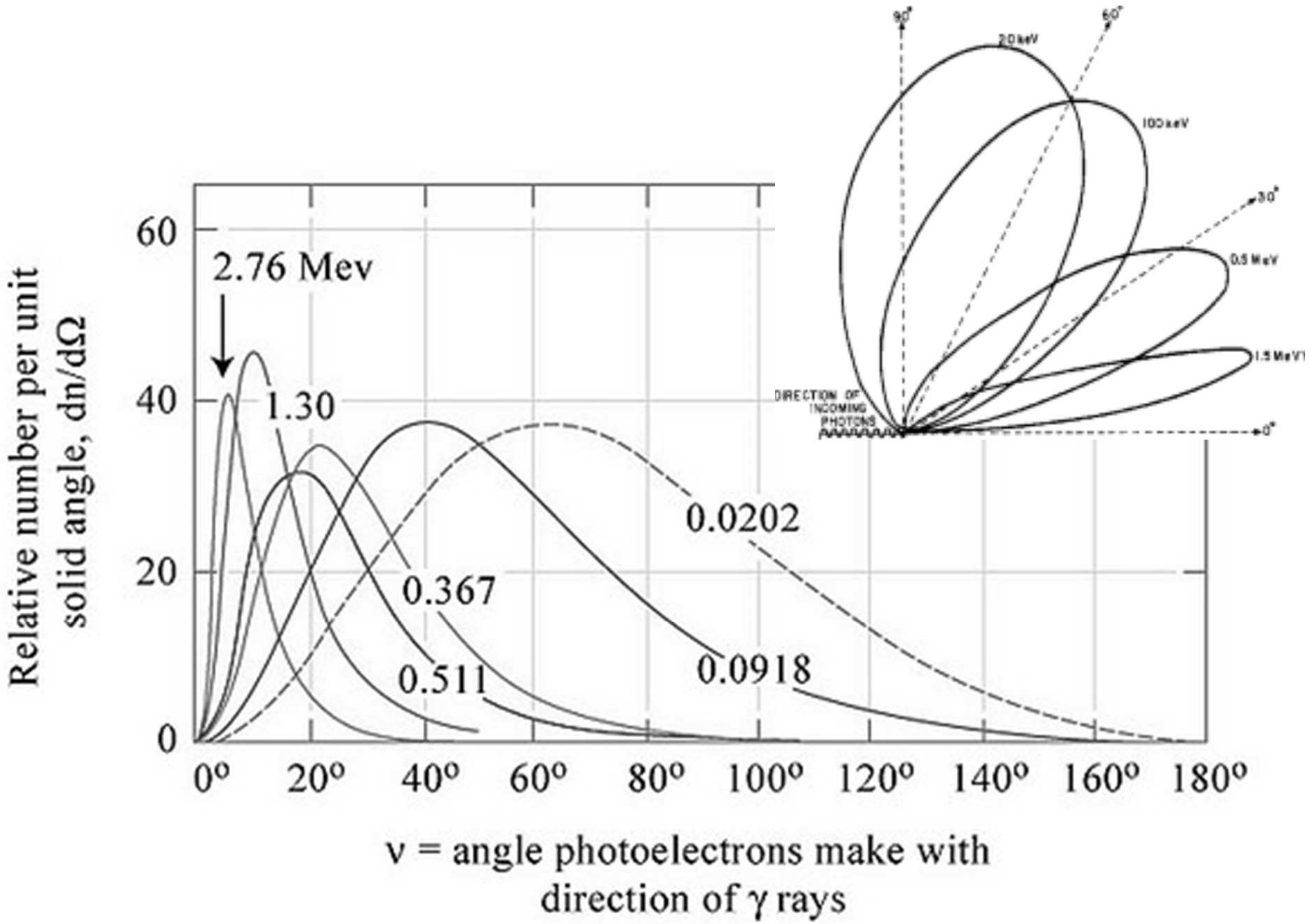
Photoelectric Absorption (cont.)

