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COMPUTATION OF IMPROVED COMPTON SCATTERING MOMENTUM TRANSFER

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ABSTRACT

It is shown that typical approximations in the electron momentum transfer used in modeling incoherent scattering from a bound electron can lead to inaccuracies in computing exit energies for low energy photons. It is suggested that improved calculated quantities may be obtained without some of these approximations.

Key Words: Compton scattering, photons

1. INTRODUCTION

In Compton scattering the differential scattering cross section per electron is the same for all atoms. The relation representing the scattering cross section is based on scattering from free electrons and is described by the Klein-Nishina formula [1]. The electron binding effects and motion are ignored. The Waller-Hartree theory [2] provides a more accurate description of Compton scattering, in which electron binding effects are approximately accounted for through the incoherent scattering function. The incoherent scattering functions are tabulated in the Lawrence Livermore National Laboratory Evaluated Photon Data Library (EDPL 97) [3]. However, this theory only provides the cross section differential in the scattering angle, while the Doppler broadening of the Compton line, caused by the momentum distribution of the target electrons, is not accounted for.

An improved description of the Compton scattering is obtained by using the relativistic impulse approximation (IA) described by Ribberfors [4,5], which incorporates binding effects and Doppler broadening in a consistent way. The IA yields a double differential cross section differential in the energy and direction of the scattered photon. Monte Carlo transport codes such as EGS4 [6] and Penelope [7] have incorporated simplifications of Ribberfors' formula. A key element of the IA procedure is to make use of information on the electron momentum distributions known as the Compton profiles to calculate the scattered photon exit energy.

In this paper the impact of approximations currently implemented in several Monte Carlo codes on the incoherent scattering cross section and scattered photon exit energy is investigated. The recommended approach yields improved incoherent scattering functions which are consistent with the values published in EDPL 97.

2. Incoherent Scattering

Consider the incoherent scattering event for an unpolarized photon of energy E and momemtum $\vec{k}$ that is absorbed and a secondary (Compton) photon of energy E' and momentum $\vec{k}'$ is emitted in the direction $\vec{\Omega}$ relative to the direction of the incident photon. In the so-called impulse approximation developed by Ribberfors the differential cross section is proportional to the Compton profile. The central point of this approximation is that the final-state wave function of the excited outgoing electron is treated as a plane wave so that the target potential is assumed to be constant during the collision. The Compton double differential cross section for photon scattering into the final state ($E', \vec{\Omega}$) calculated from the relativistic IA [4] is given by

$$\frac{d^2\sigma_{in}}{dE'd\vec{\Omega}} = \frac{r_e^2}{2}\frac{E'm}{Eq}\left[1+\left(\frac{p_Z}{mc}\right)^2\right]^{-1/2} XJ\left(p_Z\right) \tag{1}$$

where r_e is the classical electron radius, m is the electron mass, c is the speed of light, and q is the modulus of the photon momentum transfer vector, $\vec{q} = \vec{k} - \vec{k}'$. The projection of the initial electron momentum on the direction of the photon momentum transfer vector is p_Z.

The projection of the initial electron momentum on the direction of the momentum transfer vector is defined as

$$p_Z = \vec{p}\cdot\vec{q}\,/\,q \tag{2}$$

where

$$q = \left\|\vec{q}\right\| \tag{3}$$

$$q = \frac{1}{c}\sqrt{E'^2 - 2EE'\cos\theta + E^2} \tag{4}$$

θ is the photon scattered angle

X is defined as

$$X = \frac{R}{R'} + \frac{R'}{R} + 2\left(\frac{1}{R}+\frac{1}{R'}\right) + \left(\frac{1}{R}+\frac{1}{R'}\right)^2 \tag{5}$$

$$R = \frac{E}{mc^2}\left\{\left[1+\left(\frac{p_z}{mc}\right)^2\right]^{1/2} + \frac{E - E'\cos\theta}{cq}\frac{p_z}{mc}\right\} \tag{6}$$

$$R' = R - \frac{EE'}{m^2c^4}(1-\cos\theta) \tag{7}$$

$J\left(p_Z\right)$ is the Compton profile and is defined as,

$$J\left(p_Z\right) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \left|\psi\left(\vec{p}\right)\right|^2 \, dp_x dp_y \tag{8}$$

