Electron-Gamma Inter-transport Modeling

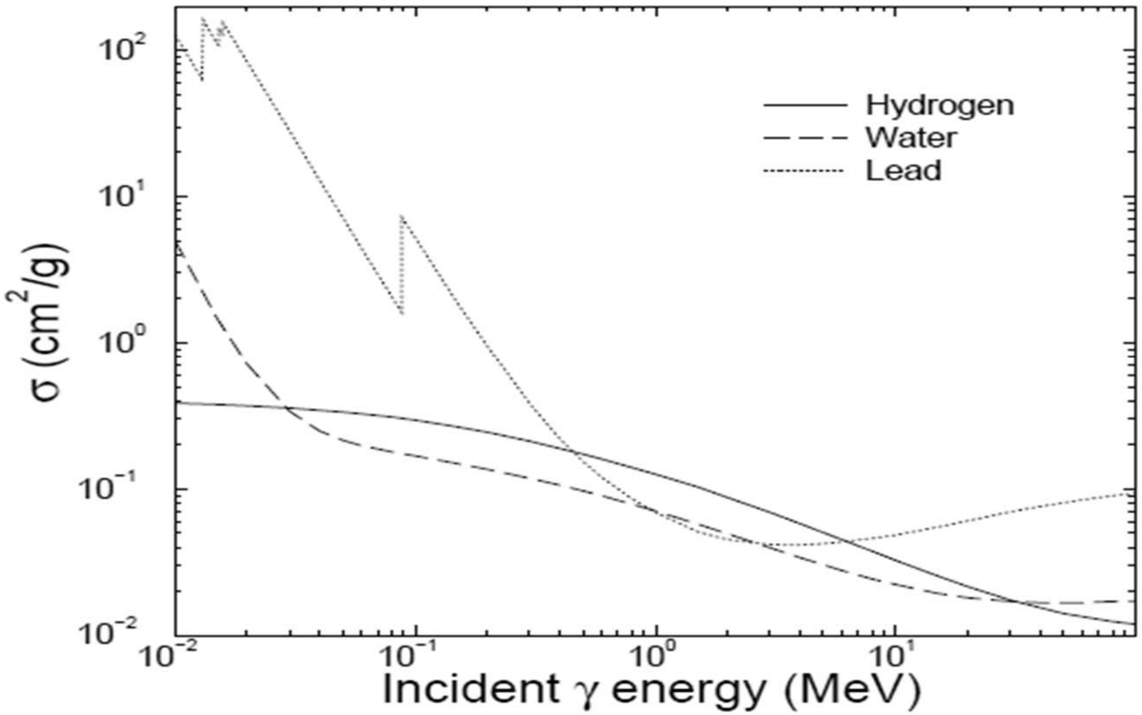
SNU/NUKE/EHK

Photon Transport Scheme

Interaction Modes of Relative Importance

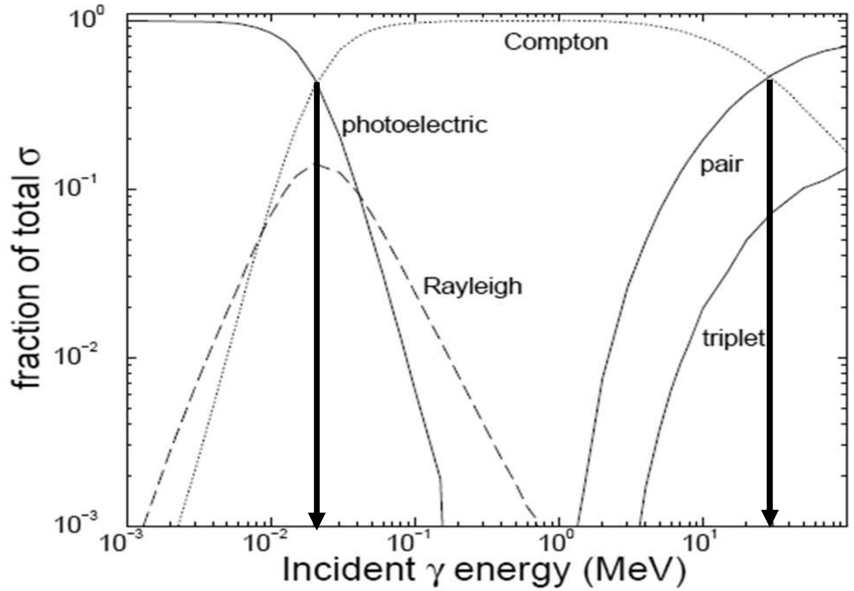
- ✓ Compton dominance region gets narrower with Z-value.
- ✓ At high energy, the Z^2 dependence of pair production is evident.
- ✓ At lower energies the $Z^n (n > 4)$ dependence of the photoelectric cross section is quite evident.