✓ A useful approximation that applies in the regime where the photoelectric effect is dominant (E<100 keV) is:

$$\sigma_{\rm ph}(E_\gamma) \propto \frac{Z^4}{E_\gamma^3}$$

which is often employed for simple analytic calculations. (However, most Monte Carlo codes employ a table look-up for the photoelectric interaction.)

✓ Angular distributions of the photoelectron can be determined according to the theory of Sauter. Although Sauter's theory is relativistic, it appears to work in the non-relativistic regime as well.


60
40
20
0
2.76 Mev
1.30
0.511
0.367
0.0918
0.0202
0°
20°
40°
60°
80°
100°
120°
140°
160°
180°
Relative number per unit solid angle, dn/dΩ
ν = angle photoelectrons make with direction of γ rays
90°
60°
30°
0°
20 keV
100 keV
0.5 MeV
1.5 MeV
DIRECTION OF INCOMING PHOTONS

Rayleigh Scattering

- ✓ the (dominantly) elastic scattering of light or other electromagnetic radiation by particles much smaller than the wavelength of the light.
- ✓ coherent scattering with no energy loss of photon.
- ✓ The cross section is at least an order of magnitude less than that of photoelectric cross section.
- ✓ There exists a photon in the final state in contrast to photoelectric effect (vs. an electron).
- ✓ The coherent interaction is an elastic (no energy loss) scattering from atoms. It is not good enough to treat molecules as if they are made up of independent atoms. The molecular structure matters!

Rayleigh Scattering (cont.)

✓ The Rayleigh differential cross section has the following form:

$$\sigma_{\mathrm{coh}}(E_\gamma, \Theta) = \frac{r_e^2}{2}(1 + \cos^2\Theta)[F(q, Z)]^2$$

where r_e is the classical electron radius (2.8179×10^{-13} cm), θ is the angle b/w the photon directions prior to and following a scattering, q is the momentum-transfer parameter, $q = (E_\gamma/hc)\sin(\theta/2)$, and F (q, Z) is the atomic form factor.

– The atomic form factor, or atomic scattering factor, is a measure of the scattering amplitude of a wave by an isolated atom.

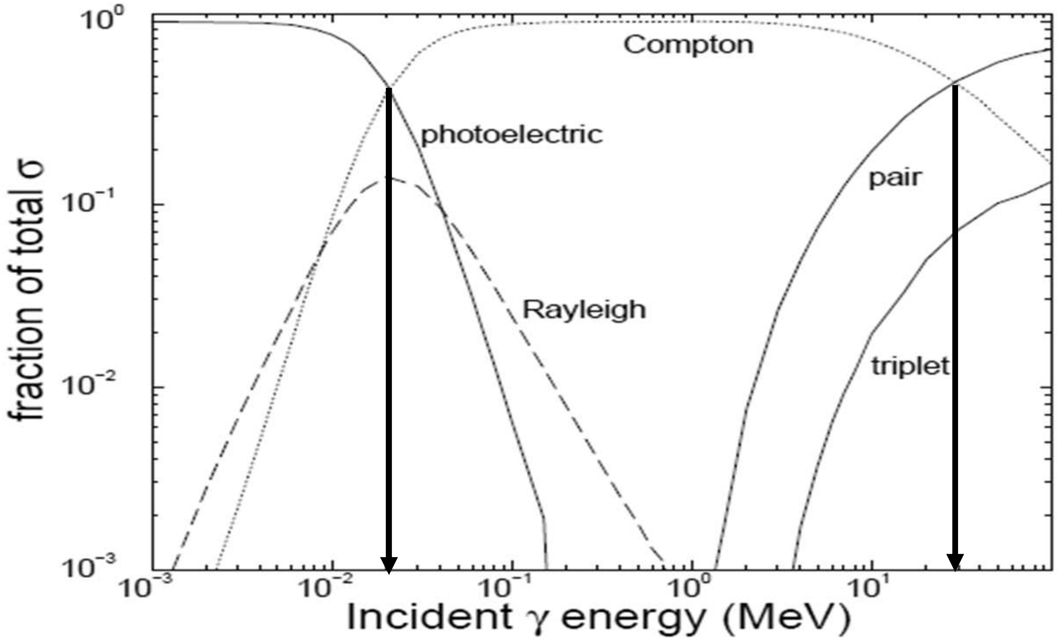
– X-rays are scattered by the electron cloud of the atom and hence the scattering amplitude of X-rays increases with the atomic number, Z, of the atoms in a sample.

