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Abstract

LSCAT(low-energy photon-scattering expansion for the EGS4[1] code) is a group of files used to calculate keV-photon transport by EGS4 with an expanded physical model. In the original version released in 1995 [2], linearly polarized photon scattering[4], bound Compton scattering and Doppler broadening of the Compton-scattered photon energy[5] were taken into account. The LSCAT program was further extended to include electron impact ionization (EII). The structure of the LSCAT program was changed to join "General treatment of photoelectric related phenomena for compounds and mixtures in EGS4" [3]. This report describes the physical models employed and relevant modification of EGS4 and PEGS4. This document also describes how to use the files, flag setting in a PEGS4 input and in a user code, and the contents of the files.

Contents

1 Method of calculation

1.1 Double differential Compton scattering cross section for a linearly polarized photon

Let consider a photon-scattering system as shown in Fig. 1. One completely linearly polarized photon, whose propagation vector and polarization vector are $\vec{k_0}$ and $\vec{e_0}$, is scattered at point O. The scattering polar and azimuth angles are θ and ϕ. The propagation vector of the scattered photon is $\vec{k}$.

Ribberfors derived a double-differential Compton-scattering cross section for an unpolarized photon using the relativistic impulse approximation [6]. By modifying Ribberfors' formula, a double-differential Compton-scattering cross section for a linearly polarized photon is prepared for the following calculation:

$$\left(\frac{d^2\sigma}{d\Omega dk}\right)_{bC,i} = \frac{r_0^2}{4}\left(\frac{k_c k}{k_0^2}\right)\left(\frac{k_c}{k_0}+\frac{k_0}{k_c}-2+4\cos^2\Theta\right)\frac{dp_z}{dk}J_i(p_z), \quad (1)$$

where

$$p_z = -137\frac{k_0-k-k_0k(1-\cos\theta)/m_0c^2}{\hbar c|\vec{k_0}-\vec{k}|}, \quad (2)$$

$$\frac{dp_z}{dk} = \frac{137k_0}{\hbar c|\vec{k_0}-\vec{k}|k_c}-\frac{p_z(k-k_0\cos\theta)}{(\hbar c)^2|\vec{k_0}-\vec{k}|^2}, \quad (3)$$

$$k_c = \frac{k_0}{1+\frac{k_0}{m_0c^2}(1-\cos\theta)}, \quad (4)$$

and

$$\hbar c|\vec{k_0}-\vec{k}| = \sqrt{k_0^2+k^2-2k_0k\cos\theta}. \quad (5)$$

Here, the subscript "bC " denotes *Compton scattering by a bound electron.* Subscript "i " denotes the shell number, which corresponds to each (n,l,m)-th sub-shell; r_0 is the classical electron radius, k_0 and k are the incident and scattered photon energies, respectively, and k_c is the Compton-scattered photon energy for an electron at rest, Θ is the angle between the incident polarization vector $\vec{e_0}$ and the scattered polarization vector $\vec{e}$, p_z is the projection of the electron pre-collision momentum on the photon-scattering vector in atomic units, $\hbar c$ is a conversion constant, $J_i(p_z)$ is the Compton profile of the i-th sub-shell[7], θ is the scattering polar angle, and m_0c^2 is the electron rest mass. Due to electron binding, the cross section given by Eq.(1) is 0 when $k > k_0 - I_i$. Here, I_i is the binding energy of an electron in the i-th shell.

Eq.(1) is used in LSCAT in the case that the user requires all of the linearly polarized photon scattering, Doppler broadening, incoherent scattering function and bound Compton scattering cross section in Compton-scattering calculations.

1.2 Linearly polarized photon scattering

In this section, formula for sampling the azimuth angle of photon scattering and the scattered polarization vector are derived. In this process, the relationship between the Compton- and Rayleigh-scattering formulas for a linearly polarized and unpolarized photon is shown. The electron-binding effect is ignored here, and will be described in 1.3.

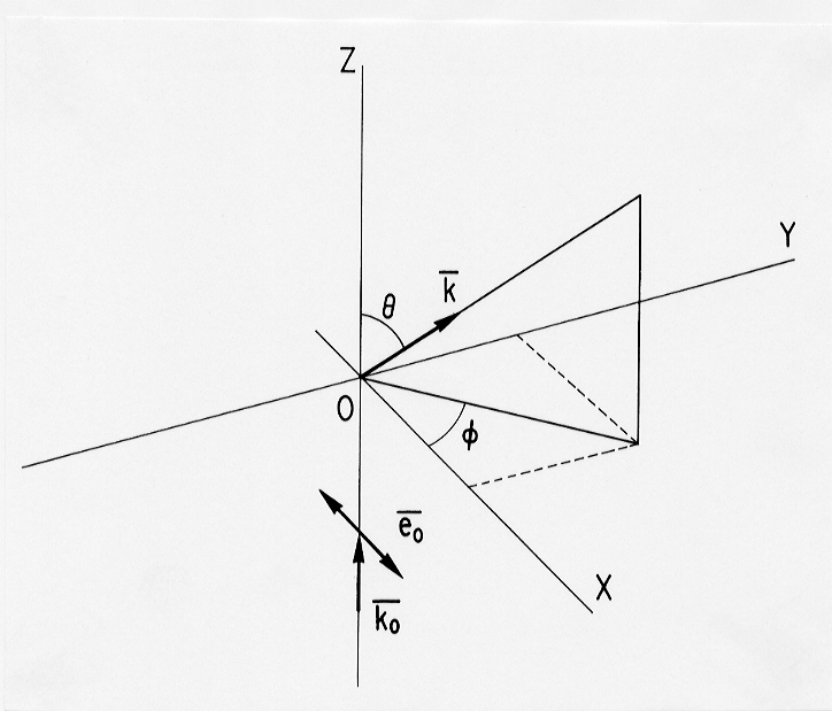

Figure 1: Photon scattering system. An incident photon toward the Z-direction is scattered at point O. The propagation vector $\vec{k_0}$ and polarization vector $\vec{e_0}$ of an incident photon are parallel to $\vec{e_z}$ and $\vec{e_x}$, respectively. Here, $\vec{e_z}$ and $\vec{e_x}$ are unit vectors along the z- and x-axis. The scattering polar angle is θ and the scattering azimuth angle from the plane of $\vec{e_0}$ is ϕ. The scattered propagation vector is $\vec{k}$.

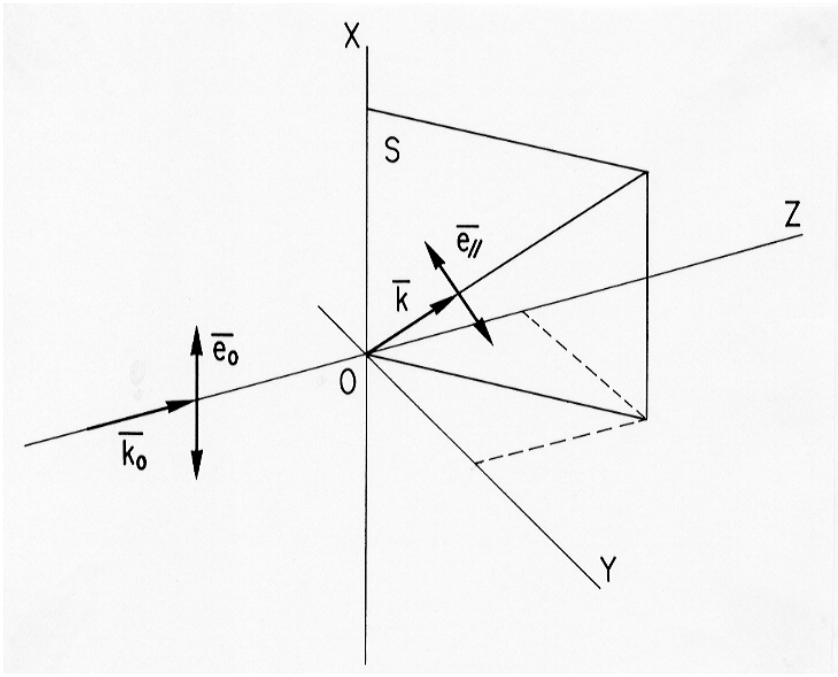

Figure 2: Direction of the polarization vector of the scattered photon. Plane S contains $\vec{e_0}$ and $\vec{k}$. $\vec{e_{\parallel}}$ is in plane S, and is perpendicular to $\vec{k}$. $\vec{e_{\perp}}$ is perpendicular to plane S.

1.2.1 Equations for a lineally polarized photon using the polarization vector (Compton)

The Compton-scattering cross section of a free electron for a linearly polarized photon (Klein-Nishina formula [8]) is derived by integrating Eq.(1) concerning k while ignoring the electron-binding effect by putting $I_i = 0$,

$$\left(\frac{d\sigma}{d\Omega}\right)_{fC} = \frac{1}{4} r_0^2 \left(\frac{k_c}{k_0}\right)^2 \left(\frac{k_c}{k_0} + \frac{k_0}{k_c} - 2 + 4\cos^2\Theta\right). \tag{6}$$

Eq.(6) is used for a Compton-scattering calculation with linear polarization in the case that any electron-binding effect is ignored.

1.2.2 Equations for a lineally polarized photon using the polarization vector (Rayleigh)

The elastic scattering of a photon by one electron is called Thomson scattering. The Thomson-scattering cross section per electron for a linearly polarized photon is[9]

$$\left(\frac{d\sigma}{d\Omega}\right)_{T} = r_0^2 \cos^2\Theta. \tag{7}$$

The elastic scattering of a photon by an atom is referred to as Rayleigh scattering in this report. The Rayleigh scattering for a linearly polarized photon is calculated by the product of Eq.(7) and the square of the atomic form factor ($F(x, Z)$). Here, x is the momentum transfer calculated by Eq.(25) and Z is the atomic number.

1.2.3 Polarization vector of a scattered photon

According to Heitler[10], two directions are considered for $\vec{e}$, *i.e.* $\vec{e}$ is either in the same plane as $\vec{e_0}$ ($\vec{e_\parallel}$) or is perpendicular to $\vec{e_0}$ ($\vec{e_\perp}$). As shown in Fig.2, $\vec{e_\parallel}$ is in the plane S, which contains $\vec{k}$ and $\vec{e_0}$, and is also perpendicular to $\vec{k}$. $\vec{e_\perp}$ is perpendicular to the plane S. Under the condition that $\vec{k_0} \parallel \vec{e_z}$ and $\vec{e_0} \parallel \vec{e_x}$, as shown in Figs.1 and 2, these two polarization vectors, $\vec{e_\parallel}$ and $\vec{e_\perp}$, are derived as the following functions of θ and ϕ :

$$\vec{e_\parallel} = N\vec{e_x} - \left(\frac{1}{N}\sin^2\theta\cos\phi\sin\phi\right)\vec{e_y} - \left(\frac{1}{N}\cos\theta\sin\theta\cos\phi\right)\vec{e_z} \tag{8}$$

and

$$\vec{e_\perp} = \left(\frac{1}{N}\cos\theta\right)\vec{e_y} - \left(\frac{1}{N}\sin\theta\sin\phi\right)\vec{e_z}. \tag{9}$$

Here, $N = \sqrt{\cos^2\theta\cos^2\phi + \sin^2\phi}$, $\vec{e_x}, \vec{e_y}, \vec{e_z}$ are unit vectors along the x-, y- and z-axis, respectively, and $\vec{e_\parallel}$ and $\vec{e_\perp}$ are treated as normalized vectors.