total photon σ vs. photon energy

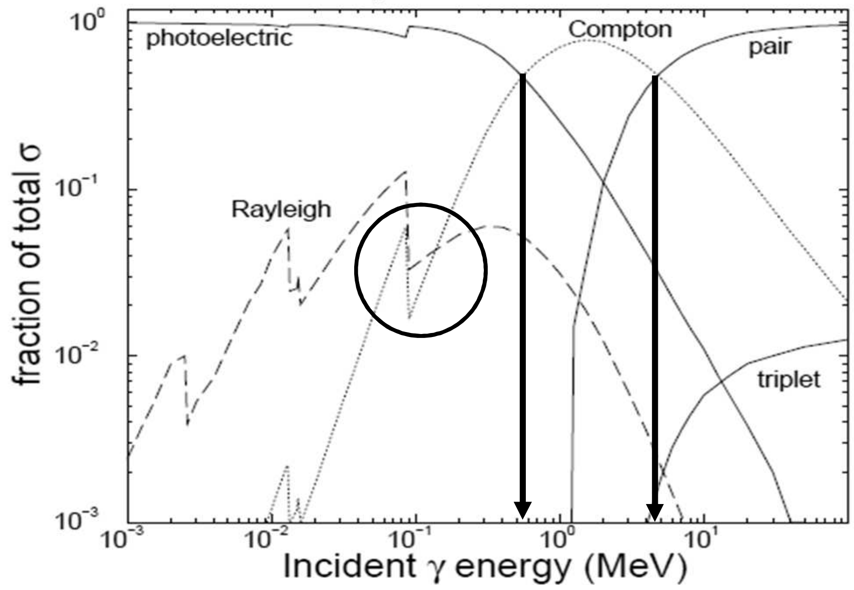


Interaction Modes of Relative Importance (cont.)

Components σ in C



Components σ in Pb



→ *Photon transport simulation in consideration of*

1. *Rayleigh scattering (The X-section rises rapidly with decreasing energy and becomes significant at higher energy with greater Z.)*
2. *photoelectric absorption*
2. *Compton scattering*
3. *pair production*

Components σ in Pb

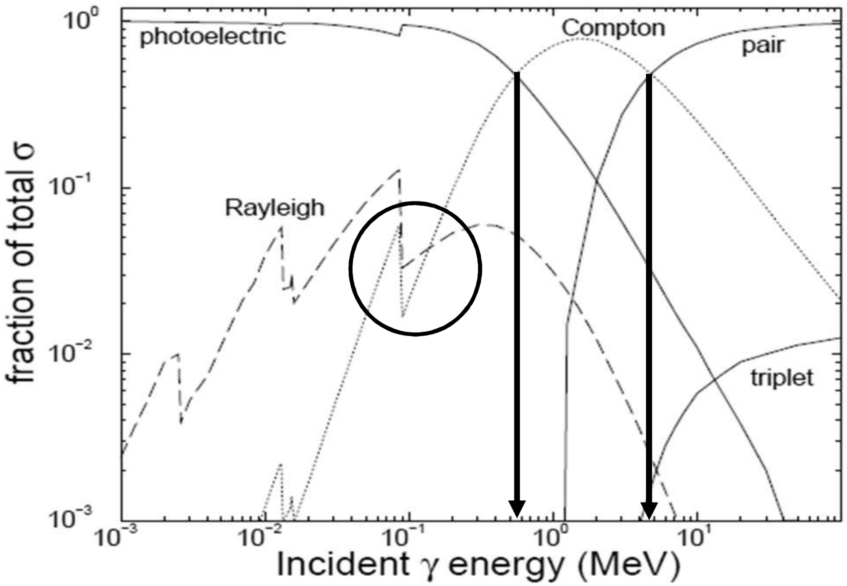


Table 1-1. Electron binding energies (continued).