– Tables of the form factors published by Hubbell and Øverbø are available.

Relative Importance of Interaction Modes

- ✓ <u>For carbon</u>, a moderately low-Z material, note three distinct regions of single interaction dominance: photoelectric below 20 keV, pair above 30 MeV and Compton in between.
- ✓ The almost order of magnitude depression of the Rayleigh and triplet contributions is some justification for the relatively crude approximations.

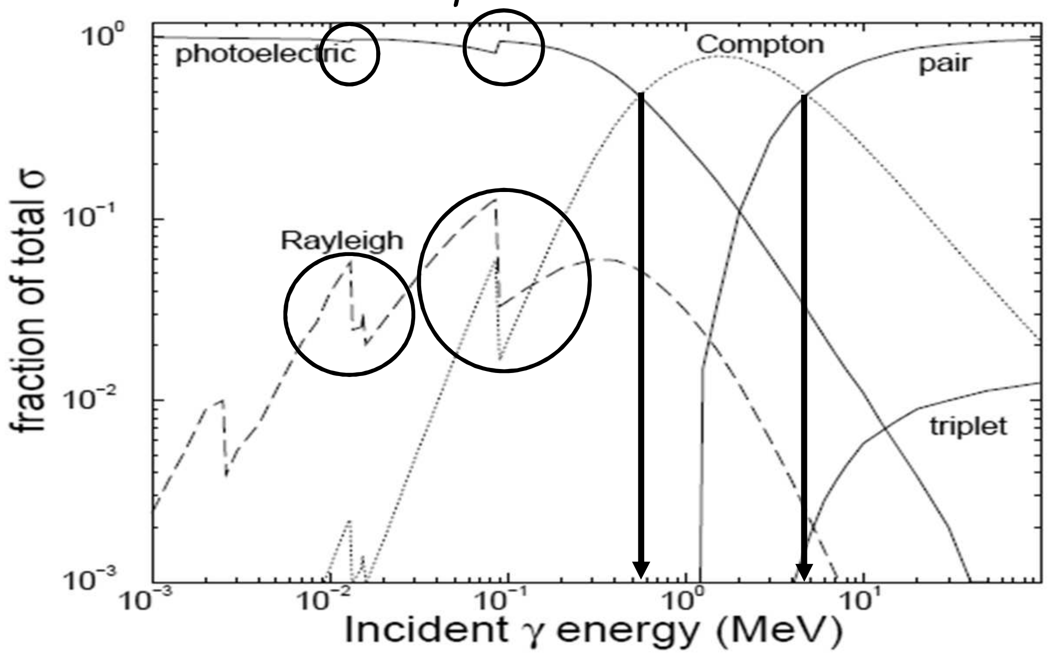
Components σ in C



Relative Importance of Interaction Modes (cont.)

- ✓ For lead, the "Compton dominance" section is much smaller, now extending only from 700 keV to 4 MeV.
- ✓ Note quite a complicated structure below about 90 keV, the K-shell binding energy of the lead atom. Below this threshold, atomic structure effect becomes very important.