1.2.4 Equations for a lineally polarized photon using the scattering angle

Eqs.(6) and (7) for these two directions of $\vec{e}$ become

$$\left(\frac{d\sigma}{d\Omega}\right)_{fC,\parallel} = \frac{1}{4}r_0^2\left(\frac{k_c}{k_0}\right)^2\left\{\frac{k_c}{k_0} + \frac{k_0}{k_c} - 2 + 4\left(1 - \sin^2\theta\cos^2\phi\right)\right\}, \tag{10}$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{fC,\perp} = \frac{1}{4}r_0^2\left(\frac{k_c}{k_0}\right)^2\left(\frac{k_c}{k_0} + \frac{k_0}{k_c} - 2\right), \tag{11}$$

and

$$\left(\frac{d\sigma}{d\Omega}\right)_{T,\parallel} = r_0^2(1 - \sin^2\theta\cos^2\phi), \tag{12}$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{T,\perp} = 0. \tag{13}$$

By adding Eqs.(10) and (11), Eqs.(12) and (13), respectively, the following Compton-scattering cross section and the Thomson-scattering cross section for θ and ϕ are obtained:

$$\left(\frac{d\sigma}{d\Omega}\right)_{fC} = \frac{1}{2}r_0^2\left(\frac{k_c}{k_0}\right)^2\left(\frac{k_c}{k_0} + \frac{k_0}{k_c} - 2\sin^2\theta\cos^2\phi\right) \tag{14}$$

and

$$\left(\frac{d\sigma}{d\Omega}\right)_{T} = r_0^2(1 - \sin^2\theta\cos^2\phi). \tag{15}$$

1.2.5 Equations for an unpolarized photon

The Compton- and Thomson-scattering cross sections per electron for unpolarized photons are obtained by averaging Eqs.(14) and (15) with respect to ϕ :

$$\left(\frac{d\sigma}{d\Omega}\right)_{fC,U} = \frac{1}{2}r_0^2\left(\frac{k_c}{k_0}\right)^2\left(\frac{k_c}{k_0} + \frac{k_0}{k_c} - \sin^2\theta\right) \tag{16}$$

and

$$\left(\frac{d\sigma}{d\Omega}\right)_{T,U} = \frac{1}{2} r_0^2 \left(1 + \cos^2\theta\right). \tag{17}$$

The Rayleigh-scattering cross section per atom for an unpolarized photon ($(d\sigma/d\Omega)_{R,U}$) is obtained as a product of the square of the atomic form factor ($F(x,Z)$) and Thomson-scattering cross section ($(d\sigma/d\Omega)_{T,U}$),

$$\left(\frac{d\sigma}{d\Omega}\right)_{R,U} = F^2(x,Z) \left(\frac{d\sigma}{d\Omega}\right)_{T,U}. \tag{18}$$

1.2.6 Sampling of the scattering azimuth angle and polarization vector

In LSCAT, ϕ is sampled for the determined θ according to Eqs.(14) and (15). The direction of the scattered polarization vector is then calculated. It is shown in Eqs.(10) and (11) that a completely linearly polarized photon is depolarized in Compton scattering according to some depolarization probability. This depolarization probability, $1 - P$, is

$$1 - P = \left(\frac{k}{k_0} + \frac{k_0}{k} - 2\right) \Big/ \left(\frac{k}{k_0} + \frac{k_0}{k} - 2\sin^2\theta\cos^2\phi\right). \tag{19}$$

In Compton scattering, either a polarized or depolarized photon is sampled according to this depolarization probability. When the scattered photon is polarized, the direction of the polarization vector is calculated according to Eq.(8). When the scattered photon is depolarized, the direction of the polarization vector is sampled from the direction between $\vec{e_\parallel}$ and $\vec{e_\perp}$, shown as Eqs.(8) and (9), respectively, at random. In Rayleigh scattering, since there is no probability for depolarization, the direction of $\vec{e}$ is always calculated according to Eq.(8).

1.2.7 Transformation to the laboratory system

In the scattering system used here, $\vec{k_0}$ and $\vec{e_0}$ are in the direction of $\vec{e_z}$ and $\vec{e_x}$, respectively, as shown in Fig.1, whereas $\vec{k_0}$ and $\vec{e_0}$ may be in an arbitrary direction in the laboratory system. The scattering and laboratory systems are connected via three rotations, which are calculated from the direction of $\vec{k_0}$ and $\vec{e_0}$ in the laboratory system. Using these three rotations, $\vec{k}$ and $\vec{e}$ are transformed from the scattering system to the laboratory system (See Appendix E).

1.2.8 Limit of the present code in linearly polarized photon scattering

- Circularly polarized photon scattering is ignored and elliptically polarized photon scattering is treated as partially linearly polarized photon scattering.
- Characteristic X-rays and bremsstrahlung photons are assumed to be unpolarized.

1.3 Bound Compton scattering and Doppler broadening

In this section, formula for sampling the scattered photon energy and the scattering polar angle while considering electron binding effect and Doppler broadening are derived. In this process, the relation among the total bound Compton cross section (σ_{bC}), the incoherent scattering function ($S(x,Z)$), and the cut off in the Doppler-broadened Compton-scattered photon spectrum is shown.

1.3.1 Double-differential bound Compton-scattering cross section

The double-differential Compton cross section of a bound electron for an unpolarized photon is obtained by averaging Eq.(1) concerning the polarization vector of the incident and scattered photons:

$$\left(\frac{d^2\sigma}{d\Omega dk}\right)_{bC,i} = \frac{r_0^2}{2}\left(\frac{k_c k}{k_0^2}\right)\frac{dp_z}{dk}\left(\frac{k_c}{k_0}+\frac{k_0}{k_c}-\sin^2\theta\right)J_i(p_z). \tag{20}$$

By substituting Eq.(3) into Eq.(20) after eliminating the second term on the right-hand side of Eq.(3), one obtains an equivalent formula to Eq.(3) of ref.[6]. When photon transport is performed while considering σ_{bC}, $S(x,Z)$ and Doppler broadening, and ignoring linearly polarized photon scattering, Eq.(20) is used for Compton-scattering calculations.

1.3.2 Differential-bound Compton-scattering cross section

The differential Compton cross section of a bound electron is obtained by integrating Eq.(20) concerning k based on the assumption that $k = k_c$ in the second term on the right-hand side:

$$\left(\frac{d\sigma}{d\Omega}\right)_{bC,i} = \frac{r_0^2}{2}\left(\frac{k_c}{k_0}\right)^2\left(\frac{k_c}{k_0}+\frac{k_0}{k_c}-\sin^2\theta\right)S_i^{IA}(k_0,\theta,Z), \tag{21}$$

where

$$S_i^{IA}(k_0,\theta,Z) = \int_{-\infty}^{p_{i,max}} J_i(p_z)dp_z. \tag{22}$$

Here, Z is the atomic number and $S_i^{IA}(k_0,\theta,Z)$ is the incoherent scattering function of the i-th shell electrons in the impulse approximation calculated by Ribberfors and Berggren[11] and $p_{i,max}$ is obtained by putting $k = k_0 - I_i$ in Eq.(2). $S_i^{IA}(k_0,\theta,Z)$ converges to the number of electrons in each sub-shell when $p_{i,max} \to \infty$. The differential Compton cross section of one whole atom is obtained by summing Eq.(21) for all of the sub-shells:

$$\left(\frac{d\sigma}{d\Omega}\right)_{bC}^{IA} = \frac{r_0^2}{2}\left(\frac{k_c}{k_0}\right)^2\left(\frac{k_c}{k_0}+\frac{k_0}{k_c}-\sin^2\theta\right)S^{IA}(k_0,\theta,Z), \tag{23}$$

where

$$S^{IA}(k_0,\theta,Z) = \sum_i S_i^{IA}(k_0,\theta,Z). \tag{24}$$

Here, $S^{IA}(k_0,\theta,Z)$ is the incoherent scattering function of an atom in the impulse approximation. Another incoherent scattering function ($S^{WH}(x,Z)$), based on Waller-Hartree theory[12], was widely used to treat the electron-binding effect on the angular distribution of a Compton-scattered photon. Here, x is the momentum transfer in Å,

$$x = \frac{k_0(\mathrm{keV})}{12.399}\sin\left(\frac{\theta}{2}\right). \tag{25}$$

Using $S^{WH}(x,Z)$, the differential Compton scattering cross section is

$$\left(\frac{d\sigma}{d\Omega}\right)_{bC}^{WH} = \frac{r_0^2}{2}\left(\frac{k_c}{k_0}\right)^2\left(\frac{k_c}{k_0}+\frac{k_0}{k_c}-\sin^2\theta\right)S^{WH}(x,Z). \tag{26}$$

The close agreement of $S^{IA}(k_0,\theta,Z)$ and $S^{WH}(x,Z)$ for several atoms was shown in ref.[11]. Namito et al [24] pointed out the difference of S^{IA} and S^{WH} in the low-energy region. In LSCAT, Eq.(26) is used for Compton-scattering calculations when incoherent scattering function ($S(x,Z)$) is taken into account.

1.3.3 Total bound Compton-scattering cross section and photon mfp

By integrating Eq.(26) concerning the solid angle (Ω), the total bound Compton-scattering cross section of an atom is obtained,

$$\sigma_{bC}^{WH} = \int^{4\pi} \left(\frac{d\sigma}{d\Omega}\right)_{bC}^{WH} d\Omega. \tag{27}$$

If the electron-binding effect in the total Compton-scattering cross section is considered in LSCAT, Eq.(27) is used for the simulation. The photon mean-free path is calculated using σ_{bC} instead of σ_{fC}(total free Compton-scattering cross section).

1.3.4 Sampling of mfp, Compton scattering, polar angle and energy of a scattered photon

In the improved Compton-scattering routine in the EGS4 code, the distance to the next photon interaction point is sampled using the photon mean-free path, evaluated by σ_{bC} taken from the DLC-99/HUGO[13, 14, 15]; the probability of Compton scattering in that interaction is calculated using σ_{bC}. After θ is sampled according to Eq.(26), using $S^{WH}(x, Z)$ taken from ref.[13], the electron sub-shell number is sampled using the number of electrons in each sub-shell. Then, $p_{i,max}$ is calculated by putting $k = k_0 - I_i$ in Eq.(2) for the sampled θ. The p_z is sampled in the interval $(0, 100)$ using a normalized cumulative density function(c.d.f.) of $J_i(x)$,

$$\xi = \frac{\int_o^{p_z} J_i(x)dx}{\int_0^{100} J_i(x)dx}. \tag{28}$$

Here, ξ is a random number between $(0, 1)$. The p_z value on the right-hand side of Eq.(28), corresponding to the sampled ξ, is used for the calculation. The distribution of p_z is equal to the normalized $J_i(p_z)$. "100" in Eq.(28) comes from the upper limit of the p_z value in ref.[7]. The speed down of the Compton-scattering routine in the improved EGS4 is negligible, since sampling of p_z is carried out quickly by the c.d.f. method. When $p_z > p_{i,max}$, it is rejected, and the shell number "i" and p_z are sampled again. This sampling is continued until $p_z < p_{i,max}$ is satisfied. Then, another rejection by $\frac{k}{k_0}$, which corresponds to the second term on the right-hand side of Eq.(20), is performed. Hereby, the scattered photon energy (k) and the polar angle (θ) were sampled according to Eq.(20).

Together with the azimuth angle(ϕ) and scattered polarization sampling described in the previous subsection, scattered-photon sampling following Eq.(1) is performed. The formulas used in each simulation mode are summarized in Table.1.

1.3.5 Limit of the present code in Bound Compton scattering and Doppler broadening

- The Compton profile of a free atom is used. To treat a compound material, a mixture of free atoms is assumed and any molecular effect on the Compton profile is ignored.

- The Compton-scattered electron energy and direction are calculated using the energy-conservation and the momentum-conservation law and assuming that no energy absorption by atoms in the Compton scattering occurs. Then, the electron binding energy is

Table 1: Formulas concerning each simulation mode.

Eq.	Simulation mode
1	Compton scattering with LP, σ_{bC}, $S(x,Z)$ and DB.
6	Compton scattering with LP.
7	Rayleigh scattering with LP.
20	Compton scattering with σ_{bC}, $S(x,Z)$ and DB.
26	Compton scattering with σ_{bC} and $S(x,Z)$.
27	Compton scattering with σ_{bC}.

subtracted from the recoil electron energy. Also, the electron binding energy is deposited locally.

1.3.6 Modification regarding bound Compton scattering from the 1995 version

1. The electron binding energy was subtracted from the recoiled electron energy. Also, this electron binding energy is deposited locally with IARG=4.
2. The variable `ICPROF` was changed into a dimension, `ICPROF(IM)`.
3. Variables `F1 - F5` in `COMPT` were changed from single precision to double precision. [1]
4. `F5>0` was changed into `F5>1.0E-10` to avoid any numerical problem.
5. `MXNS` (Maximum number of shells) was increased from 28 to 100. This was necessary to treat a compound or mixture which contains heavy elements.
6. "$S(x,Z)/Z = 1$ for $x > 80$" was added.

1.4 Electron impact ionization

1.4.1 EII cross section

A modification of the EGS4 code was made in order to include K-shell electron-impact ionization (EII) by using six different cross sections of EII: (1) Casnati's [16] (2) Kolbenstvedt-revised [17] (3) Kolbenstvedt-original [18] (4) Jakoby's [19] (5) Gryziński's [20] (6) Gryziński-relativistic [20]. A list of these cross sections is given shown in the description on `IMPACT` in Table. 6. A guideline to select an adequate EII cross section is described in ref. [21].

EII is treated as being a part of Møller scattering in the EGS4 code. Neither the electron mean-free path nor the stopping power were modified by including EII. The EII cross section of an element in a compound and mixture is assumed to be proportional to the atomic density of that element.

[1] These variables are used to calculate of k from p_z. Previously, a binning effect of k might occur in the case that a fine energy bin (order of 0.1%) is used. This modification was made to avoid such an binning effect.

1.4.2 Sampling of EII

The ratio of the K-shell EII cross section of J-th element in a material to the Møller scattering cross section is calculated by the following equation:

$$R(E,J) = \frac{\sum_{j=1}^{J} \Sigma_{\mathrm{EII},j}(E)}{\Sigma_{\mathrm{Moller}}(E)}, \tag{29}$$

$$\Sigma_{\mathrm{EII},j}(E) = p_j \, \sigma_{\mathrm{EII},j}(E) \, \rho \frac{N_0}{W}, \tag{30}$$

where
$R(E,J)$ = the cumulative distribution function of the ratio of the K-shell EII cross section of the J-th element in a material to the Møller scattering cross section at electron energy E,
$\Sigma_{\mathrm{Moller}}(E)$ = macroscopic Møller scattering cross section at electron energy E,
$\Sigma_{\mathrm{EII},j}(E)$ = macroscopic EII cross section of the j-th element at electron energy E,
$\sigma_{\mathrm{EII},j}(E)$ = microscopic EII cross section of the j-th element at electron energy E,
p_j = proportion by number of the j-th element in the material,
ρ = density of a material,
N_0 = Avogadro's number,
W = Atomic, molecular and mixture weight for an element, for a compound, and for a mixture.