Where the $\psi\left(\vec{p}\right)$ is the wave function of the bound electrons in the momentum representation. The term $\left|\psi\left(\vec{p}\right)\right|^2$ is the momentum density distribution of the electron system before scattering.

In the Hartree-Fock approximation for closed-shell configurations, the momentum distribution of the electrons in an atomic shell is obtained by adding the contributions of the orbitals in that shell. The function $J(p_Z)$ and the Compton profile for shell *i*, $J_i(p_Z)$, are both bell-shaped and symmetric about $p_Z = 0$. The normalization

$$\int_{-\infty}^{\infty} J_i(p_Z) dp_Z = 1 \tag{9}$$

is assumed.

Tables of atomic and shell-wise Hartree-Fock Compton profiles for all elements have been published by Biggs *et al* [8]. Contributions from different electron shells are considered separately, so that the atomic or molecular Compton profile is the sum of one-electron shell Compton profiles $J_i(p_Z)$ for shell *i*.

The Compton profiles are related to the incoherent scattering function, $S(x,Z)$ by:

$$S(x,Z) = \sum_i Z_i \int_{-\infty}^{p_{z,i}^{\max}} J_i(p_Z)\, dp_z \tag{10}$$

p_Z is expressed in atomic units of $me^2/\hbar$, the average electron momentum in the ground state of hydrogen, Z_i is the number of electrons in shell *i*, and $p_{z,i}^{\max}$ is the highest p_Z value for which an electron in the *i*th orbital shell can be excited. The arguments of the incoherent scattering function are $x = E^*\sin(\theta/2)$, and Z is the number of electrons for the atom. The incoherent scattering functions in EPDL97 are those of Hubbell [9,10,11].

Monte Carlo transport codes such as EGS4 [6] and Penelope [7] have incorporated simplifications of Ribberfors' formula to obtain a representation of the incoherent differential scattering cross section of the form.

$$\frac{d\sigma_{in}}{d\Omega} \propto \sum_i \int_{-\infty}^{p_{z,i}^{\max}} F(p_z) J_i(p_Z)\, dp_z \tag{11}$$

A method is presented that improves the largest possible value of p_Z, $p_{z,i}^{\max}$, for a given shell *i* by eliminating some traditional approximations.

2.1. Electron momentum transfer

An expression for p_Z and $p_z^{\max}$ are obtained by using the conservation of momentum and energy.

$$E + E_e = E' + E_e' - E_i \tag{12}$$

$$\vec{k} + \vec{p} = \vec{k}' + \vec{p}' \tag{13}$$

where

E, E' are the photon energies before and after collision

E_e , E_e' are the electron energies before and after collision

E_i is the binding energy of the orbital electron

$\vec{k}$, $\vec{k}'$ are the photon momentum before and after collision with moduli $\frac{E}{c}$ and $\frac{E'}{c}$

$\vec{p}$, $\vec{p}'$ are the electron momentum before and after a collision

The projection of the electron momentum on the scattering photon vector is defined by equation (2) together with the following relations.