Components σ in Pb

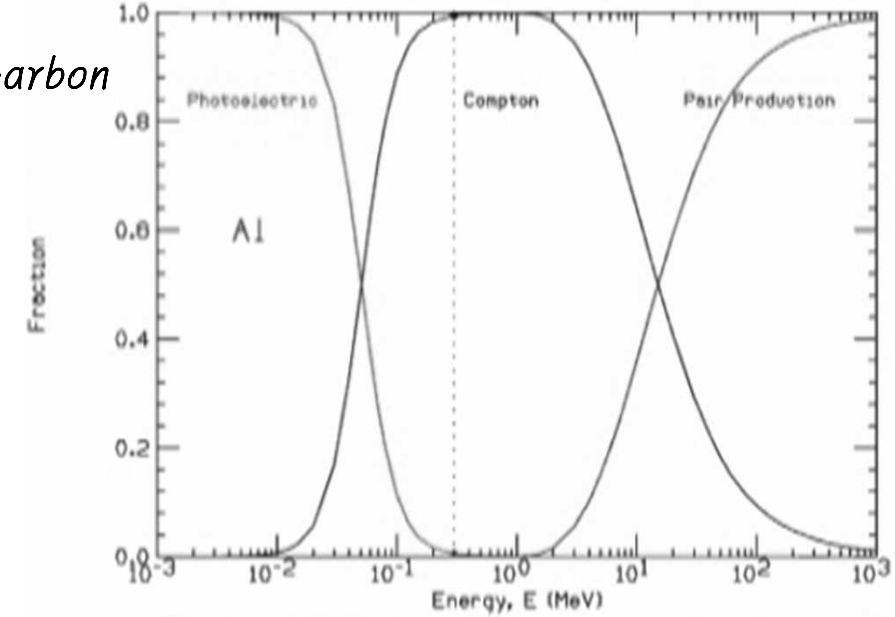


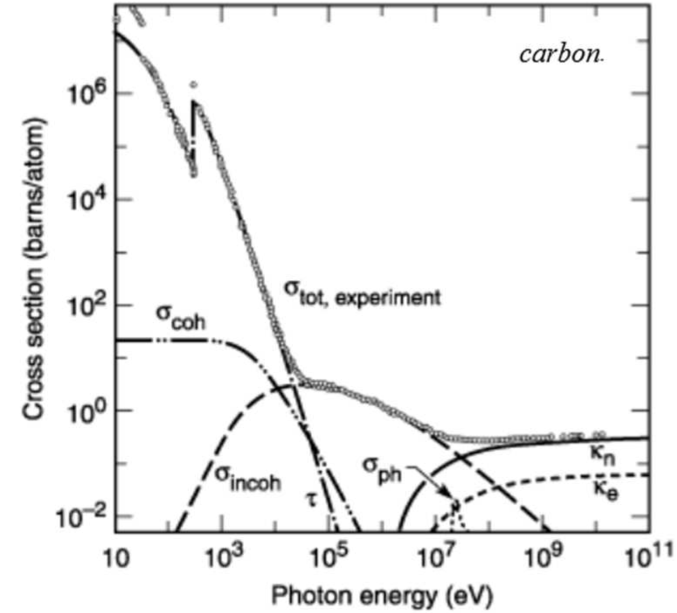
Electron binding energies

Element	K 1s	L_1 2s	L_2 $2p_{1/2}$	L_3 $2p_{3/2}$	M_1 3s	M_2 $3p_{1/2}$	M_3 $3p_{3/2}$	M_4 $3d_{3/2}$	M_5 $3d_{5/2}$
82 Pb	88005	15861	15200	13035	3851	3554	3066	2586	2484

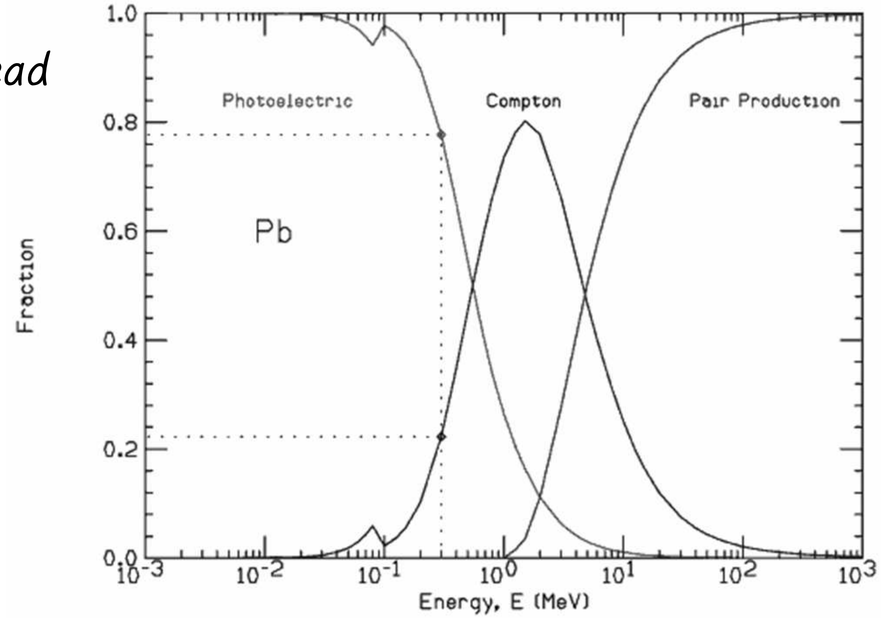
relative contribution by process vs. photon energy