$R(E,J)$ is calculated in `pegs4nb.mor`, output in material data. In the EGS4 calculation, a K-shell vacancy creation by EII is sampled using $R(E,J)$.

1.4.3 K-X ray emission and energy deposition

After a K-shell vacancy creation by EII, the emission of a K-X ray is sampled using the K-shell fluorescence yield [22]. This part is common as the calculation after a K-shell vacancy creation by the photoelectric effect. [3] The difference is that no Auger electron nor cascade particle is followed in the case of EII. The directions of the K-X ray is assumed to be isotropic. In the case of K-X-ray emission, the K-X ray energy is sampled from up to the 10 K-X ray energies listed in [22] according to the relative yield of the K-X ray. In the case that a K-X ray is emitted, the difference in E_B (K shell binding energy) and the K-X ray energy is deposited locally. In the case that no K-X ray is generated (i.e. Auger electron emission), E_B is deposited locally.

1.4.4 Energy and direction of electrons after EII

The energy and direction of electrons after EII are treated in an approximate way. E_B is subtracted from the energy of either one of the two electrons related to the Møller scattering. In the case that neither of the two electron has kinetic energy greater than E_B, E_B is subtracted from the energy of both electrons while keeping the ratio of the kinetic energies unchanged. The directions of the electrons after EII are treated as being the same as the electrons after Møller scattering.

1.4.5 Modification after the NIM paper

The implementation of EII into the EGS4 code was described in ref [21]. The following points were modified from the description in ref [21]:

Table 2: New `IARG` and `IAUSFL` values for EII

`IARG`	`IAUSFL`	Situation
25	26	An EII interaction is about to occur.
26	27	Returned to MOLLER after a call to EII was made.

1. Previously, the K-X ray energy is sampled from up to the 4 K-X ray energies. Now, the K-X ray energy is sampled from up to the 10 K-X ray energies listed in [22]. This is due to a change in the treatment of the photoelectric effect-related phenomena in the EGS4 code [3]. [2]

2. EII of any element in a compound or mixture is treated.

3. The fluorescent yield is taken from Table 3 of ref.[22]. (In a previous calculation in the NIM paper, the fluorescent yield from Table. 10 of [23] was used.)

After K-shell vacancy creation, only the K-X ray is followed. Nether a K-Auger electron nor a cascade photon or electron is followed. The EII in L and the higher shells are treated as free-electron Møller scattering, as is in the default EGS4.

1.5 Modification of specifications for AUSGAB

1.5.1 Modification of the definition of IARG=4

The definition of `IARG=4` is expanded because, "Part of particle energy is deposited due to the binding energy." This situation occurs in one of the following 3 cases:

1. A photoelectric interaction has occurred and the difference in the electron binding energy and the secondary particle (X ray or Auger electron) energy is deposited.

2. Compton interaction has occurred and the electron binding energy is deposited locally. This is enabled only when the Doppler-broadening option is turned on.

3. The K-shell EII has occurred and the difference between the electron binding energy and the secondary particle (K-X ray) energy is deposited. This is enabled only when the EII option is turned on.

1.5.2 Extension of IARG and IAUSFL for EII

To call `AUSGAB` before and after an EII interaction, the range of the `IARG` and `IAUSFL` values were extended as shown in Table 2.

[2] A K-X ray calculation model in photoelectric effect-related phenomena in EGS4 was modified. [3] This modification in EII was made due to the effect of this modification because the EII calculation and photoelectric effect calculation use a common subroutine to calculate the K-X ray.

1.6 Outline of the modification of EGS4 subroutines

The following EGS4 subroutines were newly created for LSCAT:

- `SUBROUTINE APHI`:
  - Azimuth-angle(ϕ) sampling at Compton and Rayleigh scattering while considering the effect of photon linear polarization.
  - Calculation of $\vec{e}$.
  - Conversion from the scattering system to the laboratory system.
- `SUBROUTINE EII`
  - Subtracted E_B from the scattered-electron energy.
  - Set splitting number of EII K-X.
  - Call subroutine `KSHELL` to judge the X-ray/Auger emission and determine the X ray energy.
  - Energy deposition.
  - Store EII K-X ray in STACK and apply splitting to it.
- `SUBROUTINE RAYLEI`:

  Rayleigh scattering of a linearly polarized photon.

The following EGS4 subroutines were modified for LSCAT:

- `SUBROUTINE COMPT`:

  Linear polarization, $S(x,Z)/Z$ and Doppler broadening are added.
- `SUBROUTINE ELECTR`

  Return to `SHOWER` after calling `MOLLER` if the particle at the top of the `STACK` is a photon.
- `SUBROUTINE HATCH`:

  Read in $S(x,Z)/Z$, Compton profile and EII/Moller ratio (*R(E,J)*).
- `SUBROUTINE MOLLER`:

  Call `SUBROUTINE EII` using *R(E,J)*.

These subroutines (except for `SUBROUTINE ELECTR`) were contained in `kek4n.mor`. Flowchart of `SUBROUTINE APHI`, Doppler-broadening part of `SUBROUTINE COMPT` and `SUBROUTINE EII` were shown in Appendix H. The modification of `SUBROUTINE ELECTR` was contained in `kek4macn.mor` together with other macros for LSCAT. A list of LSCAT in `kek4macn.mor` is shown in Appendix G.3. In `kek4n.mor` and `kek4macn.mor`, the subroutines and macros for "General treatment of photoelectric related phenomena for compounds and mixtures in EGS4" [3] were also contained.

2 How to calculate

The main part of `LSCAT` consists of the following 3 programs: [3]

- `kek4n.mor`: Contains subroutines for LSCAT and a general treatment of photoelectric-related phenomena.
- `kek4macn.mor`: Contains macros for LSCAT and a general treatment of photoelectric-related phenomena and other kek macros.
- `pegs4nb.mor`: Prepare σ_{bC}, $S(x,Z)/Z$, Compton profile and the EII/Moller ratio for the EGS4 calculation.

Two user codes are made as a sample for the photon-scattering part and EII part of LSCAT:

- `ucbcomp4.mor`: A sample user's code to demonstrate how the photon-scattering part of LSCAT works.
- `ucbrem.mor`: A sample user's code to demonstrate how the EII part of LSCAT works.

This section describes how these files are used and how the flag variables are set. The contents of all the files in the distribution package are given in Appendix B.

2.1 Linearly polarized photon scattering

2.1.1 ucbcomp4.mor

To see linearly polarized photon scattering quickly, one can run `ucbcomp4.mor`. This is an EGS4 user code which is used to calculate the spectra of a scattered photon. The calculation geometry is shown in Fig.3. The details of the measurement and geometry are described in ref.[24].

The source is a mono-energy, mono-directional partially linearly polarized synchrotron-radiation photon beam. In Fig.3, the propagation and polarization vectors of the source are indicated by $\vec{k_0}$ and $\vec{e_0}$. The scattering sample is placed at point O. The normal vector of the sample is $(-\frac{1}{2}, -\frac{1}{\sqrt{2}}, \frac{1}{2})$. The scattered photon is detected by Ge-1 and Ge-2. In the calculation, scattered photons toward the X and Y directions are detected. (The opening angle of the detector is 5° in the calculation.) To run `ucbcomp4.mor`, type in

```
negs4run ucbcomp4.mor cic3.dat
```

Do not select "`use PRESTA`" in `negs4run`. The output is written in `mortjob.out6`. Due to source-photon linear polarization, the number of scattered photons in the horizontal direction is about 6-times more than that in the vertical direction in `mortjob.out6`. The average of the scattered photons in the horizontal and vertical directions is shown in Fig.4(a).

While `ucbcomp4.mor` includes both linear polarization and bound Compton scattering, each approximation can be turned on/off independently. The influence of the photon linear polarization can be seen by the `ucbcomp4.mor` calculation after changing `LPOLAR(I)=1;` into

[3] In the 1995 version of LSCAT, the subroutines and macros for LSCAT were contained in a file named `LSCAT.MOR`. Now, the LSCAT subroutines and macros are contained in `kek4n.mor` and `kek4macn.mor`, and `LSCAT.MOR` is no longer used.

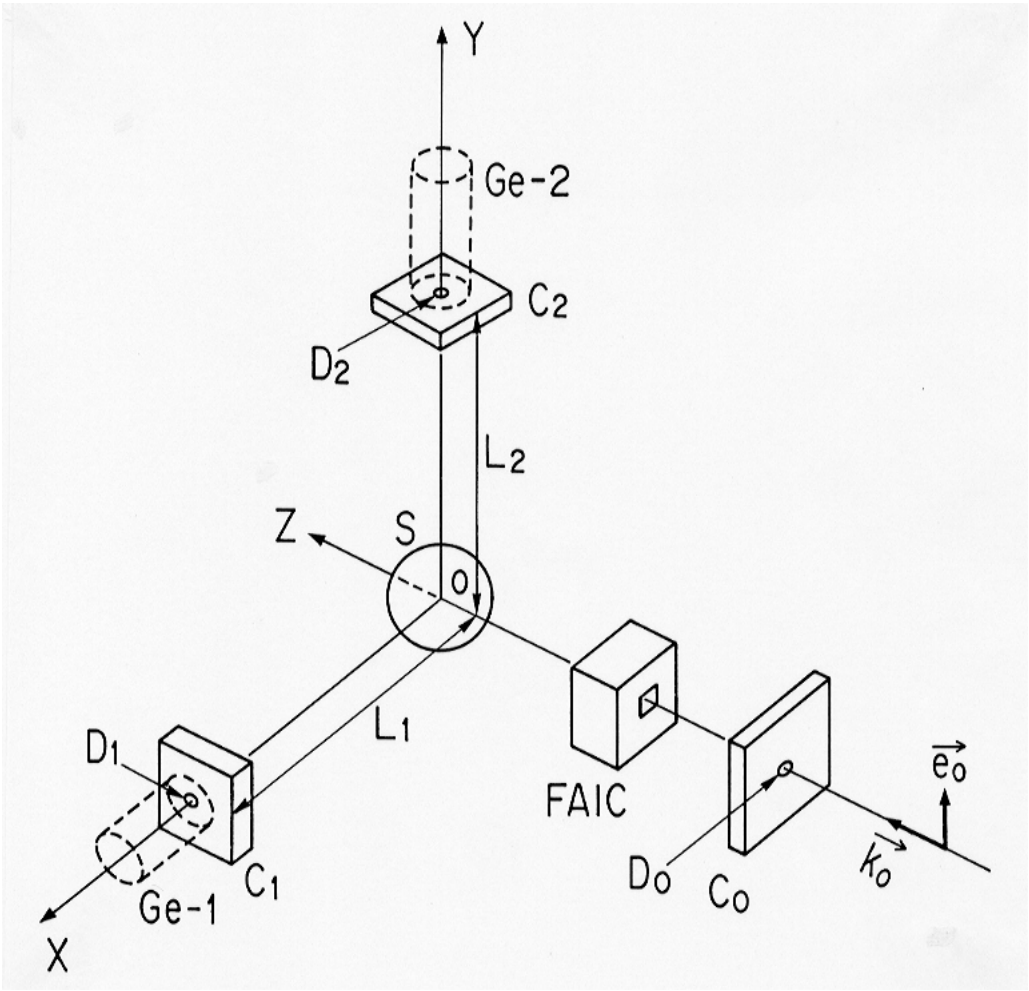

Figure 3: Geometry used in `ucbcomp4.mor`.

Table 3: Flag variable for a linearly polarized photon.

Linear polarization	LPOLAR(I)*
On	1
Off	0

* I is the region number where the switch is turned on/off.

LPOLAR(I)=0;. The calculated intensity of a scattered photon apparently differs from the measurement in the case that linearly polarized photon scattering is ignored. Search "LPOL" to find lines related to linear polarization in ucbcomp4.mor.

2.1.2 One's own user code

Linearly polarized photon scattering can be turned on/off by the LPOLAR(I) flag in the user's code, as shown in Table. 3 (I is the region number where the switch is turned on). Add

```
COMIN/MISC/;
```

to a user code if this was not included. This common contains LPOLAR(I).

In the case that linearly polarized photon scattering is turned on, the user should set the UF(1), VF(1), WF(1) and PVAL values in one's own user code. The degree of linear polarization is set by the PVAL value. UF(1), VF(1) and WF(1) are the polarization vector of the source photons. The polarization vector should be normalized and should be perpendicular to the propagation vector. UF(1), VF(1) and WF(1) are set inside the CALL SHOWER loop, depending on PVAL. Examples of linearly polarized or unpolarized photon source coding are shown next.

Completely linearly polarized photon source In the case that the photon source is completely linearly polarized, the propagation vector is along the z-direction and the polarization vector is along the y-direction, the source description is as follows:

```
UI=0.0; VI=0.0; WI=1.0;
UFI=0.0; VFI=1.0; WFI=0.0;

DO I=1,NCASES ["START OF SHOWER CALL LOOP"
UF(1)=UFI; VF(1)=VFI; WF(1)=WFI;
CALL SHOWER(IQI,EISING,XI,YI,ZI,UI,VI,WI,IRI,WTI);
]
```

Partially linearly polarized photon source If the source propagation vector is along the z-direction and the polarization vector is along the y-axis with $P = 0.85$, as is ucbcomp4.mor, make the user's code as follows:

```
UI=0.0; VI=0.0; WI=1.0;
PVAL=0.85;
PRATIO=0.5+PVAL*0.5;

DO I=1,NCASES ["START OF SHOWER CALL LOOP"
```

```
$RANDOMSET VALUE;
IF(VALUE.LT.PRATIO)[UFI=0.0; VFI=1.0; WFI=0.0;]
ELSE[UFI=1.0; VFI=0.0; WFI=0.0;]
UF(1)=UFI; VF(1)=VFI; WF(1)=WFI;
CALL SHOWER(IQI,EISING,XI,YI,ZI,UI,VI,WI,IRI,WTI);
]
```

The following shows incorrect examples of partially polarized photon-source coding.