(in eV)

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 $3d_{5/2}$	N_1 4s	N_2 $4p_{1/2}$	N_3 $4p_{3/2}$
82 Pb	88005	15861	15200	13035	3851	3554	3066	2586	2484	891.8†	761.9†	643.5†

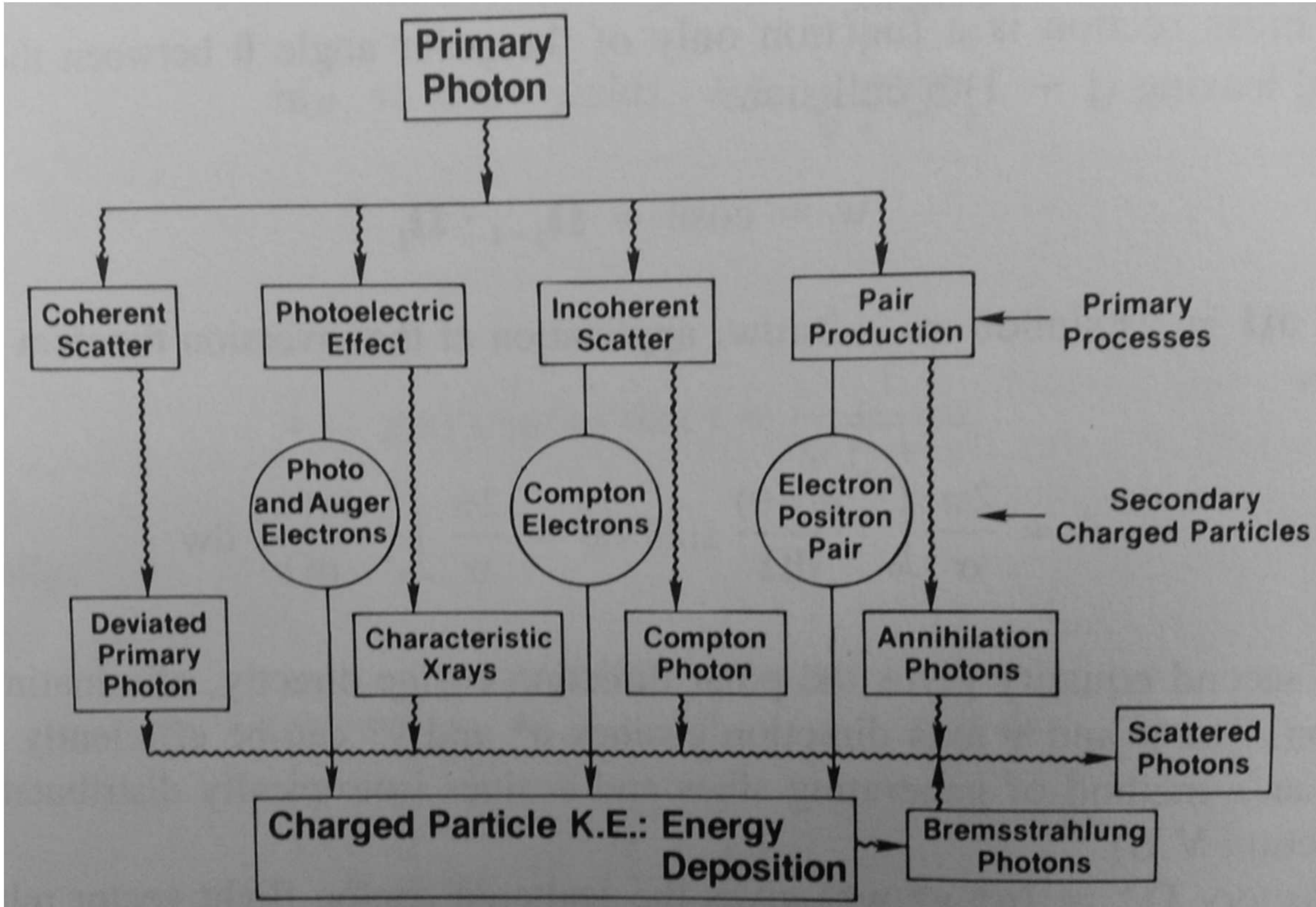


FIGURE 6. Principal mechanisms of photon scattering and energy deposition in the 10 keV to 10 MeV energy range.

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.

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.

Photon Transport Logic Flow:
photon transport cutoff energy P_{cutoff}

- ✓ Initial photon energy E_γ
- ✓ Photons that fall below P_{cutoff} are absorbed on the spot. In reality, low-energy photons are absorbed by the photoelectric process and vanish.
- ✓ In materials of atomic number lower than 20, the binding energy of K-shell electrons is less than 5 keV.