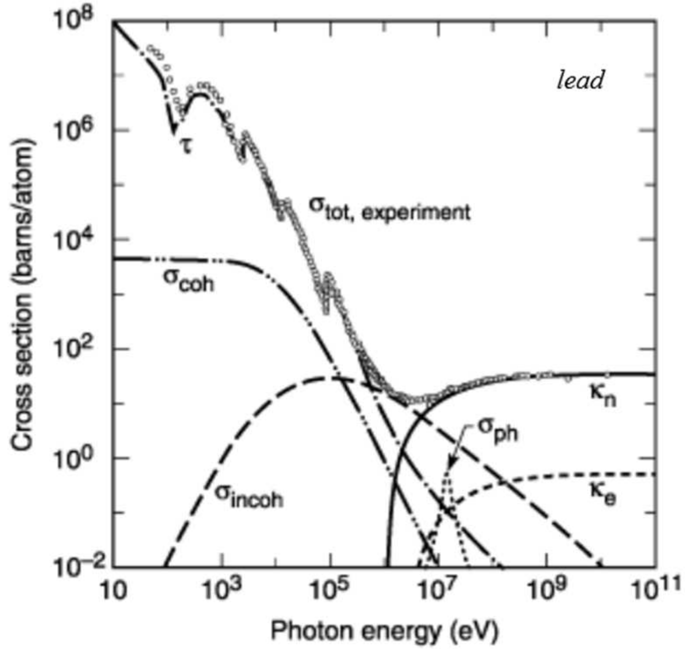
Carbon





Lead

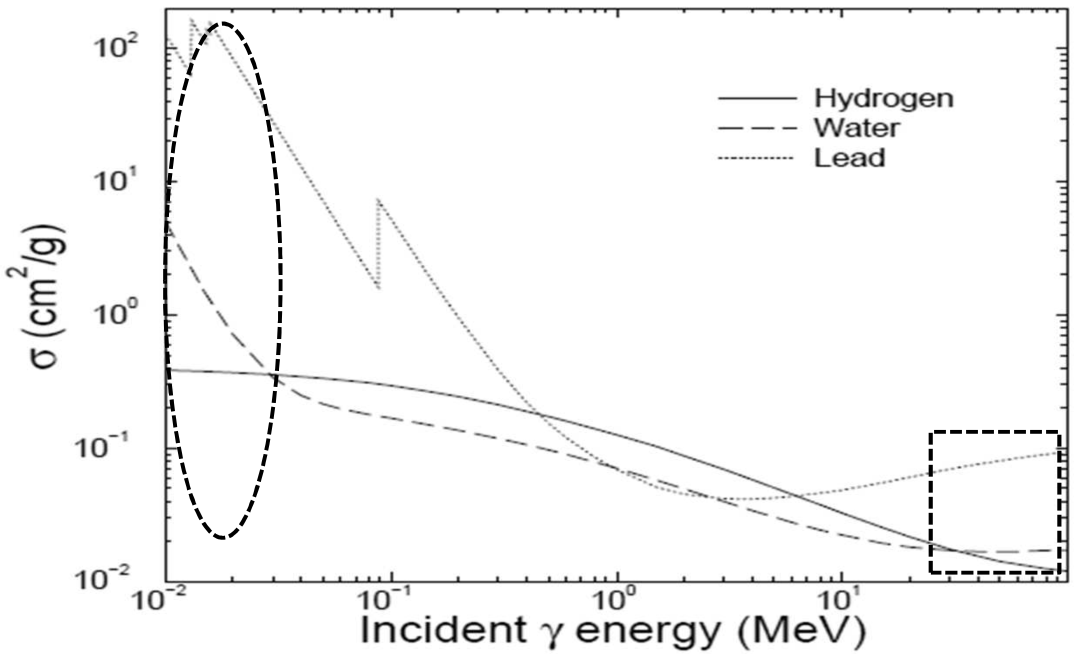




Total Cross Section

- ✓ Compton dominance region gets narrower with Z-value.
- ✓ At high energy, the Z^2 dependence of pair production is evident in the lead.
- ✓ At lower energies the $Z^n (n > 4)$ dependence of the photoelectric cross section is quite evident.