- Set `UF(1)`, `VF(1)` and `WF(1)` outside the shower-call-loop. Since `$RANDOMSET` for setting the source photon polarization is executed only once, partial linear polarization is not simulated.
- `UFI=1-PVAL; VFI=PVAL; WFI=0.0;`

  is another example of incorrect coding, because the main polarization direction becomes some direction between the x- and y-axis in this case.

Unpolarized photon source In a photon-transport simulation considering linear polarization, an unpolarized photon source is automatically generated by setting

`UF(1)=0.0; VF(1)=0.0; WF(1)=0.0;`

in the shower call loop.

2.2 Bound Compton scattering and Doppler broadening

2.2.1 ucbcomp4.mor

To see photon transport with bound Compton scattering and Doppler broadening quickly, one can run `ucbcomp4.mor` again. Type in

```
negs4run ucbcomp4.mor cic3.dat
```

and do not select "`USE PRESTA`" in `negs4run`. See `mortjob.out6` for the output. The scattered-photon spectra calculated using `ucbcomp4.mor` are shown in Fig.4. "CP" means σ_{bC}, *S(x,Z)/Z* and Doppler broadening are considered and "S" means σ_{bC} and *S(x,Z)/Z* are considered. Both are smeared by a Gaussian function to model the detector resolution. Thus, the output of `ucbcomp4.mor` is slightly different from Fig.4.

The influence of Doppler broadening can be seen by repeating the `ucbcomp4.mor` calculation after changing `IPROFR(I)=1;` into `IPROFR(I)=0;`. As shown in "S" line in Fig. 6, the calculated spectra of a Compton-scattered photon differs from a measurement, apparently in the case that Doppler broadening is ignored.

2.2.2 Make cross-section file including σ_{bC}, $S(x,Z)/Z$ and $J_i(p_z)$

It is necessary to prepare σ_{bC}, *S(x,Z)/Z* and a Compton profile before performing a low-energy photon-transport calculation considering these things. First, compile `pegs4nb.mor` by:

```
pegs4nbcompile
```

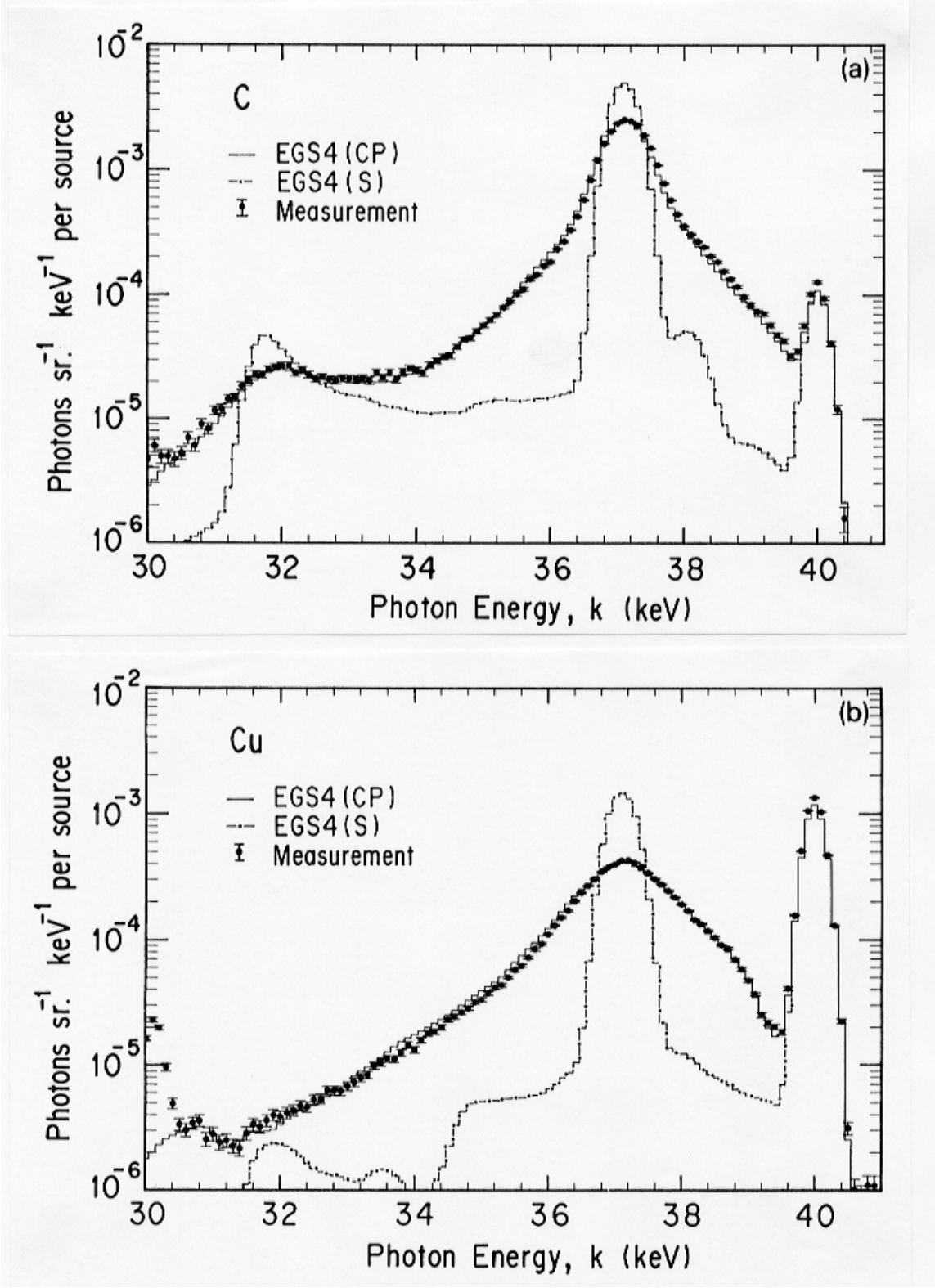

Figure 4: Comparison of the photon spectra scattered by C and Cu samples.

All additional features of `pegs4nb.mor` to produce cross-section files, including σ_{bC}, $S(x,Z)/Z$ and Compton profile, are controlled via optional flags in namelist `INP`. The name of the flags and their functions are summarized in Table 6.

To make material data, including σ_{bC}, *S(x,Z)/Z* and Compton profile, the input file is:

```
ELEM
 &INP IBOUND=1,INCOH=1,ICPROF=3,IRAYL=1 &END
C-ICPROF3-PHOTX                C
C
ENER
 &INP AE=0.512,UE=0.711,AP=.001,UP=0.2 &END
TEST
 &INP &END
PWLF
 &INP &END
DECK
 &INP &END
```

This is `cic3.inp`. `ICPROF=3` produces a normalized cumulative density function of $J_i(p_z)$, which corresponds to the right-hand side of Eq.(28). `ICPROF=4` is used only when PWLF of p_z vs $J_i(p_z)$ is necessary. To simulate photon transport with Doppler broadening, σ_{bC} and $S(x,Z)/Z$ must be considered. Thus, if `ICPROF`$\neq$`0`, `IBOUND` and `INCOH` must be 1. The reason is an electron-binding effect on the Doppler-broadening affects the angular distribution of the Compton-scattered photon and total Compton scattering (as mentioned in section 1). An input other than the part between `&INP` and `&END` can be changed according to the pegs4 input rule. Run `pegs4nb.mor` by type in;

```
pegs4nbrun cic3.inp cic3a.dat z006.dat
```

`cic3.inp` and `z006.dat` are examples of input and Compton profile input files. `z006.dat` is contained in `scp31.tar`. Specify the Compton-profile data file corresponding to the elements. (The way to calculate a for compound or mixture is described later.)

The following two examples of pegs4nb input are useful only in special cases, like comparing EGS4 with other codes in the same approximation.

To make material data, including σ_{bC} and *S(x,Z)/Z*, the input file is:

```
ELEM
 &INP IBOUND=1,INCOH=1 &END
C-INCOH                        C
C
ENER
 &INP AE=0.512,UE=0.711,AP=.001,UP=0.2 &END
TEST
 &INP &END
PWLF
 &INP &END
DECK
 &INP &END
```

To simulate photon transport with $S(x,Z)$, σ_{bC} must be used. Thus, `IBOUND` must be 1 if `INCOH`$=1$. If a user is interested in σ_{bC} only, the input is

```
ELEM
 &INP IBOUND=1 &END
C-BOUND                         C
C
ENER
 &INP AE=0.512,UE=0.711,AP=.001,UP=0.2 &END
TEST
 &INP &END
PWLF
 &INP &END
DECK
 &INP &END
```

INCOH=0 and ICPROF=0 is automatically set. In the case that the Compton profile is not necessary, leave the third operand blank in pegsnb4run execution.

Preparing Compton profile file for compound and mixture (1) In the case that the material is either a compound or a mixture, the user must to make a special Compton profile file.

A short program makescpr.mor was made to produce the Compton profile for a compound and a mixture. Place makescpr.mor and shellwise Compton profile files in the same directory. Key in

```
mortrun makescpr.mor
```

Program asks, either compound or mixture, number of elements (NE), relative numbers of atoms (PZ, for compound), relative amount of atom by weight (RHOZ, for mixture) and atomic number (Z).

For example, specify "0 (for compound)", input 2 for NE, 2 and 1 for PZ, 1 and 8 for Z. Then, the Compton profile for water is written in newscpr.dat. [4] You can then prepare a Compton profile for your own input.

The makescpr.mor and Compton profile files can be placed in different directories. In this case, modify the contents of variable FILENM in makescpr.mor so that the location of the Compton profile is specified in FILENM.

Preparing Compton profile file for compound and mixture (2) An alternative way (to run pegs4nb for a compound and a mixture without running makescpr.mor) is possible.

Place pegs4nb.exe and the Compton profile files in the same directory. Or, modify the contents of FILENM in pegs4nb.mor so that the location of the Compton profile is specified in FILENM and compile pegs4nb.mor.

Modify ICPROF=3 into ICPROF=-3 (or modify ICPROF=4 into ICPROF=-4) in pegs4 input and run pegs4nb.exe. All of the necessary Compton profile files are automatically read in and a material data file is created. pgs4job.ssl is a Compton profile file for the material.

[4] Here, the first sub-shell corresponds to the H-1s sub-shell. The second to fourth sub-shells correspond to O-1s to the O-2p subshell. Like this, all of the sub-shells of all elements in a compound or a mixture are treated as sub-shells of one element.

Error message on SUN If you run `pegs4nb.mor` on a SUN work station, you will get the following error message:

```
Note: the following IEEE floating-point arithmetic exceptions
occurred and were never cleared; see ieee_flags(3M);
Inexact:  Underflow;
Sun's implementation of IEEE arithmetic is discussed in
the Numerical Computation Guide.
```

Ignore this message, since it is produced from the original NRCC version, `pegs4.mortran`, and the output seems to be correct, even if this message is printed out.

How to make plural material data To make plural material data, run `pegs4nb.mor` for each material. (ex. run pegs4nb.mor 3 times to make data for 3 materials) and join them using a unix (ex. `cat`, `cp`) or a DOS command (ex. `COPY`). Specify a different output file name for each pegs4nbrun; otherwise, the output is automatically overwritten.

2.2.3 One's own user code

To do photon transport considering σ_{bC}, $S(x, Z)$ and Doppler broadening (DB), the user should set the flag variables in one's own user code. Add

```
COMIN/MISC/;
```

to a user code if this was not included. This common contains flag variables.

Switches for each simulation mode are listed in Table 4. As described above, to simulate photon transport including Doppler broadening, $S(x, Z)$ and σ_{bC} must be considered. To do this:

1. Specify `IBOUND=1`, `INCOH=1` and `ICPROF=3` in `pegs4nbrun` job.
2. Specify `INCOHR(I)=1` and `IPROFR(I)=1` in user's code.

Also, to simulate photon transport including $S(x, Z)$, σ_{bC} must be considered. To do this, specify:

1. `IBOUND=1` and `INCOH=1` in `pegs4nbrun` job.
2. `INCOHR(I)=1` in user's code.

Also, to simulate photon transport including σ_{bC} only specify:

1. `IBOUND=1` in `pegs4nb.mor`.
2. No modification is necessary in the user's code.

To switch σ_{bC} and σ_{fC} in the user's code, do as follows:

- Make material data with σ_{bC} and name it as (for example) 'Material-bC'.
- Make material data with σ_{fC} and name it as (for example) 'Material-fC'.
- Specify either 'Material-bC' or 'Material-fC' in the user's code.