→ P_{cutoff} = 5 keV of choice

E_B (eV)

Element	K 1s
1 H	13.6
2 He	24.6*
3 Li	54.7*
4 Be	111.5*
5 B	188*
6 C	284.2*
7 N	409.9*
8 O	543.1*
9 F	696.7*
10 Ne	870.2*
11 Na	1070.8†
12 Mg	1303.0†
13 Al	1559.6
14 Si	1839
15 P	2145.5
16 S	2472
17 Cl	2822.4
18 Ar	3205.9*
19 K	3608.4*
20 Ca	4038.5*
21 Sc	4492
22 Ti	4966

Photon Transport Logic Flow:

Step 1. Determine the next interaction distance s.

✓ pdf: $p(s)ds = \mu_t \cdot exp(-\mu_t s)ds$,
where $\mu_t = \mu_R + \mu_{pe} + \mu_{CS} + \mu_{pp}$

- μ_R , μ_{pe} , μ_{CS} and μ_{pp} are mutually exclusive events.
- μ's are specific to the photon energy E_γ and medium.

✓ cdf: $P(s) = 1 - exp(-\mu_t s)$

→ $s = -ln\ \xi/\mu_t$ with a random number ξ.

Photon Transport Logic Flow:

Step 2. Determine whether collision without or with energy loss

✓ pdf: $p_R = \mu_R/\mu_t$ and

$p_{NR} = \mu_{NR}/\mu_t = 1 - p_R$,

where $\mu_{NR} = \mu_{pe} + \mu_{CS} + \mu_{pp}$

✓ cdf: $P_R = p_R$, $P_{NR} = p_R + p_{NR} = 1$

→ coherent (Rayleigh) scattering if $\xi \leq P_R$, Go to Step 2-1.

otherwise, collision with energy loss.

Step 2-1. determine the scattering angle θ

Photon Transport Logic Flow:

Step 3. Determine the mode of collision with energy-loss

✓ pdf: $p_{pe} = \mu_{pe}/\mu_{NR}$,

$p_{CS} = \mu_{CS}/\mu_{NR}$, and

$p_{pp} = \mu_{pp}/\mu_{NR}$.

where $\mu_{NR} = \mu_{pe} + \mu_{CS} + \mu_{pp}$

✓ cdf: $P_{pe} = p_{pe}$, $P_{CS} = p_{pe} + p_{CS}$, $P_{pp} = p_{pe} + p_{CS} + p_{pp} = 1$.

→ photoelectric absorption if $\xi \leq P_{pe}$,

Compton scattering if $P_{pe} < \xi \leq P_{CS}$ or

Pair production if $P_{CS} < \xi \leq P_{pp} = 1$

Photon Transport Logic Flow:
at Rayleigh scattering (cont.)

✓ Sampling of the scattering angle:

$$\frac{d\sigma_R(\theta)}{d\Omega} = \frac{r_e^2}{2}(1 + \cos^2\theta)[F_T(q)]^2$$

where r_e = the classical electron radius and $F_T(q)$ = the total molecular form factor calculated under the assumption of independent atoms:

$$[F_T(q)]^2 = \sum_{i=1}^{N_e} p_i [F(q, Z_i)]^2$$

from $F(q, Z_i)$, the atomic form factor for element Z_i.