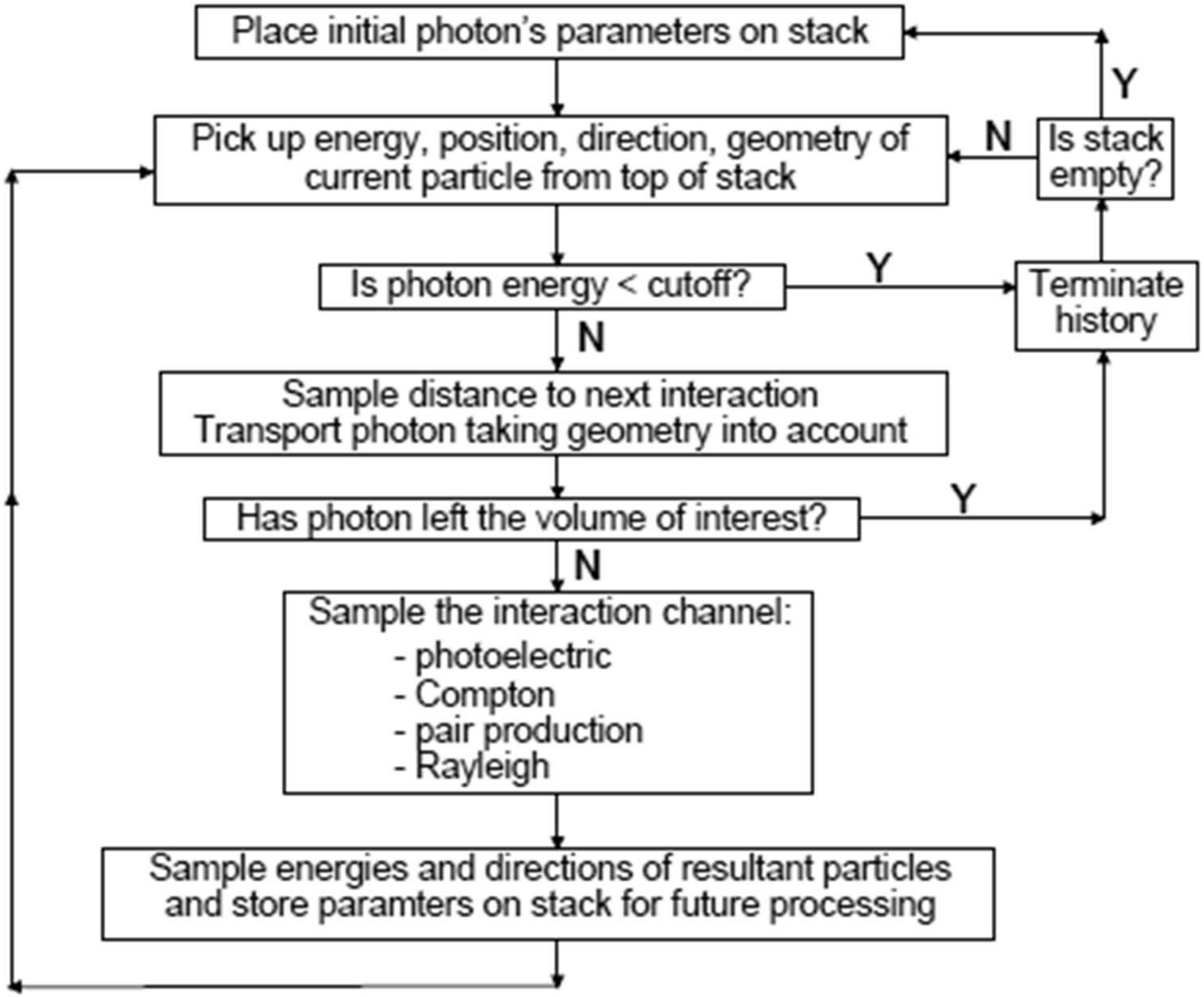
Total Photon σ vs. Photon Energy



Photon Transport: Logic Flow

- It is simplified by ignoring electron creation and considering that the transport occurs in only a single volume element and a single medium.
- Imagine that an initial photon's parameters are present at the top of an array called STACK, an array that retains particle phase space characteristics for processing.
- There is a photon transport cutoff defined. Photons that fall below this cutoff are absorbed "on the spot". In "real life" low-energy photons are absorbed by the photoelectric process and vanish.

Ex. photon transport logic flow (EGS4)



Photon Transport: Logic Flow (cont.)

- ✓ The initial characteristics of a photon entering the transport routine and first tested to see if the energy is below the transport cutoff.
- ✓ If it is below the cutoff, the history is terminated. If the STACK is empty then a new particle history is started.
- ✓ If the energy is above the cutoff then the distance to the next interaction site is chosen.
- ✓ The photon is then transported, that is "stepped" to the point of interaction. If the photon, by virtue of its transport, has left the volume defining the problem then it is discarded.

Photon Transport: Logic Flow (cont.)

- ✓ Otherwise, the branching distribution is sampled to see which interaction occurs. Having done this, the surviving particles (new ones may be created, some disappear, the characteristics of the initial one will almost certainly change) have their energies, directions and other characteristics chosen from the appropriate distributions.
- ✓ The surviving particles are put on the STACK. Lowest energy ones should be put on the top of the STACK to keep the size of the STACK as small as possible.
- ✓ Then the whole process takes place again until the STACK is empty and all the incident particles are used up.

Problem Definition

- Define the problem geometry
  - the physical description of the geometry and the material constituents.
  - All particle interactions, flight paths and escapes from the problem geometry are based on this description.
- Define the source
  - The source may be a pdf from which the start particles are selected or a specific set of starting points, directions, energies, and times.

Random Walk

- Select a source particle