Table 4: Flag values for each calculation mode

Mode		Input for pegs4nb	User Code
Compton Scatt. cross section	σ_{bC}	IBOUND=1	
$S(x,z)/Z$ rejection	Yes	INCOH=1	INCOHR(I)=1*
Doppler Broadening	Yes	ICPROF=3	IPROFR(I)=1*
Compton Scatt. cross section	σ_{bC}	IBOUND=1	
$S(x,z)/Z$ rejection	Yes	INCOH=1	INCOHR(I)=1
Compton Scatt. cross section	σ_{bC}	IBOUND=1	
$S(x,z)/Z$ rejection	No		
Compton Scatt. cross section	σ_{fC}		
$S(x,z)/Z$ rejection	No		

* I is the region number where the switch is turned on/off.

2.3 Electron impact ionization

2.3.1 ucbrem.mor

To see the K-X ray from EII quickly, one can run `ucbrem.mor`. This is an EGS4 user code which is used to calculate the spectra of a produced photon. The calculation geometry is shown in Fig.5. The details of the measurement and geometry are described in refs.[21, 25, 26]. The calculation conditions were as follows. An electron beam of 100 keV was incident on the Sn sample (target thickness, 21.6 mg/cm^2) normally. The photon was detected by two detectors at $\theta = 70°$ and 110°. To run `ucbrem.mor`, type in

```
negs4run ucbrem.mor sn.dat
```

Select "`Use PRESTA`" in `negs4run`. `sn.dat` is material data which contain the EII/Moller ratio made from Casnati's EII formula. The output is written in `mortjob.output` and `mortjob.7out`. The calculated spectra and measurement are shown in Fig. 6. By applying a gauss smear to the calculated spectra, the calculation and measurement agree well, as shown in Fig.3 of ref.[21]. The contribution of K-X ray from EII can be seen by repeating the `ucbrem.mor` calculation after changing `IMPACR(I)=1;` as `IMPACR(I)=0;` in the `ucbrem.mor`. As shown in Fig. 6, the K-X ray intensity becomes 3- or 5-times weaker at $\theta = 70°$ and 110°, respectively, in the case that EII is ignored.

2.3.2 Make a cross-section file including EII

It is necessary to prepare the EII/Moller ratio before performing an electron-photon transport calculation considering EII. Compile `pegs4nb.mor` if it has not yet been compiled,

```
pegs4nbcompile
```

All additional features of `pegs4nb.mor` to produce the EII/Moller ratio are controlled via optional flags in namelist `INP`. In the PEGS4 calculation, `IMPACT=1-6` in the input file enables

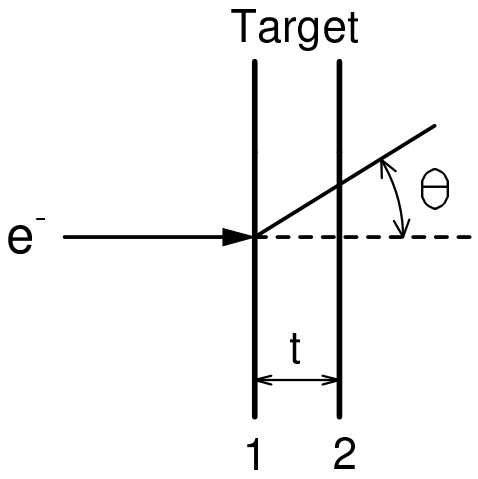

Figure 5: Geometry used in `ucbrem.mor`.

an EII cross-section preparation; `IMPACT=0` or no mention of `IMPACT` turns off the EII cross-section preparation. The choice of the EII cross section formula is controlled via the a value of `IMPACT`, as shown in Table 6. For example, following pegs4nb input specifies making material data with the EII cross section in Casnati's formula:

```
ELEM
 &INP IMPACT=1 &END
SN                              SN
SN
ENER
 &INP AE=0.512,UE=10.511,AP=0.001,UP=10.0 &END
TEST
 &INP &END
PWLF
 &INP &END
DECK
 &INP &END
```

Assuming this input file is saved in `sn.inp`, run `pegs4nb.mor` by type in;

```
pegs4nbrun sn.inp pegs4.out
```

Material data with the EII cross section are written in `pegs4.out`.

2.3.3 One's own users code

EII can be turned on/off in the user code by setting a flag `IMPACR(I)`. `IMPACR(I)=1` and `IMPACR(I) =0` specifies the inclusion and ignorance of EII in region I, respectively, as shown in Table 5. Add

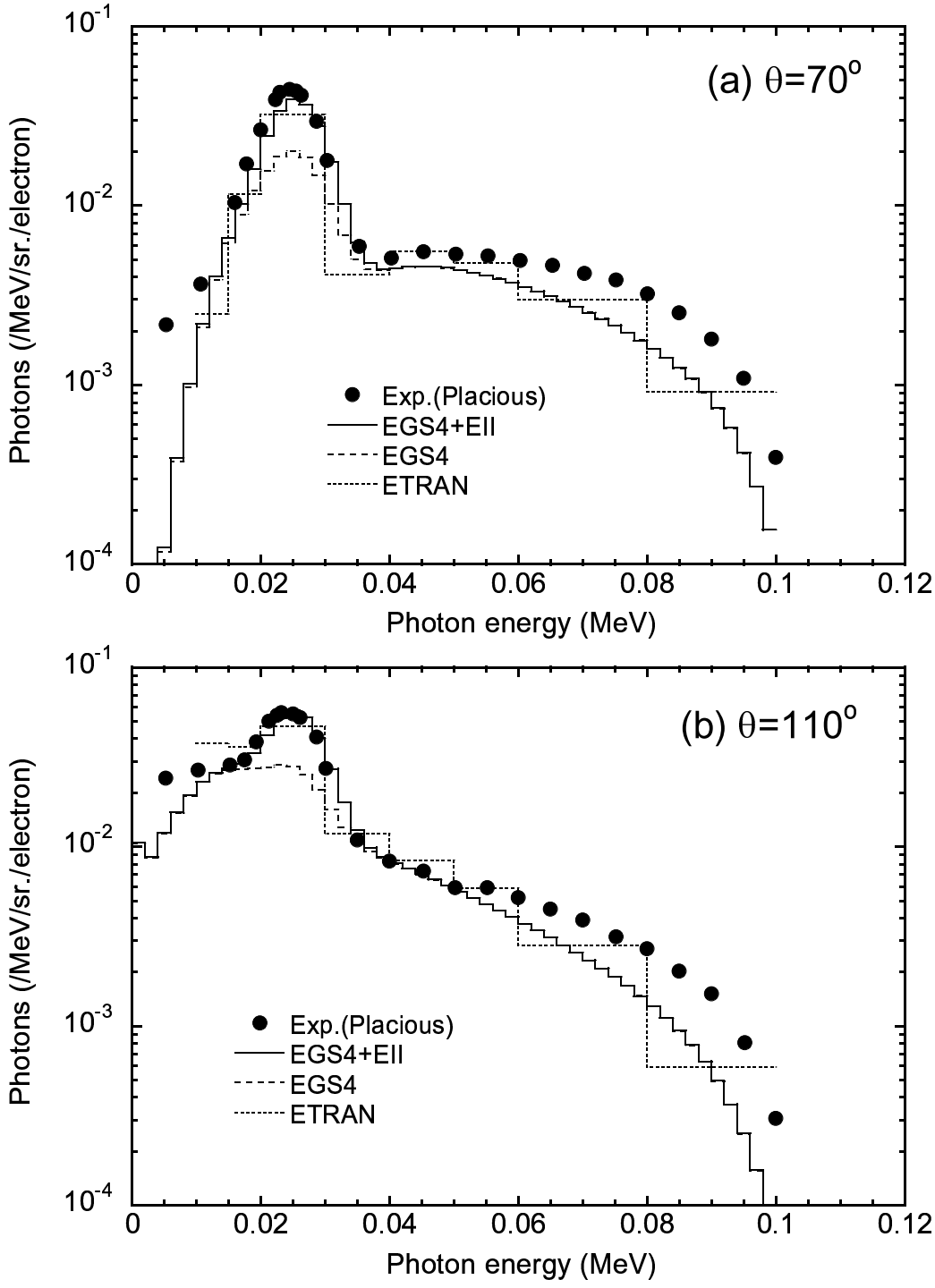

Figure 6: Spectra of the bremsstrahlung and K-X rays from a Sn target.

Table 5: Flag values for EII.

EII	IMPACR(I)*
On	1
Off	0

* I is the region number where the switch is turned on/off.

```
COMIN/MISC,EIICOM/;
```

to the user code if this was not included. This common contains flag variables.

Particle splitting can be applied to EII induced K-X rays to increase the calculation efficiency. To apply a splitting to EII K-X, specify

```
IEISPL=1;
NEISPL=n;
```

where `n` is the number of splittings. In the case that particles overflow the `common/stack`, the number of splittings is automatically reduced.

Acknowledgment

A bug fix in the Compton-scattering routines (Page 8) was triggered by information from users. Dr. R. Capote (Center for Applied Studies on Nuclear Development in Havana) pointed out the necessity to modify 2 and 4. Dr. A. Weidemann (Physikalisches Institut IV in Erlangen, Germany) pointed out the binning effect, which was fixed by modification 3. Dr. A. Carlsson pointed out a bug on $S(x, Z)$, which was fixed by modifying 6. Dr. H. Tawara of KEK also pointed out the necessity of modifying 2 and 6.

Dr. J. M. Heumann pointed out a bug in the EII part of `pegs4nb.mor`. Dr. L. Tavora (Univ. of Surrey) pointed out a bug in shellwise Compton profile files. A discussion with Dr. J. O'Meara (McMaster Univ.) was useful for clarifying the description of the rotation calculation in linearly polarized photon scattering (Appendix E).

Dr. A. Taibi of Univ. College London provided a form factor and coherent scattering cross section files in which the interference effect is considered. He also provided a modification of `pegs4nb.mor` to handle these files.

The authors express thanks to all of them.

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APPENDIX

A How to get files

Get the following files using anonymous ftp from `ftp.kek.jp` (130.87.34.28);

`/kek/kek_egs4/kek_improve/kek_improve.tar.Z`	for unix.
`/kek/kek_egs4/kek_improve/kek_improve.exe`	for PC.
`/kek/kek_egs4/kek_improve/scp31.tar.Z`	Shell-wise Compton profile for unix.
`/kek/kek_egs4/kek_improve/scp31.exe`	Shell-wise Compton profile for PC.

On unix machine, Uncompress and extract files by

```
uncompress kek_improve.tar.Z
tar xvf - < kek_improve.tar
```

On PC, extract files by

```
kek_improve
```

This is a self-extraction file.

Send e-mail when you take these files, writing:

- Your name, institute and e-mail address.
- A brief paragraph on the purpose you are using LSCAT.

e-mail: yoshihito.namito@kek.jp
Fax: 81-298-64-1993.

B Contents of files

- `bcomp.dat`

  The bound total Compton cross section (σ_{bC}) for all elements ($Z = 1 \sim 100$). `pegs4nb.mor` automatically picks up this as an input file (unit= 11). Made using DLC-99 [13].

- `cic3.dat`

  An example of the output of `pegs4nb.mor` and an example input for `ucbcomp4.mor`.

- `cic3.inp`

  An example of an input for `pegs4nb.mor` (unit=5). See the description of `pegs4nb.mor` for the meaning of additional flags in namelist INP.

- `csitl.dat`

  Input for `ucphotol.mor`.

- `egs4blkn.mor`

  Added initialization for flags.

- `egs4n.mor`

  Subroutine edgset and photo were removed.

- `ics_x.dat`

  Coherent scattering cross section with interference effect. x is the first letter of materials (Water, PMMA, Fat, Muscle, Kidney, Liver and Blood).

- `iff_x.dat`

  Form factor with an interference effect which is named in the same fashion as the coherent-scattering cross-section files.

- `incoh.dat`

  The incoherent scattering function ($S(x, Z)$) for all elements ($Z = 1 \sim 100$). `pegs4nb.mor` automatically picks up this as an input file (unit= 12). Made using DLC-99 [13].

- `kek4macn.mor`

  Includes macros for lscat. `negs4run` automatically picks up it.

- `kek4n.mor`

  Includes subroutines for lscat. `negs4run` automatically picks up it.

- `makescpr.mor`

  Short program to prepare a Compton profile for a compound and a mixture.

- `negs4run` (unix) or `negs4run.bat` (PC)

  C shell script (unix) or batch file (PC) to run EGS4 user's code. `kek4macn.mor` and `kek4n.mor` are automatically added to the user's code.

- `pegs4nbcompile` (unix) or `pegs4nbcom.bat` (PC)

  C shell script (unix) or batch file (PC) to compile `pegs4nb.mor` and make `pegs4nb.exe`.

- `pegs4nbrun` (unix) or `pegs4nbrun.bat` (PC)

  C shell script (unix) or batch file (PC) to run `pegs4nb.exe`.

- `pegs4nb.mor`

  `pegs4nb.mor` is made from `pegs4.mor` (NRCC-unix version). Bound Compton cross section(σ_{bC}), incoherent scattering function ($S(x, Z)/Z$), Doppler broadening and EII were added.

- `sn.dat`

  Material data for `ucbrem.mor`. EII/Moller ratio using Casnati's formula was contained.

- `ucbcomp4.mor`

  An EGS4 user code used to calculate the spectra of a scattered photon. Switches to enable the photon scattering part of LSCAT is contained.

- `ucbrem.mor`

  An example user's code to calculate with EII.

- `ucphotol.mor`

  EGS4 user code to calculate L-X rays from the first element to check L-X ray emission.