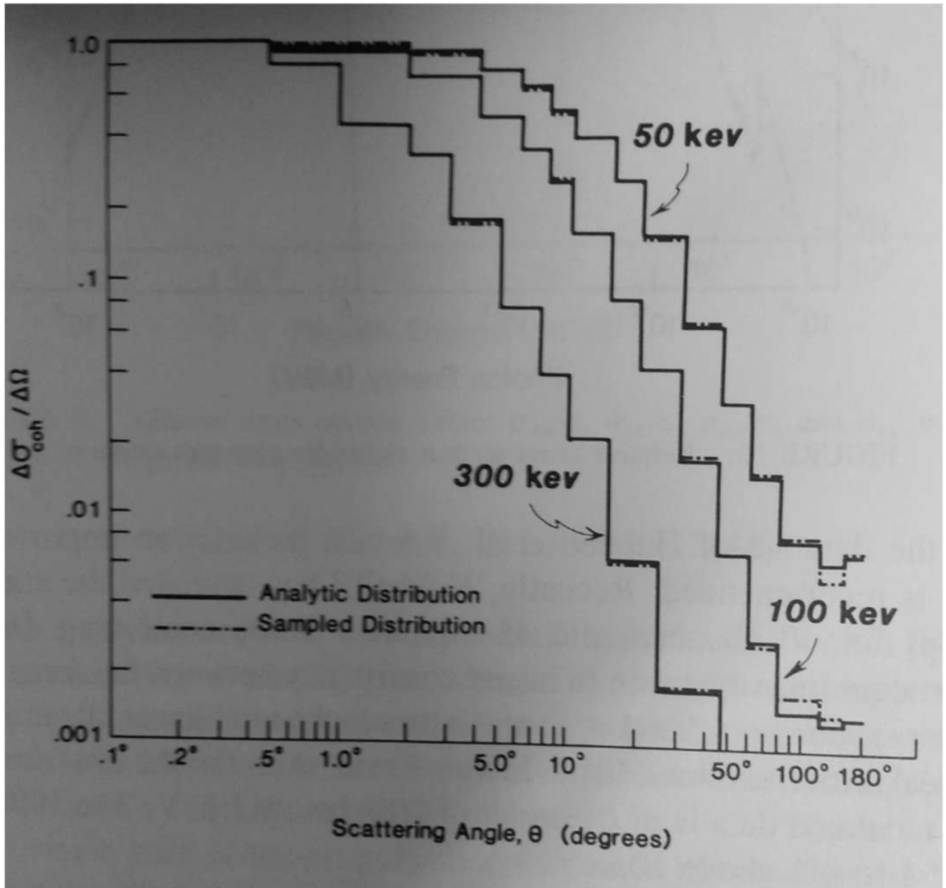


FIGURE 12. Angular distribution of 50, 100, and 300 keV photons coherently scattered in platinum. Broken lines indicate sample averages based upon 250,000 samples using the technique of Equation 51.

angular distribution of photons coherently scattered in platinum

Photon Transport Logic Flow:

at Rayleigh scattering (cont.)

✓ The cross section* <u>for individual atom</u> is given

$$\check{\Sigma}_{coher,partial}(Z,\check{k}) = \frac{N_a \rho}{M} X_0 \left(\frac{1 \times 10^{-24} cm^2}{barn}\right) \sigma_{coher}(Z,\check{k}) \quad (barns)$$

where k =photon energy in unit of m_0c^2, N_a = Avogadro number, ρ = density, M = molecular weight and X_0 = radiation range.
(*E. Storm and HI Israel, :Photon cross sections from 1 keV to 100 MeV for elements Z=1 to Z=100" , Atomic Data and Nuclear Data Tables 7, 1970)

✓ The total cross section for all the atoms acting independently is

$$\check{\Sigma}_{coher}(\check{k}) = \sum_{i=1}^{N_e} p_i \, \check{\Sigma}_{coher,partial}(Z_i,\check{k})$$

p_i = number density proportion

Photon Transport Logic Flow:
at Rayleigh scattering (cont.)

✓ In actual, both the molecular structure and the structure of medium affect the form factor and thus the coherent scattering:

Table 2.16.1
Total Cross Section (10^{-24} cm^2/molecule) for Coherent Scattering from Water[a]

Photon Energy (keV)	Free O + 2 Free H[b]	Free H_2O Molecule	Liquid Water
20	2.65	2.92	2.46
60	0.417	0.444	0.392
100	0.161	0.170	0.151

[a] From Johns and Yaffe[66]— note that effects on scattering angle are more dramatic than for total cross sections.
[b] Value used in EGS4/PEGS4.

Photon Transport Logic Flow:

at photoelectric absorption

✓ Keep the photoelectron of $E_{pe} = E_\gamma - E_{BE}$ at STACK, if $E_{pe} > E_{cutoff}$. (electron transport cutoff energy)
Otherwise,
deposit the energy E_{pe} at the interaction spot.

✓ Whether or not, fluorescence photon emission

→ emission of fluorescence photon at $E_\gamma = E_{BE}$ if $\xi \leq Y_F$

(The fluorescence yield Y_F is specific to the medium.)

→ otherwise, deposit the energy E_{BE} of Auger electron at the interaction spot.

Photon Transport Logic Flow:

at Compton scattering

- ✓ Keep the Compton electron of $E_{CS}(E_{\gamma},\theta) = E_{\gamma} - E_{\gamma'}$ at STACK if $E_{CS}(E_{\gamma},\theta) > E_{cutoff}$.
  Otherwise,
  deposit the energy $E_{CS}(E_{\gamma},\theta)$ at the interaction spot.

- ✓ If $E_{\gamma'} > P_{cutoff}$, determine next interaction distance s.
  otherwise,
  deposit the energy $E_{\gamma'}$ at the interaction spot, and then go to STACK and pick out a photon at lowest energy.