  - A photon is selected from the source distribution to be given an initial position, energy, time, and direction of travel.

- Determine the collision point
  - A collision site for the photon is selected from the exponential distribution of collisions along its path.
  - The cross sections of the materials through which the photon is traveling are used to obtain the probability of collisions per unit path length.

Random Walk (cont.)

- Determine the type of interaction
  - Once a point of interaction is chosen, the total cross section is apportioned pro rata among the elements (vs. nuclear species) present.
  - After selecting an element (vs. a nuclear species), the cross section for that element (vs. species) is used to determine which type of interaction has occurred.
  - An alternative technique for handling interaction cross section is to average or "mix" the cross sections so that one combined set contains the features of all the constituents.
  - A multi-group formulation is also possible, in which the photon energies (vs. neutron energies) are cast into a set of discrete bins or groups, and a table of group-averaged cross sections is used to determine the interactions.

Random Walk (cont.)

- Determine the result of interaction:

  the result of the interaction is selected from one or more of the following alternatives:

  1. death of the photon (vs. neutron) by absorption (or reduction of the "weight" of the particle by non-absorption probability)
  2. production of secondary particles, such as in photoelectric absorption or pair production (vs. fission), or
  3. scattering of the tracked particle through some angle selected from the particular angular scattering characteristics of the atom (vs. nucleus) encountered.

Random Walk (cont.)

- Complete the history
  - All secondary particles, as well as the scattered photon (vs. neutron), are tracked to determine subsequent collision points and products.
  - This process is continued until the initial photon (vs. neutron) and all its secondary particles produced by the initial photon (vs. neutron) either die or escape from the problem geometry.

Presentation of Result

- Compute the response of interest
  - Use the result of random walk to calculate the detector response, which may be done simultaneously with the random walk or by means of a post-random walk process.