$$\vec{q} = \vec{p} - \vec{p}' \tag{15}$$

$$\vec{q} = \vec{k}' - \vec{k} \tag{16}$$

And the square of it's modulus is

$$q^2 = \|\vec{q}\|^2 = \frac{1}{c^2}\left(E'^2 - 2EE'\cos\theta + E^2\right) \tag{17}$$

$$\|\vec{p}'\|^2 = p'^2 = p^2 - 2\vec{p}\cdot\vec{q} + q^2 \tag{18}$$

where

$$2\vec{p}\bullet\vec{q} = p^2 - p'^2 + q^2 \tag{19}$$

$$2p_z q = p^2 - p'^2 + q^2 \tag{20}$$

$$p_Z = \frac{p^2 - p'^2 + q^2}{2q} \tag{21}$$

For a given particle (i.e. an electron), the total energy E_T , momentum, and mass relation is:

$$E_T^2 = \left(m_e c^2\right)^2 + c^2 p^2 \tag{22}$$

Solving for the momentum yields

$$p = \sqrt{\frac{E_T^2}{c^2} - {m_e}^2 c^2} \tag{23}$$

The total electron energy E_T is equal to the electron kinetic energy E_e plus the rest mass energy $m_e c^2$

$$p = \sqrt{\frac{\left(E_e + m_e c^2\right)^2}{c^2} - {m_e}^2 c^2} \tag{24}$$

after rearranging terms,

$$p^2 c^2 = E_e^2 + 2mc^2 E_e \tag{25}$$

also

$$p'^2 c^2 = E_e'^2 + 2mc^2 E_e' \tag{26}$$

Using the previous relations, p_Z is expressed now as

$$p_Z = \frac{-\frac{1}{c^2}\left\{\left(E-E'-E_i\right)^2+2\left(E-E'+E_i\right)\left(mc^2+E_e\right)\right\}+\frac{1}{c^2}\left(E'^2-2EE'\cos\theta+E^2\right)}{\frac{2}{c}\sqrt{E'^2-2EE'\cos\theta+E^2}} \tag{27}$$

The approximation found in literature is to assume E_i and E_e are small, thus yielding

$$p_Z \approx \frac{\frac{EE'}{c^2}\left(1-\cos\theta\right)-\left(E-E'\right)\left(mc^2/c^2\right)}{\frac{1}{c}\sqrt{E'^2-2EE'\cos\theta+E^2}} \tag{28}$$

Using cgs units (cm, gm, sec) and the electron charge in esu units, $\underline{p}_Z$ is expressed as

$$\underline{p}_Z \approx \frac{1}{\alpha}\left\{\frac{\frac{EE'}{mc^2}\left(1-\cos\theta\right)-\left(E-E'\right)}{\sqrt{E'^2-2EE'\cos\theta+E^2}}\right\} \tag{29}$$

where

$\underline{p}_Z$ is p_Z in atomic units of $me^2/\hbar$

$\alpha = e^2/\hbar c$, is the fine structure constant (dimensionless).

The highest p_Z value for which an electron in the ith orbital shell can be excited is obtained by setting $E' = E - E_i$ in the previous equation, and assures that sufficient energy is transferred to the electron to set it free.

$$\underline{p}_{z,i}^{\max} \approx \frac{1}{\alpha}\left\{\frac{E_i+\left(E^2-EE_i\right)\left(1-\cos\theta\right)/mc^2}{\sqrt{2E\left(E-E_i\right)-2E\left(E-E_i\right)\cos\theta+E_i^2}}\right\} \tag{30}$$

The relation for $\underline{p}_{z,i}^{\max}$ in equation (30) is used in several photon transport codes and appears in many technical papers. This relation for $\underline{p}_{z,i}^{\max}$ could lead to significant errors at low energies. For certain elements such as oxygen, photons in the keV range are not much larger than the electron binding energies for the lowest orbital (~514 eV). The approximation used to obtain equations (29) and (30) can lead to inaccuracies in computing the photon exit energy and differential scattering cross section in the tens of keV range.