Compton Scattering

- ✓ The differential cross section of photons scattered from a single <u>free</u> 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 (~511 keV/c^2); and $P(E_\gamma,\theta)$ is the ratio of photon energy after and before the collision:

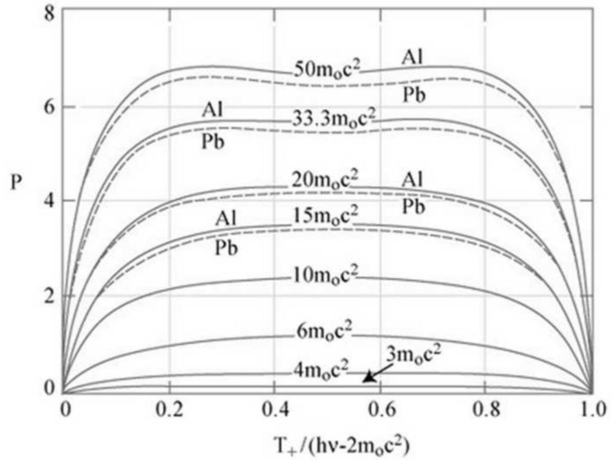
$$E_\gamma'/\ E_\gamma = P(E_\gamma,\theta) = \frac{1}{1+(E_\gamma/m_e c^2)(1-\cos\theta)}$$

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

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

Photon Transport Logic Flow:

at pair production



- ✓ Determine the energy E_N for electron and E_P for positron

  where $E_N + E_P = E_\gamma - 1.02$ (in MeV) and

  $0 < \{E_N$ and $E_P\} < E_\gamma - 1.02$ (in MeV) of the same chance

- ✓ Keep the electron at STACK, if $E_N > E_{cutoff}$.
  Otherwise, deposit the energy E_N at the interaction spot.

- ✓ Keep the positron at STACK, if $E_P > E_{cutoff}$.
  Otherwise, deposit the energy E_P at the interaction spot.

Electron Transport Scheme

Electron Transport Logic Flow:
electron transport cutoff energy E_{cutoff}

- ✓ Initial electron energy E_{el}
- ✓ Electrons that fall below E_{cutoff} are absorbed on the spot.
- ✓ In water medium, the electron range is about 3 μm at 10 keV.

→ E_{cutoff} = 10 keV of choice

Electron Transport Logic Flow:

Step 1. Determine the next interaction distance s.

✓ pdf: $p(s)ds = \Sigma_t \cdot exp(-\Sigma_t s)ds$,
where $\Sigma_t = \Sigma_{col} + \Sigma_{rad} + \Sigma_{anni}$ ($\Sigma_{anni} = 0$ for negatron)

– Σ_{col}, Σ_{rad} and Σ_{anni} are mutually exclusive events.

– Σ's are specific to the electron energy E_{el} and medium.

✓ cdf: $P(s) = 1-exp(-\Sigma_t s)$

$\rightarrow s = -ln\, \xi/\Sigma_t$ with a random number ξ.

Electron Transport Logic Flow:

Step 2. Determine whether collisional, radiative or absorptional

✓ pdf: $p_{col} = \Sigma_{col}/\Sigma_t$,

$p_{rad} = \Sigma_{rad}/\Sigma_t$, and

$p_{anni} = \Sigma_{annih}/\Sigma_t$.

where $\Sigma_t = \Sigma_{col} + \Sigma_{rad} + \Sigma_{anni}$ ($\Sigma_{anni} = 0$ for negatron)

✓ cdf: $P_{col} = p_{col}$, $P_{rad} = p_{col} + p_{rad}$, $P_{anni} = p_{col} + p_{rad} + p_{anni} = 1$.

→ collisional energy loss if $\xi \le P_{col}$,

radiative energy loss if $P_{col} < \xi \le P_{rad}$ (= 1, for negatron)

annihilation if $P_{rad} < \xi \le P_{anni}$ (= 1, for positron)

✓ Collisional cross section

$$\Sigma_{col}(E, Z) = \sigma_{col}(E, Z) \cdot \underline{N_A} \cdot \rho(Z)/M(Z) \qquad (N_A \text{ with no unit})$$

where $\sigma_{col}(E, Z)$ is the integral of the differential cross sections over 4π solid angle. (ex. Moller for negatron or Bhabha for positron)

$$\frac{d\sigma}{d\Omega} = \frac{e^4}{32\pi^2 E_{\mathrm{cm}}^2}\left[\frac{1+\cos^4\frac{\theta}{2}}{\sin^4\frac{\theta}{2}} - \frac{2\cos^4\frac{\theta}{2}}{\sin^2\frac{\theta}{2}} + \frac{1+\cos^2\theta}{2}\right] \quad : \text{Bhabha}$$

$$\frac{d\sigma}{d\Omega} = \frac{d\sigma}{d\Omega}(\theta) = \frac{d\sigma}{d\Omega}(-\theta) = \frac{d\sigma}{d\Omega}(\pi - \theta) \quad : \text{Moller}$$