C How to Implement in Your System

C.1 PEGS4 and material data

Compile `pegs4nb.mor` with `pegs4nbcompile` (`pegs4nb_com.bat`). Create material data with `IBOUND=1`, `INCOH=1`, `ICPROF=3`, `IMPACT=n` option by running `pegs4nb` with `pegs4nbrun` (`pegs4nbrun.bat`). The meaning of each flag was described in 2.2.2, 2.3.2 and Appendix D.

C.2 EGS4 related

The procedure to run EGS4 with this implementation depends on your current system.

1. Running EGS4 in KEK-way
   By using `negsrun` (`negs4run.bat` and `negs4runp.bat`), the following things are automatically performed:
   - Replace `kek4mac.mortran` (`kek4mac.mor`) with `kek4macn.mor`.
   - Replace `kek4.mortran` (`kek4.mor`) with `kek4n.mor`.
   - Replace `egs4block.mortran` (`egs4blok.mor`) with `egs4blkn.mor`.
   - Replace `egs4.mortran` (`egs4.mor`) with `egs4n.mor`.
   - Delete `SUBROUTINE`s related `PHOTO` those are not included in the original EGS4 and ones related to `LSCAT`.
2. Running EGS4 in another way:
   - Put `kek4macn.mor` after `egs4mac.mortran` (`egs4mac.mor`).
   - Put `kek4n.mor` after your user code.
   - Replace `egs4block.mortran` (`egs4blok.mor`) with `egs4blkn.mor`.
   - Replace `egs4.mortran` (`egs4.mor`) with `egs4n.mor`.
   - Delete `SUBROUTINE`s related `PHOTO` those are not included in the original EGS4 and ones related to `LSCAT`.

C.3 User code

- Delete macros and `SUBROUTINES`s copied from the previous version of `LSCAT` from your user code and `SUBROUTINE`s related `PHOTO`.
- Add `COMIN/MISC,EIICOM/;`
- Set flags, `LPOLAR(I)`, `INCOHR(I)`, `IPROFR(I)`, `IMPACR(I)`. See 2.1.2, 2.2.3, 2.3.3, and Table 7 for the description of flags.

Table 6: New flags in namelist INP.

Flags	value	Function
IBOUND	0	Use free Compton cross section σ_{fC} (Default).
	1	Use bound Compton cross section σ_{bC}.
ICPROF	0	Turn off any Compton profile (Default).
	1	(Not use)
	2	(Not use)
	3	Turn on shell-wise Compton profile.
		Output cumulative density function(cdf) of $J_i(p_z)$.
	4	Turn on shell-wise Compton Profile. Output p_z-$J_i(p_z)$.
IMPACT	0	Turn off EII cross section (Default).
	1	EII cross section using Casnati's formula [16].
	2	EII cross section using Kolbenstvedt's rev. formula [17].
	3	EII cross section using Kolbenstvedt's formula [18].
	4	EII cross section using Jakoby's formula [19].
	5	EII cross section using Gryziński's formula [20].
	6	EII cross section using Gryziński's Relativistic formula. [20].
INCOH	0	Turn off incoherent scattering function $S(x,Z)/Z$ (Default).
	1	Turn on incoherent scattering function $S(x,Z)/Z$.
IRAYL	0	Turn off Coherent scattering cross section (Default).
	1	Output form factor in c.d.f. form and Rayleigh scattering cross section.
	2	Output form factor in c.d.f. form and Rayleigh scattering cross section.
		Interference effect is considered.
	3	Output form factor in the form of "x vs $F^2(x,Z)$".
IXRAY	0	Turn off ratio of photoelectric effect cross section of each element (Default).
	1	Turn on ratio of photoelectric effect cross section of each element.

D New flags for pegs4nb

New flags for pegs4nb input are summarized in Table.6. The binding effect in Compton scattering and electron impact ionization were already mentioned. The way to use the `IXRAY` variable is described in ref. [3].

The interference effect in coherent scattering was first incorporated into pegs4 by Leliveld et al [27] and expanded to 7 materials (Water, PMMA, Fat, Muscle, Kidney, Liver and Blood) by Taibi [28] using form factors measured by Peplow and Verghese [29]. When `IRAYL=2` is selected, specify:

- The molecular form factor files `iff_x.dat`, where x stands for the first letter of the materials. For example, the form-factor data for water are contained in `iff_w.dat`.
- The coherent cross-section files, `ics_x.dat`, which are named in the same fashion as the form factor data files.

in `pegs4nbrun` job.

E Scattering and Laboratory Systems

This appendix describes the relation of the laboratory system, which is used in the default EGS4 simulation, to the scattering system used in Compton and Rayleigh scattering routines for linearly polarized photons.

The laboratory system, in which $\vec{k_0}$ and $\vec{e_0}$ are in arbitrary directions, and the scattering system, in which $\vec{k_0}$ is parallel to $\vec{e_z}$ and $\vec{e_0}$ is parallel to $\vec{e_x}$, is transformed to each other by three rotations. $\vec{e_z}$ and $\vec{e_x}$ are unit vectors parallel to the z- and x-axies. Two rotations are necessary to make $\vec{k_0} \parallel \vec{e_z}$. These rotations were described by Cashwell and Everett. [30] The default EGS4 already treats these rotations. According to Ref.[30] notation, this $\mathbf{A^{-1}}$ matrix is

$$\mathbf{A^{-1}} = \begin{pmatrix} \frac{uw}{\rho} & \frac{vw}{\rho} & -\rho \\ \frac{-v}{\rho} & \frac{u}{\rho} & 0 \\ u & v & w \end{pmatrix}. \tag{31}$$

Here, $\rho = \sqrt{1-w^2}$. This matrix is written with an inverse sign, since $\mathbf{A}$ is mainly used for a transformation from the scattering system to the laboratory system. It is clear that

$$\mathbf{A^{-1}} \begin{pmatrix} u \\ v \\ w \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{32}$$

In the laboratory system, $\vec{e_0} \perp \vec{k_0}$; rotation by $\mathbf{A^{-1}}$ does not change this relation. As $\mathbf{A^{-1}}$ makes $\vec{k_0} \parallel \vec{e_z}$, $\mathbf{A^{-1}}$ moves $\vec{e_0}$ onto the x-y plane. In Fig. 7, $\vec{k_0}$ and $\vec{e_0}$ after two rotations by the $\mathbf{A^{-1}}$ matrix is shown. Another rotation by an angle $(-\omega)$ along the z-axis is necessary to make $\vec{e_0} \parallel \vec{e_x}$. The $\cos\omega$ and $\sin\omega$ are calculated using

$$\mathbf{A^{-1}}\vec{e_0} = \begin{pmatrix} \cos\omega \\ \sin\omega \\ 0 \end{pmatrix}. \tag{33}$$

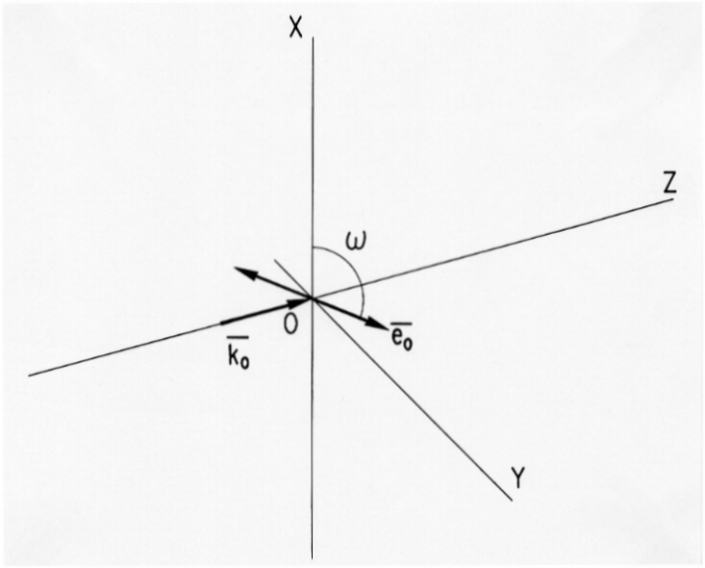

Figure 7: Direction of $\vec{k_0}$ and $\vec{e_0}$ after two rotations by $\mathbf{A}^{-1}$. While $\vec{k_0}$ is already parallel to $\vec{e_z}$, another rotation along the z-axis is necessary to make $\vec{e_0} \parallel \vec{e_x}$.

By these three rotations, $\vec{k_0}$ and $\vec{e_0}$ in the laboratory system are transferred to those in the scattering system. The scattered photon propagation vector ($\vec{k}$) and the polarization vector ($\vec{e}$) are transferred from the scattering system to the laboratory system by an inverse of these three rotations after Compton or Rayleigh scattering.

The relationship of $\vec{k_0}$, $\vec{k}$, $\vec{e_0}$ and $\vec{e}$ in laboratory system and those in scatter system are:

$$\begin{aligned} \vec{k_0}(\text{lab}) &= \mathbf{A}\cdot\mathbf{B}\cdot\vec{k_0}(\text{scatter}), \\ \vec{e_0}(\text{lab}) &= \mathbf{A}\cdot\mathbf{B}\cdot\vec{e_0}(\text{scatter}), \\ \vec{k}\ (\text{lab}) &= \mathbf{A}\cdot\mathbf{B}\cdot\vec{k}\ (\text{scatter}), \\ \vec{e}\ (\text{lab}) &= \mathbf{A}\cdot\mathbf{B}\cdot\vec{e}\ (\text{scatter}), \end{aligned} \tag{34}$$

where

$$\mathbf{B} = \begin{pmatrix} \cos\omega & -\sin\omega & 0 \\ \sin\omega & \cos\omega & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{35}$$

F Modification of pegs4nb.mor

Appendix F,G,H and I are attached to this report to help users who must understand the contents of LSCAT in detail.

F.1 Photon scattering

Modified part

- `COMIN/RSLTS/`: Added variables of $S(x,Z)/Z$ and $J_i(p_z)$ for output.

- `NAMELIST/INP`: Added flags for σ_{bC}, $S/Z(x,Z)$ and $J_i(p_z)$.
- `MAIN`
  - Read in σ_{bC}, $S(x,Z)/Z$ and $J_i(p_z)$.
  - PWLF (PieceWise Linear Fit) for $S(x,Z)/Z$, $J_i(p_z)$. Flowchart of PWLF of $J_i(p_z)$ is shown in Appendix H.
- `BLOCK DATA`
  - Added default values for PWLF of $S(x,Z)/Z$ and $J_i(p_z)$.
  - Set default value for `IBOUND`, `INCOH`, `ICPROF` and `IMPACT`.
- `SUBROUTINE LAY`
  - Added flags of $S(x,Z)/Z$ and $J_i(p_z)$.
  - Output $S(x,Z)/Z$.
  - Output $J_i(p_z)$.
- `FUNCTION COMPTM`: Calculate the total Compton scattering cross section using σ_{bC} or σ_{fC}.

New COMINs and NAMELISTs

- `COMIN/SFCOM`: $S(x,Z)/Z$ data.
- `COMIN/CPCOM`: $J_i(p_z)$ data.
- `NAMELIST/BCOMDT`: Input σ_{bC}.
- `NAMELIST/ISCADT`: Input $S(x,Z)/Z$.
- `NAMELIST/CPRFDT`: (Not use)
- `NAMELIST/SCPRDT`: Input $J_i(p_z)$.

New SUBROUTINES

- `CFUNS`: (Not use).
- `CFUNS2`: (Not use).
- `CFUNS3`: $\int_0^{p_z} J_i(x)dx / \int_0^{100} J_i(x)dx - p_z$ interpolation for PWLF.
- `CFUNS4`: $p_z - J_i(p_z)$ interpolation for PWLF.
- `RFUNS2`: $x - F(x,Z)$ interpolation for PWLF. Used by `IRAYL=2` input. Output *x-F(x,Z)* table. (Added to calculate Rayleigh scattering intensity.)
- `SFUNS`: $x - S(x,Z)/Z$ interpolation for PWLF.

New FUNCTION

- CPRFIL: $p_z - J_i(p_z)$ interpolation. Integrand of FUNCTION QD.