We derive the relation for $\underline{p}_z^{\max}$ starting from equation (27) by assuming that only the electron energy, E_e, is neglible. Equation (27) reduces to:

$$p_Z \approx \frac{-\frac{1}{c^2}\left\{\left(E-E'-E_i\right)^2+2\left(E-E'+E_i\right)\left(mc^2\right)\right\}+\frac{1}{c^2}\left(E'^2-2EE'\cos\theta+E^2\right)}{\frac{2}{c}\sqrt{E'^2-2EE'\cos\theta+E^2}} \tag{31}$$

and expressed in atomic units of $me^2/\hbar$ to yield

$$\underline{p}_Z \approx \frac{1}{\alpha}\left[\frac{\left(-\frac{1}{mc^2}\right)\left\{\left(E-E'-E_i\right)^2+2\left(E-E'+E_i\right)\left(mc^2\right)\right\}+\frac{1}{mc^2}\left(E'^2-2EE'\cos\theta+E^2\right)}{2\sqrt{E'^2-2EE'\cos\theta+E^2}}\right] \tag{32}$$

As noted previously, $\underline{p}_{z,i}^{\max}$ is obtained by assuming that $E' = E - E_i$ in equation (32).

$$\underline{p}_{z,i}^{\max} \approx \frac{1}{\alpha}\left[\frac{1}{2mc^2}\sqrt{2E\left(E-E_i\right)-2E\left(E-E_i\right)\cos\theta+E_i^2}\right] \tag{33}$$

The photon exit energy E' is obtained by solving equation (27) for p_Z derived previously.

$$E' = \frac{a+\sqrt{b}}{c} \tag{34}$$

where

$$\begin{aligned} a = &-2mc^2\left(E_i+E\right)+E_i\left(E_i-2E\right)\left(E_i-E+E\cos\theta\right)+ \\ &mc^2\left(E_i^2+2E_iE-2E^2+2E\left(E_i-E\right)\cos\theta\right)+ \\ &2\alpha^2\left(mc^2\right)^4 E\underline{p}_z^2\cos\theta \end{aligned} \tag{35}$$

$$\begin{aligned} b = &-\left(-\left(mc^2-E_i+E-E\cos\theta\right)^2+\alpha^2\left(mc^2\right)^4\underline{p}_z^2\right)\times \\ &\left(-\left(E_i\left(E_i-2E\right)+2mc^2\left(E_i+E\right)\right)^2+4\alpha^2\left(mc^2\right)^4E^2\underline{p}_z^2\right)+ \\ &\left(\left(E_i\left(E_i-2E\right)+2mc^2\left(E_i+E\right)\right)\left(mc^2-E_i+E-E\cos\theta\right)-2\alpha^2\left(mc^2\right)^4Ep_z^2\cos\theta\right)^2 \end{aligned} \tag{36}$$

$$c = -2\left(mc^2-E_i-E-E\cos\theta\right)^2+2\alpha^2\left(mc^2\right)^4 \tag{37}$$

3. Results

We applied the previously discussed approximations on the oxygen atom since it is a component of both air and water. Figure 1 shows the shellwise Compton profile data for oxygen from Biggs. The Compton profile for the first orbital decreases gradually with $\underline{p}_Z$ compared to the higher orbitals. Therefore the integral of the Compton profile for the first orbital over the range of $\underline{p}_Z$ will be more sensitive to the value of $\underline{p}_{z,i}^{\max}$ for $\underline{p}_Z$ values greater than 3. Figure 2 shows a comparison of values of $\underline{p}_{z,i}^{\max}$ for 25 keV and 200 keV incident photons scattered over the range of scattering angles. The new procedure for calculating $\underline{p}_{z,i}^{\max}$, calculated with equation (33),

yields a lower value than the old procedure from equation (30). For small scattering angles, the old procedure for calculating $\underline{p}_{z,i}^{\max}$ increases rapidly in value. Figure 3 shows the percent difference between both approaches for 25 keV and 200 keV. The differences for the higher incident energy photons are small except for small scattering angles. The difference for the 25 keV photons increases with decreasing scattering angle.