✓ *Radiative cross section*

$$\Sigma_{rad}(E, Z) = \Sigma_{Brem}(E, Z)$$

$$-\left(\frac{d\check{E}}{dx}\right)_{Brem} = \int_0^{E_0} \check{k}\left(\frac{d\check{\Sigma}_{Brem}}{d\check{k}}\right) \cdot d\check{k}$$

$\sigma_{brem}(k)$: *Koch and Motz, Rev. Mod. Phys. (1959)*

$$\frac{dE}{dx} = 4\alpha N_A \frac{Z^2}{A} r_e^2 \cdot E \ln\frac{183}{Z^{\frac{1}{3}}}$$

$$-\frac{dE}{dx} = \frac{E}{X_0}$$

with $\rho X_0 = \dfrac{\rho A}{4\alpha N_A Z^2 r_e^2 \ln\frac{183}{Z^{\frac{1}{3}}}}$

[Radiation length in g/cm²]

$$\rightarrow E = E_0 e^{-x/X_0}$$

After passage of one X_0 electron has lost all but $(1/e)^{th}$ of its energy

[i.e. 63%]

✓ *Absorptional cross section*

$$\Sigma_{anni}(E, Z) = \sigma_{anni}(E, Z) \cdot N_A \cdot \rho(Z)/M(Z) \quad (N_A \text{ with no unit})$$

$$\sigma(Z,E) = \frac{Z\pi r_0^2}{\gamma+1}\left[\frac{\gamma^2+4\gamma+1}{\gamma^2-1}\ln\left(\gamma+\sqrt{\gamma^2-1}\right)-\frac{\gamma+3}{\sqrt{\gamma^2-1}}\right] \quad : \text{Heitler}$$

E = total energy of the incident positron

$\gamma = E/m_e c^2$

r_0 = classical electron radius

Electron Transport Logic Flow:

Step 3-1. If collisional, determine the energy loss and the scattering angle (either positron or negatron)

- ✓ pdf: $p_{col}(E, \theta_i) = d\sigma(E, \theta)/d\Omega$ at θ_i
- ✓ cdf: $P_{col}(E, \theta_i)$ = integral of $d\sigma(E, \theta)/d\Omega$ from $\theta' = 0$ to θ_i

  and $P_{col}(\pi) = 1$.

$$\frac{d\sigma}{d\Omega} = \frac{e^4}{32\pi^2 E_{\rm cm}^2}\left[\frac{1+\cos^4\frac{\theta}{2}}{\sin^4\frac{\theta}{2}} - \frac{2\cos^4\frac{\theta}{2}}{\sin^2\frac{\theta}{2}} + \frac{1+\cos^2\theta}{2}\right]$$: Bhabha

$$\frac{d\sigma}{d\Omega} = \frac{d\sigma}{d\Omega}(\theta) = \frac{d\sigma}{d\Omega}(-\theta) = \frac{d\sigma}{d\Omega}(\pi-\theta)$$: Moller

→ scattering angle = θ_i if $P_{col}(\theta_{i-1}) \le \xi \le P_{col}(\theta_i)$ and calculate the energy loss $E_{loss}(\theta_i)$ for momentum and energy conservation.

Electron Transport Logic Flow:

Step 3-1. If collisional, determine the energy loss and the scattering angle (cont.)

- ✓ If $E_{loss}(\theta_i) \geq AE$, store the electron of E_{loss} at STACK for later tracing,
- ✓ If $E_{cutoff} \leq E_{loss}(\theta_i) \leq AE$, go to CSDA route with $E_{loss}(\theta_i)$, or
- ✓ If $E_{loss}(\theta_i) \leq E_{cutoff}$, dissipate the energy $E_{loss}(\theta_i)$ at the collision spot.

Electron Transport Logic Flow:

Step 3-1. If collisional, determine the energy loss and the scattering angle (cont.)

- ✓ The energy of the primary electron after collision is

$$E'(\theta_i) = E - E_{loss}(\theta_i)$$

- ✓ If $E'(\theta_i) \geq AE$, keep tracing the primary electron of E',
- ✓ If $E_{cutoff} \leq E'(\theta_i) \leq AE$, go to CSDA route with $E'(\theta_i)$, or
- ✓ If $E'(\theta_i) \leq E_{cutoff}$, dissipate the energy $E'(\theta_i)$ at the collision spot.