F.2 EII

1. A variable IMPACT was added to COMMON/EIMPACT and NAMELIST/INP/ as a flag to select this option and to specify the EII cross section. To set the initial value for IMPACT, the following statements were added to BLOCK DATA:

```
"DATA FOR COMMON EIMPACT"
DATA IMPACT/0/; "IMPACT=0 MEANS NOT INCLUDE ELECTRON IMPACT IONIZATION"
"                         DATA"
"                       1 to 6 MEANS INCLUDE EII DATA"
```

2. A new function EIITM was added to calculate the K-shell EII cross section. EIITM was also added to $FUNCTIONS as a 2-dimensional function.

```
"*********************************************************************"
"                                                                  KEK"
FUNCTION EIITM(E,ZVAL);
"                                                 17 DEC 1999/1730/YN"
"*********************************************************************"
"***TOTAL CROSS SECTION FOR ELECTRON IMPACT IONIZATION               "
COMIN/DERCON,EIMPACT,PHPAIR,PMCONS,MIXDAT,MOLVAR/;

J=ZVAL;
EKBMEV=EKEDGE(J)*0.001;

"Insert to avoid divide 0.   11/16/99 HH and YY"
IF(EKBMEV.EQ.0.0) [EIITM=0.0; RETURN;]

X=(E-RM)/EKBMEV;
NISMALL=2; "Number of K electron in atom"

IF(X.GT.1.001)[

  "Relativistic correction factor                          "
  "Derived by Grizinski, Phys. Rev. vol 138, A322 (1965)   "
  "Formulated by Quarles, Phys. Rev. A vol 13, 1278 (1976) "
  CAPI=EKEDGE(J)/RM/1000.0;
  CAPE=(E-RM)/RM;
  FR1=(2.0+CAPI)/(2.0+CAPE);
  FR2=(1.0+CAPE)/(1.0+CAPI);
  FR3=(CAPI+CAPE)*(2.0+CAPE)*(1.0+CAPI)**2;
  FR4=CAPE*(2.0+CAPE)*(1.0+CAPI)**2+CAPI*(2.0+CAPI);
  RFACT=FR1*FR2**2*(FR3/FR4)**1.5;

"Casnati+relativisity. J.Phys.B vol 15, 155 (1982) Eq.(8)"
IF(IMPACT.EQ.1)[
  SMALLA0=5.292E3; "First Bohr Radius in 10**-12cm"
  CAPI0=13.606E-3; "Rydberg energy in keV"
  CAPU=(E-RM)/(EKEDGE(J)*0.001);
  SMALLD0=-0.0318; SMALLD1=0.3160; SMALLD2=-0.1135;
  SMALLB0=10.57;   SMALLB1=-1.736; SMALLB2=0.317;
  SPHI=(EKEDGE(J)/CAPI0)**(SMALLD0+SMALLD1/CAPU+SMALLD2/CAPU**2);
  SPSI=SMALLB0*EXP(SMALLB1/CAPU+SMALLB2/CAPU**2);
  QCAP=NISMALL*SMALLA0**2*RFACT*(CAPI0/EKEDGE(J))**2*SPHI*SPSI
      *ALOG(CAPU)/CAPU;
  ] "End of Casnati+Rel."

"Kolbenstvedt, Revised, Phys. Rev. A2,1429(1970)"
IF(IMPACT.EQ.2) [
```

```
  CAPE=(E-RM)/RM; CAPE1=CAPE+1.0; CAPE2=CAPE+2.0; CAPI=EKBMEV/RM;
  SMALPH=1.0/137.036;
  EKE0=0.5*(SMALPH*ZVAL)**2*RM*1000.0; "I_0"
  QCAPA=CAPE1*CAPE1/CAPI/CAPE/CAPE2; "barn/atom"
  QDIST2=0.275*(EKE0/EKEDGE(J))**3*((1.-16./13.*(1.-EKEDGE(J)/EKE0))*
  (ALOG(2.*CAPE*CAPE2/CAPI)-CAPE*CAPE2/(CAPE1*CAPE1))-55./78.-
  32./39.*(1.-EKEDGE(J)/EKE0));
  QCLOSE=0.99*(1.0-CAPI/CAPE*(1.0-CAPE*CAPE/2.0/CAPE1/CAPE1+
  (2.0*CAPE+1.0)/CAPE1/CAPE1*ALOG(CAPE/CAPI)));
  QCAP=QCAPA*(QDIST2+QCLOSE);
  ] "End of Kolbenstvedt (1970)"


"Kolbenstvedt, J. Appl. Phys. 38,4785(1967)"
IF(IMPACT.EQ.3) [
  CAPE=(E-RM)/RM; CAPE1=CAPE+1.0; CAPE2=CAPE+2.0; CAPI=EKBMEV/RM;
  QCAPA=CAPE1*CAPE1/CAPI/CAPE/CAPE2; "barn/atom"
  QDIST=0.275*(ALOG(1.19*CAPE*CAPE2/CAPI)-CAPE*CAPE2/(CAPE1*CAPE1));
  QCLOSE=0.99*(1.0-CAPI/CAPE*(1.0-CAPE*CAPE/2.0/CAPE1/CAPE1+
  (2.0*CAPE+1.0)/CAPE1/CAPE1*ALOG(CAPE/CAPI)));
  QCAP=QCAPA*(QDIST+QCLOSE);
  ] "End of Kolbenstvedt (1967)"

"Jakoby et al, J. Phys C9,487(1987)"
IF(IMPACT.EQ.4) [
  BETA2A=(1.0+(E-RM)/RM)**(-2);
  BETA2=1.0-BETA2A;
  BETA02=1.0-(1.0+EKEDGE(J)/(RM*1000))**(-2);
  FCAP1=254.9/(EKEDGE(J)*BETA2);
  FCAP2=ALOG(BETA2/BETA2A)-BETA2;
  FCAP3=1.0-BETA02/BETA2;
  FCAP4=ALOG(1.0/BETA02);
  FCAP5=BETA02/BETA2;
  SMA=5.14*ZVAL**(-0.48);
  SMB=5.76-0.04*ZVAL;
  SMC=0.72+0.039*ZVAL-0.0006*ZVAL**2;
  QCAP=SMA*FCAP1*(FCAP2+SMB*FCAP3+FCAP4*FCAP5**SMC);
  ] "End of Jakoby"

"Gryzinski, Phys. Rev. 138,A336(1965) Eq.22"
IF(IMPACT.EQ.5.OR.IMPACT.EQ.6)[
  QCONST=0.0656; "MeV**2*barn"
  G1=1.0/X*((X-1.0)/(X+1.0))**1.5;
  G2=1.0+0.6667*(1.0-0.5/X)*ALOG(2.7+SQRT(X-1.0));
  QCAP=QCONST*NISMALL/EKBMEV**2*G1*G2; "barn/atom"

"Relativistic correction"
"Gryzinski, Phys. Rev. 138,A322(1965) Eq.59,61"
  IF(IMPACT.EQ.6)[QCAP=QCAP*RFACT; ] "End of IMPACT.EQ.6"
  ] "End of Gryzinski"

IF(QCAP.LT.0.0)[QCAP=0.0;]

EIITM=QCAP*AN*1.0E-24/WM*RHO*RLC;  "/r.l."
] "End of X.GT.1.001"

ELSE[EIITM=0.0;]

RETURN;
END;  "END OF FUNCTION EIITM"
```

3. A new function, `EIIFUNS`, was added as an external function to calculate the ratio of the K-shell EII cross section to the Moller scattering cross section *R(E,J)* (Eq.29).

```
"*****************************************************************"
"                                                              KEK"
SUBROUTINE EIIFUNS(E,V);
"                                            17DEC1999/1730/YN "
```

```
"*********************************************************************"
"*****SUBROUTINE TO COMPUTE EII/Moller RATIO TO BE FIT.              "
REAL V($MXEL);
COMIN/MIXDAT/;
DO I=1,$MXEL [V(I)=0.0;]

AMOLL=AMOLTM(E);
IF(AMOLL.LT.1.0E-30) RETURN;

EIISUM=0.0;
DO I=1,NE [
ZVAL=Z(I);
EIISUM=EIISUM+EIITM(E,ZVAL)*PZ(I);
V(I)=EIISUM/AMOLL;
]
RETURN;
END;
```

4. The following statements were added to the `MAIN` program to do piecewise linear fitting (PWLF) of *R(E,J)* of an each element:

```
"Fit EII/Moller ratio. 16DEC1999 Y. Namito"
IF(IMPACT.GE.1) [
OUTPUT IMPACT;('0DO PWLF TO EII/MOLLER. IMPACT=',I3/);

CALL PWLF1(NEII,NALE,AE,UE,THMOLL,EPE,ZTHRE,ZEPE,NIPE,ALKE,ALKEI,
AXEII,BXEII,$MXEKE,$MXEL,AFEII,BFEII,EIIFUNS);
]
```

5. The following variables were added to `COMMON/RSLTS` to transfer the PWLF result from `MAIN` to `SUBROUTINE LAY`:
   `NEII`: Number of intervals for piece-wise linear fitting.
   `AXEII,BXEII`: Parameters to give an argument to calculate *R(E,J)*.
   `AFEII($MXEKE,$MXEL),BFEII($MXEKE,$MXEL)`: Coefficient of *R(E,J)*.

6. The following statements were added to `SUBROUTINE LAY` to output the PWLF result of *R(E,J)*.

```
IF (IMPACT.GE.1)[
DO I=1,NE [IZ(I)=Z(I);]
$ECHOWRITE(IP, :INT:) NE;
$ECHOWRITE(IP, :INT:) (IZ(I),I=1,NE);
$ECHOWRITE(IP, :INT:) NEII;
$ECHOWRITE(IP, :FLT:) BXEII,AXEII;
$ECHOWRITE(IP, :FLT:)((BFEII(I,IFUN),AFEII(I,IFUN),IFUN=1,NE),I=1,NEII);
]
```

G Modification of EGS4

G.1 Modification of Subroutine HATCH

The `SUBROUTINE HATCH` was modified as follows to include *R(E,J)* and to keep the possibility of using the material data created by the current PEGS4:

1. Reading `IBOUND`, `INCOH`, `ICPROF` and `IMPACT` in was added.

```
$ECHO READ(KMPI,:INT:)
$LGN(MSGE,MGE,MSEKE,MEKE,MLEKE,MCMFP,MRANGE(IM)),IRAYL,IBOUND,INCOH,
ICPROF(IM),IMPACT,IXRAY;
```

2. Reading *S(x,Z)/Z* in was added:

```
IF (INCOH.EQ.1) [
$ECHO READ(KMPI,:INT:) NGS(IM);
NGSIM=NGS(IM);
$ECHO READ(KMPI,:FLT:)$LGN(SCO(IM)/0,1/);
$ECHO READ(KMPI,:FLT:)($LGN(SXZ(I,IM)/0,1/),I=1,NGSIM);
IF(INCOHM(IM).NE.1) [OUTPUT IM;
(' INCOHERENT DATA AVAILABLE FOR MEDIUM',I3,
 ' BUT OPTION NOT REQUESTED.',/);]
]
```

3. Reading the Compton profile in was added:

```
{IF (ICPROF(IM).EQ.1.OR.ICPROF(IM).EQ.2) [
$ECHO READ(KMPI,:INT:) NGC(IM);
NGCIM=NGC(IM);
$ECHO READ(KMPI,:FLT:)$LGN(CCO(IM)/0,1/),CPIMEV;
$ECHO READ(KMPI,:FLT:)($LGN(CPR(I,IM)/0,1/),I=1,NGCIM);
IF(IPROFM(IM).NE.1) [OUTPUT IM;
(' TOTAL COMPTON PROFILE DATA AVAILABLE FOR MEDIUM',I3,
 ' BUT OPTION NOT REQUESTED.',/);]
]

IF (ICPROF(IM).EQ.3.OR.ICPROF(IM).EQ.4) [
$ECHO READ(KMPI,:INT:) MXSHEL(IM),NGC(IM);
NGCIM=NGC(IM);   MXSIM=MXSHEL(IM);
$ECHO READ(KMPI,:FLT:)(ELECNO(I,IM),I=1,MXSIM);
$ECHO READ(KMPI,:FLT:)(CAPIO(I,IM),I=1,MXSIM);
$ECHO READ(KMPI,:FLT:)$LGN(CCOS(IM)/0,1/);
$ECHO READ(KMPI,:FLT:)
(($LGN(CPRS(I,IS,IM)/0,1/),IS=1,MXSIM),I=1,NGCIM);

IF(IPROFM(IM).NE.1) [OUTPUT IM;
(' SHELL COMPTON PROFILE DATA AVAILABLE FOR MEDIUM',I3,
 ' BUT OPTION NOT REQUESTED.',/);]
]
```

4. Reading *R(E,J)* in was added:

```
IF(IMPACT.GE.1) [
$ECHO READ(KMPI,:INT:) NEPM(IM);
NER=NEPM(IM);
$ECHO READ(KMPI,:INT:) (IZEI(I,IM),I=1,NER);
$ECHO READ(KMPI,:INT:) NEII(IM);
$ECHO READ(KMPI,:FLT:) $LGN(EICO(IM)/0,1/);
$ECHO READ(KMPI,:FLT:) (($LGN(EII(I,IFUN,IM)/0,1/),IFUN=1,NER),
I=1,NEII(IM));

IF(IMPACM(IM).NE.1) [OUTPUT IM;
(' ELECTRON IMPACT IONIZATION DATA AVAILABLE FOR MEDIUM',I3,
 ' BUT OPTION NOT REQUESTED.',/);]
]
```

G.2 Modification of Subroutine MOLLER

The `SUBROUTINE MOLLER` was modified to call subroutine EII using *R(E,J)*. The following COMIN statement was added:

```
COMIN/ELECIN,EDGE,EPCONT,EIICOM/;      "Addition for EII 03DEC1999/YN"
```

The following statements were added at the end of the subroutine MOLLER:

```
IF(IMPACR(IR(NP)).EQ.1.AND.IEDGFL(IR(NP)).NE.0)[
    $RANDOMSET RANII;
    EKE=EIE-RM;
    ELKE2=ALOG(EKE);
    $SET INTERVAL ELKE2,EICO;
    DO IFUN=1,NEPM(MEDIUM) [
        EIIR=EII1(LELKE2,IFUN,MEDIUM)*ELKE2+EII0(LELKE2,IFUN,MEDIUM);
        IF(RANII.LT.EIIR)[ "EII occurred"
            $AUSCALL($EIIAUSB);
            IZ=IZEI(IFUN,MEDIUM); "IZ is used in Subs EII and KSHELL"
            CALL EII;
            $AUSCALL($EIIAUSA);
            RETURN;
            ] "End of EII occurred IF"
        ]
    ] "End of Electron Impact Ionization"
```