Figure 4 shows a comparison of the calculated incoherent form factors, using equation (10), with the tabulated values in EPDL 97 for photons with an incident energy of 25 keV. The calculated incoherent form factors made use of equations (30) and (33) to obtain the values of $\underline{p}_{z,i}^{\max}$. The calculated form factors using the new procedure for $\underline{p}_{z,i}^{\max}$ are in very good agreement with the tabulated data and deviate at small scattering angles. The old procedure of calculating $\underline{p}_{z,i}^{\max}$ yielded results that were noticeably different from the tabulated data. The form factors approach the value of Z, the number of electrons in the atom, at higher energies.

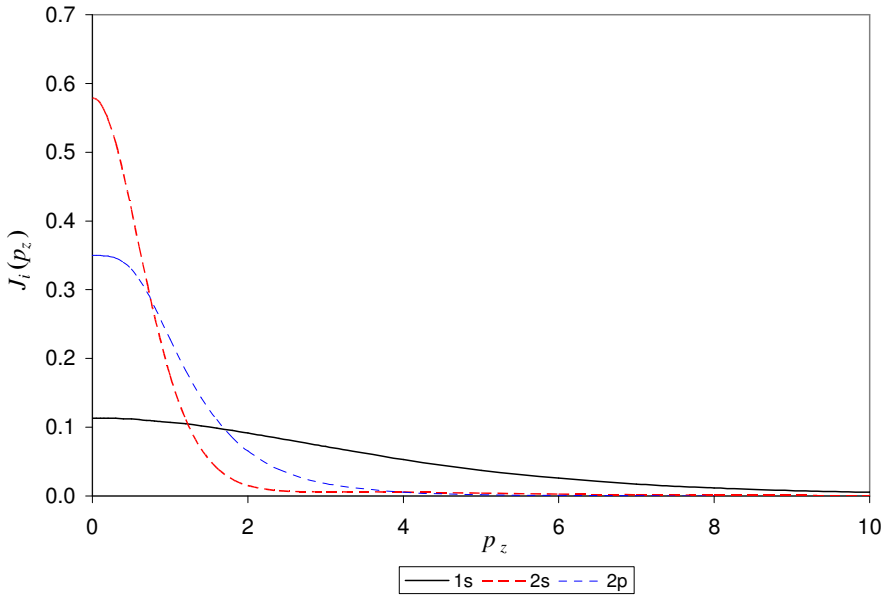

Figure 1. Compton profiles for oxygen atom

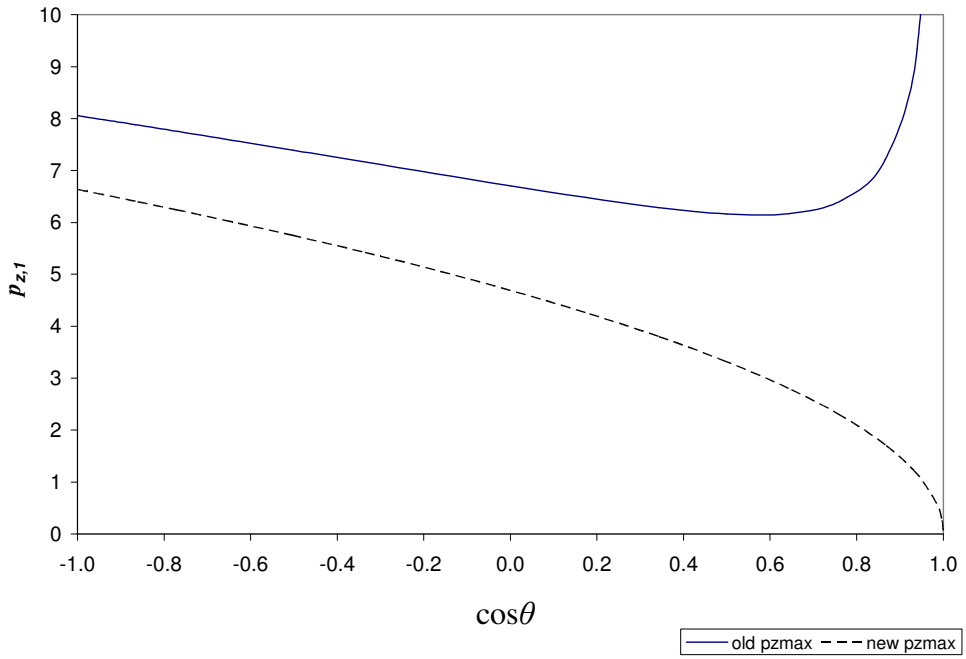

Figure 2. Maximum p_z for 25 keV photons (i=1) for oxygen

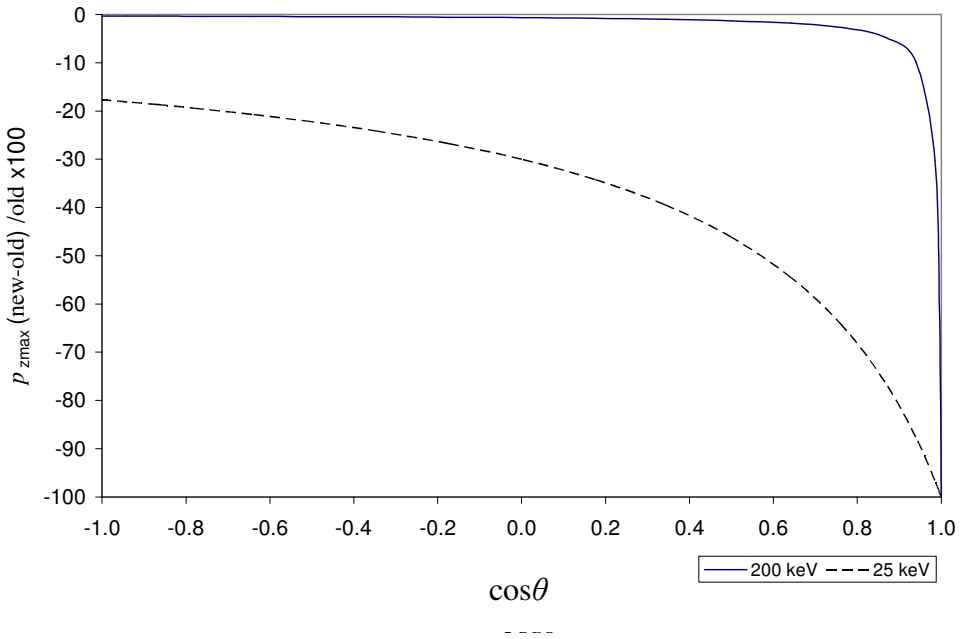

Figure 3. Comparison of p_{zmax} change for 25 keV and 200 keV photons

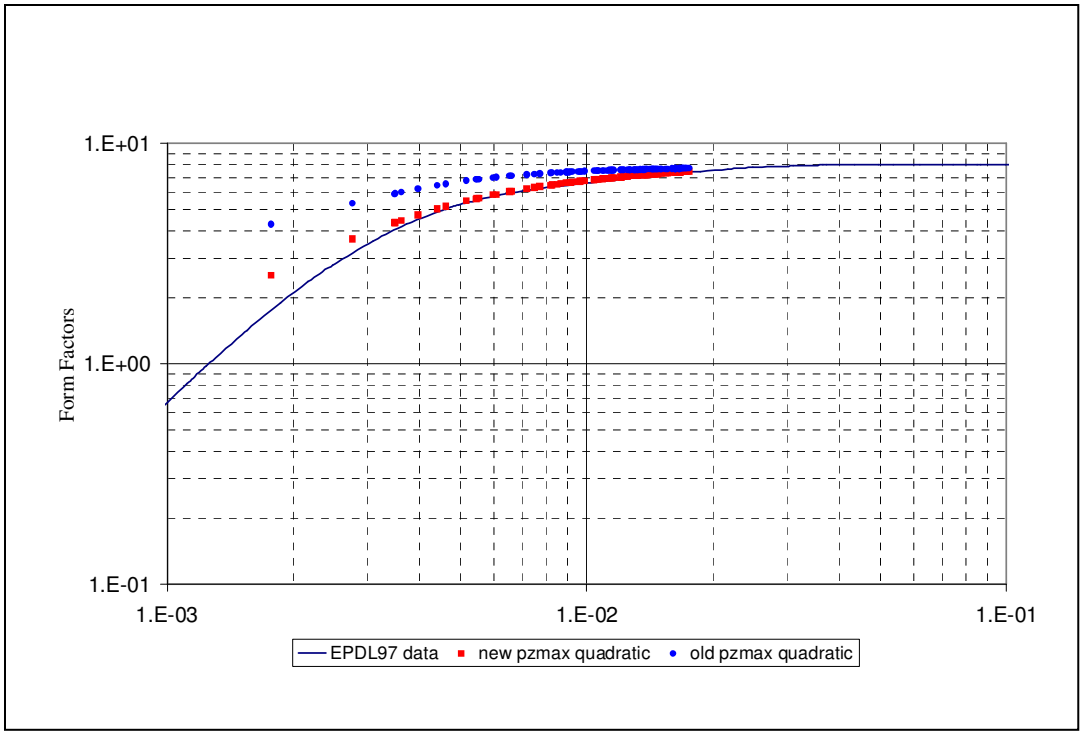

Figure 4. Comparison of calculated to tabulated form factors