Electron Transport Logic Flow:

Step 3-2. If radiative, determine the energy loss

- ✓ pdf: $p_{rad}(E, E^{i}_{loss}) = d\sigma(E, k)/dk$ at $k = E^{i}_{loss}$
- ✓ cdf: $P_{rad}(E, E^{i}_{loss})$ = integral of $d\sigma(E, k)/dk$ from $k = 0$ to E^{i}_{loss}

  and $P_{rad}(E, E) = 1$.

$$\frac{d\sigma}{dk} = \frac{d\sigma_n}{dk} + Z\frac{d\sigma_e}{dk}$$

→ energy loss = E^{i}_{loss} if $P_{rad}(E, E^{i-1}_{loss}) \leq \xi \leq P_{rad}(E, E^{i}_{loss})$.

Electron Transport Logic Flow:

Step 3-2. If radiative, determine the energy loss (cont.)

- ✓ If $E^i_{loss} \geq AP$, store the photon of E^i_{loss} at STACK for later tracing,
- ✓ If $P_{cutoff} \leq E^i_{loss} \leq AP$, go to CSDA route with E^i_{loss}, or
- ✓ If $E^i_{loss} \leq P_{cutoff}$, dissipate the energy E^i_{loss} at the collision spot.

* Conventional choice of $AP = P_{cutoff}$.

Electron Transport Logic Flow:

Step 3-2. If radiative, determine the energy loss (cont.)

- ✓ The energy of the primary electron is

$$E' = E - E^i_{loss}$$

- ✓ If $E' \geq AE$, keep tracing the primary electron of E',
- ✓ If $E_{cutoff} \leq E' \leq AE$, go to CSDA route with E', or
- ✓ If $E' \leq E_{cutoff}$, dissipate the energy E' at the collision spot.

Electron Transport Logic Flow:

Step 3-3. If absorptional, characterize the energy of annihilation photons

- ✓ $E_{\gamma 1} = E_{\gamma 2} = 0.511$ (in MeV)
  (assuming rest electron at annihilation)
- ✓ Both photons are emitted in almost the opposite directions where the direction line is arbitrary.
  - Select ξ_1 ξ_2, then $u_1 = \cos\theta_1 = 1-\xi_1$ and $\phi_1 = 2\pi\xi_2$

    Calculate $v_1 = (1-u_1^2)^{1/2} \cdot \cos\phi_1$ and

    $$w_1 = (1-u_1^2)^{1/2} \cdot \sin\phi_1$$
  - Let $u_2 = -u_1$, $v_2 = -v_1$, $w_2 = -w_1$
- ✓ Store $E_{\gamma 1}$, u_1, v_1, w_1 and start tracing with $E_{\gamma 2}$, u_2, v_2, w_2

Electron Transport Logic Flow:

Step 4. CSDA energy dissipation for electrons

- ✓ Calculate the pathlength s of an electron of E ($E_{cutoff} \le E \le AE$)

$$s = R(E) = \int_{E_{cutoff}}^{E^i_{loss}} \frac{dE'}{S(E')}$$

where $S(E) = -\frac{dE}{ds}$ is the collisional stopping power.

- ✓ Take a substep of pathlenth of s/NESTEP and select the scattering angle θ from multiple scattering distribution function $p(\theta)$. (NESTEP = W/ESTEPE)

- ✓ Take the azimuthal angle ϕ from uniform distribution at $0 \le \phi \le 2\pi$.

Electron Transport Logic Flow:

Step 4. CSDA energy dissipation for electrons (cont.)

$$p(\theta)\,d\theta = \frac{2}{\overline{\theta^2}} \exp\left(-\frac{\theta^2}{\overline{\theta^2}}\right) d\theta$$

: Gaussian distribution for θ.

✓ Calculate new directional cosines (u', v', w') of an electron at (u, v, w) after scattering by (θ, ϕ).

$$u' = u \cos\theta + \frac{uw \sin\theta \cos\phi - v \sin\theta \sin\phi}{\sqrt{1 - w^2}}$$

$$v' = v \cos\theta + \frac{vw \sin\theta \cos\phi + u \sin\theta \sin\phi}{\sqrt{1 - w^2}}$$

$$w' = w \cos\theta - \sin\theta \cos\phi \sqrt{1 - w^2}$$

except for $w \simeq 1$, in which case,

$$u' = \sin\theta \cos\phi$$

$$v' = \sin\theta \sin\phi$$

$$w' = w \cos\theta$$