4. CONCLUSIONS

It is shown that typical approximations in the electron momentum transfer used in Compton scattering modeling can lead to inaccuracies in computing the angular differential scattering cross section and exit energies for low energy photons when computing Doppler broadened angular distributions. It is suggested that improved calculated quantities may be obtained without some of these approximations.

REFERENCES

1. R. D. Evans, *The Atomic Nucleus*, McGraw-Hill Book Company, Inc. New York, USA, (1955).
2. I. Waller and D. R. Hartree, *Proceedings of the Royal Society London* **A 124,** p. 11. (1929).
3. D.E. Cullen, et al., *The Livermore Evaluated Photon Data Library*, *UCRL-50400, Volume 6, Rev. 5* (1997).
4. R. Ribberfors, "Relationship of the relativistic Compton cross section to the momentum distribution of bound electron states", *Physical Review B*, **12**, pp. 2067-2074 (1975).
5. R. Ribberfors, "Incoherent x-ray functions and cross sections", *Physical Review A*, **26**, pp. 3325-3333, (1982).

6. Y. Namito, "Implementation of the Doppler broadening of a Compton-scattered photon into the EGS4 code", *Nuclear Instruments and Methods in Physics Research*, **A 349**, pp. 489-494, (1994).
7. D. Brusa, *et al.*, "Fast sampling algorithm for the simulation of photon Compton scattering", *Nuclear Instruments and Methods in Physics Research*, **A 379**, pp. 167-175, (1996).
8. F. Biggs, *et al*., "Hartree-Fock Compton Profiles for the Elements", *Atomic Data and Nuclear Data Tables* **16**, pp. 201-309, (1975).
9. J. H. Hubbell, *et al.,* "Atomic Form Factors, Incoherent Scattering Functions, and Photon Scattering Cross Sections", *Journal of Physical Chemistry Reference Data*, **4 No.3**, pp. 471-616, (1975).
10. J. H. Hubbell, *et al.,* "Atomic Form Factors, Incoherent Scattering Functions, and Photon Scattering Cross Sections", *Journal of Physical Chemistry Reference Data*, **7**, p. 615, (1977).
11. J. H. Hubbell, "Summary of Existing Information on the use on the Incoherent Scattering of Photons Particularly on the validity of the use of the Incoherent Scattering Function", *Radiation Physical Chemistry*, **50, No.1**, pp. 113-124, (1997).