G.3 List of LSCAT macro in kek4macn.mor

```
%C80
"*********************************************************************"
"*KEK Low Energy Photon Scattering Macros        16FEB2000/1600/YN*"
"*********************************************************************"
"RAYLEIGH (COHERENT) SCATTERING MACROS WITH LINEAR POLARIZATION"
"Changed into SUBROUTINE RAILEI. 7JAN1999/YN"
REPLACE {$RAYLEIGH-SCATTERING;} WITH
  {;IF(IRAYLR(IRL).EQ.1) [
   $RANDOMSET RNNO37;
   IF (RNNO37.LE.(1.0-COHFAC)) [
   $AUSCALL($RAYLAUSB);
   CALL RAYLEI;
   $AUSCALL($RAYLAUSA);
   GOTO :PNEWENERGY:;]]
  }

REPLACE {$COMIN-COMPT;} WITH {;COMIN/DEBUG,MISC,STACK,
  THRESH,UPHIOT,USEFUL,RANDOM/;}
REPLACE {$MXSCTFF} WITH {100}
REPLACE {$MXCP} WITH {2000}
; "BUFFER FLUSH"

REPLACE {;COMIN/BCOMP/;} WITH
{;COMMON/BCOMP/ICPROF($MXMED),
$LGN(SCO($MXMED)/0,1/),$LGN(SXZ($MXSCTFF,$MXMED)/0,1/),
$LGN(CCO($MXMED)/0,1/),CPIMEV,$LGN(CPR($MXCP,$MXMED)/0,1/),
MXSHEL($MXMED),ELECNO($MXNS,$MXMED),CAPIO($MXNS,$MXMED),
$LGN(CCOS($MXMED)/0,1/),$LGN(CPRS($MXCP,$MXNS,$MXMED)/0,1/);}
"INCOHM,IPROFM,IMPACM were moved to COMMON/MEDIA.        04FEB2000/YN"
"LPOLAR,INCOHR,IPROFR,IMPACR were moved to COMMON/MISC.  04FEB2000/YN"
"Separated from USERIP                                   06FEB2000/YN"
"$MXNS was introduced.                                   16FEB2000/YN"
"NGCS was removed.                                       16FEB2000/YN"
"NGS,NGC were moved to dimension in HATCH.               16FEB2000/YN"

REPLACE {;COMIN/EIICOM/;} WITH
{;COMMON/EIICOM/IZEI($MXEPERMED,$MXMED),NEII($MXMED),
$LGN(EICO($MXMED)/0,1/),$LGN(EII($MXEKE,$MXEPERMED,$MXMED)/0,1/),
```

```
IEISPL,NEISPL,FEISPL;}
"Mod to treat multi-element EII. IZEI -- EII were added. 20DEC1999/YN"
"Mod to combine EII split. IEISPL -- FEISPL were added.  27DEC1999/YN"
"Separated from USERIP                                    06FEB2000/YN"

"-------------------------------------------------------------------"
"*** MEDIA--NAMES OF MEDIA CURRENTLY BEING USED                     "
"INCOHM,IPROFM,IMPACM were added.                      04FEB2000/YN"
"-------------------------------------------------------------------"
REPLACE {;COMIN/MEDIA/;} WITH
  {;{SETR F=$FORTVER}
   [IF] {COPY F}=1977 [;
      COMMON/MEDIA/
         $LGN(RLC,RLDU,RHO,
         MSGE,MGE,MSEKE,MEKE,MLEKE,MCMFP,MRANGE,IRAYLM,
         INCOHM,IPROFM,IMPACM($MXMED)),NMED;
     COMMON/MEDIAC/MEDIA(24,$MXMED); $TYPE MEDIA;]
   [ELSE] [;
      COMMON/MEDIA/
         $LGN(RLC,RLDU,RHO,
         MSGE,MGE,MSEKE,MEKE,MLEKE,MCMFP,MRANGE,IRAYLM,
         INCOHM,IPROFM,IMPACM($MXMED)),NMED,
         MEDIA(24,$MXMED);]
  }

"-------------------------------------------------------------------"
"*** MISC--MISCELLANEOUS COMMON                                     "
"LPOLAR,INCOHR,IPROFR,IMPACR were added                04FEB2000/YN"
"-------------------------------------------------------------------"
REPLACE {;COMIN/MISC/;} WITH
{;COMMON/MISC/KMPI,KMPO,DUNIT,NOSCAT,$LGN(MED,RHOR,IRAYLR,LPOLAR,
INCOHR,IPROFR,IMPACR($MXREG));}

"-----------------------------------------------------------------------"
"Electron Impact Ionization                                 16OCT1996/YN"
"Next macro modifies ELECTR"
"This terminates ELECTRA. W/O this, EII K-X is discarded in ELECTRA."
REPLACE {$PARTICLE-SELECTION-MOLLER}
WITH {IF(IQ(NP).EQ.0)THEN; $AUSCALL($MOLLAUSA); RETURN; ENDIF;}

"New parameter for CALL AUSGAB  before/after EII           29NOV1999/YN"
PARAMETER $MXAUS=27;
PARAMETER $MXAUSM5=22;
PARAMETER $EIIAUSB=25;
PARAMETER $EIIAUSA=26;
;
"-----------------------------------------------------------------------"

"-------------------------------------------------------------------"
"*** STACK--INFORMATION KEPT ABOUT CURRENT PARTICLES(LP Version)   "
"-------------------------------------------------------------------"
REPLACE {;COMIN/STACK/;} WITH
  {;COMMON/STACK/$LGN(E,X,Y,Z,U,V,W,UF,VF,WF,DNEAR,WT,IQ,IR,
  MDIR, LATCH($MXSTACK)),NP,MDIRI,LATCHI
  ;$ENERGY PRECISION E;}
"NSCAT,NCOMP,NRAYL was removed from STACK.  11JAN2000/YN"
;
"THIS MACRO EXCHANGES TWO POSITIONS ON THE STACK"
"NB: LATCH IS A NON-STANDARD STACK VARIABLE     "
"    REMOVE IT IF IT CAUSES PROBLEMS            "
REPLACE {$EXCHANGE-STACK(#,#);} WITH {;
```

```
FDUMMY = U({P2});     U({P2})     = U({P1});     U({P1})     = FDUMMY;
FDUMMY = V({P2});     V({P2})     = V({P1});     V({P1})     = FDUMMY;
FDUMMY = W({P2});     W({P2})     = W({P1});     W({P1})     = FDUMMY;
FDUMMY = E({P2});     E({P2})     = E({P1});     E({P1})     = FDUMMY;
FDUMMY = WT({P2});    WT({P2})    = WT({P1});    WT({P1})    = FDUMMY;
IDUMMY = IQ({P2});    IQ({P2})    = IQ({P1});    IQ({P1})    = IDUMMY;
"LATCH IS NON-STANDARD"
IDUMMY = LATCH({P2}); LATCH({P2}) = LATCH({P1}); LATCH({P1}) = IDUMMY;
"UF, VF, WF is NON-STANDARD"
FDUMMY = UF({P2});    UF({P2})    = UF({P1});    UF({P1})    = FDUMMY;
FDUMMY = VF({P2});    VF({P2})    = VF({P1});    VF({P1})    = FDUMMY;
FDUMMY = WF({P2});    WF({P2})    = WF({P1});    WF({P1})    = FDUMMY;
}
;
REPLACE {$PARTICLE-SELECTION-COMPT;} WITH
"       ========================="
  {;IF(IQ(NP)=0  &  E(NP-1)<ECUT(IR(NP-1))) [
   IQ(NP)=IQ(NP-1);IQ(NP-1)=0; T=E(NP); E(NP)=E(NP-1);
   E(NP-1)=T; T=U(NP);U(NP)=U(NP-1);U(NP-1)=T; T=V(NP);
   V(NP)=V(NP-1);V(NP-1)=T; T=W(NP);W(NP)=W(NP-1);W(NP-1)=T;
   T=UF(NP);UF(NP)=UF(NP-1);UF(NP-1)=T; T=VF(NP);VF(NP)=VF(NP-1);
   VF(NP-1)=T; T=WF(NP);WF(NP)=WF(NP-1);WF(NP-1)=T;]}
"   FOR LOW ENERGY CALCULATIONS ESPECIALLY, THIS SAVES A LOT OF SPACE  "
"   ON THE STACK BECAUSE LOW ENERGY ELECTRONS ARE DISCARDED IMMEDIATELY"
"   EVEN IF THEIR ENERGY (INCLUDING THE REST MASS) IS GREATER THAN     "
"   THE PHOTONS ENERGY                                                 "
;

REPLACE {;$UN-POLARIZED-PHOTON;} WITH
   {;/UF(NP),VF(NP),WF(NP)/=0.0;}
REPLACE {;$PARTICLE-SELECTION-BREMS;} WITH
  {;/UF(NP),UF(NP-1),VF(NP),VF(NP-1),WF(NP),WF(NP-1)/=0.0;
  IF(IBRSPL.EQ.1)[
    "SPLITTING HAS BEEN REQUESTED"
    IF((NBRSPL.GT.1).AND.((NP+NBRSPL).GE.$MXSTACK))[
      "STACK OVERFLOW IMMINENT, REDUCE NBRSPL, RAISE FBRSPL"
      LOOP[
        OUTPUT $MXSTACK,NBRSPL,(2*NBRSPL+1)/3;
        ('0*** WARNING ***. STACK SIZE = ',I4,' MIGHT OVERFLOW'/
         '                 NBRSPL BEING REDUCED, ',I4,'-->',I4/);
        NBRSPL=(2*NBRSPL+1)/3;
        FBRSPL=1.0/FLOAT(NBRSPL);
        IF(NBRSPL.EQ.1)[
          "STACK IS TOO SMALL TO ALLOW SPLITTING, SHUT IT OFF"
          OUTPUT $MXSTACK;
          ('0*** WARNING ***. STACK SIZE = ',I4,' IS TOO SMALL'/
           '                  BREMSSTRAHLUNG SPLITTING NOW SHUT OFF'/);
          IBRSPL=0;
          ]
        "KEEP LOOPING UNTIL NBRSPL IS SMALL ENOUGH"
        ]UNTIL((NP+NBRSPL).LT.$MXSTACK);
      ]
    "SHUFFLE THE ELECTRON TO THE TOP OF THE STACK"
    "NPSTRT IS A POINTER TO THE ORIGINAL LOCATION OF THE ELECTRON"
    IF(IQ(NP).EQ.0)[NPSTRT=NP-1;$EXCHANGE-STACK(NP,NP-1);]
    ELSE[NPSTRT=NP;]
    "ADJUST THE WEIGHT OF THE INITIAL PHOTON"
    WT(NP-1)=WT(NP-1)*FBRSPL;
    "STORE THE ENERGY OF THE INITIAL PHOTON"
    FRSTBR=E(NP-1);
    "RESTORE THE ELECTRON'S INITIAL ENERGY BECAUSE THE INTERACTION"
```

```
  "REDUCED IT"
  E(NP)=E(NP)+E(NP-1);
  "TELL AUSGAB THAT A BREMSSTRAHLUNG INTERACTION HAS OCCURRED"
  $AUSCALL($BREMAUSA);
  "INITIALIZE THE SPLITTING COUNTER"
  ICSPLT=1;
  WHILE(ICSPLT.LT.NBRSPL)[
    "LOOP NBRSPL-1 TIMES (TOTAL NUMBER OF PHOTONS = NBRSPL)"
    ICSPLT=ICSPLT+1;
    "TELL AUSGAB THAT A BREMSSTRAHLUNG INTERACTION WILL OCCURRED"
    $AUSCALL($BREMAUSB);
    "SAMPLE THE BREMSSTRAHLUNG INTERACTION"
    CALL BREMS;
    "SHUFFLE THE ELECTRON TO THE TOP OF THE STACK"
    IF(IQ(NP).EQ.0)[$EXCHANGE-STACK(NP,NP-1);]
    "ADJUST THE PHOTON WEIGHT"
    WT(NP-1)=WT(NP-1)*FBRSPL;
    "RESTORE THE ELECTRON'S INITIAL ENERGY"
    E(NP)=E(NP)+E(NP-1);
    "TELL AUSGAB THAT A BREMSSTRAHLUNG INTERACTION HAS OCCURRED"
    $AUSCALL($BREMAUSA);
    "END OF THE SPLITTING LOOP"
    ]
  "RESTORE THE ELECTRON'S ENERGY TO WHAT IT HAD AFTER THE"
  "FIRST INTERACTION"
  E(NP)=E(NP)-FRSTBR;
  "PUT THE ELECTRON BACK TO IT'S ORIGINAL STACK LOCATION"
  "THIS WILL PREVENT OVERFLOW BECAUSE USUALLY THE PHOTON"
  "HAS LOWER ENERGY"
  $EXCHANGE-STACK(NPSTRT,NP);
  ]
;}
```

H Flowchart

A flowchart of `SUBROUTINE APHI` is shown in Fig.8. A flowchart of a part of `SUBROUTINE COMPT`, which is related to an expansion regarding Doppler broadening, is shown in Fig.9. A flowchart of `SUBROUTINE EII` is shown in Figs. 10∼11. A flowchart of a part of `pegs4nb.mor`, which is related to an expansion of Doppler broadening, is shown in Fig.12.

I Variables and commons

The LSCAT related variables in `COMMON MISC` and `COMMON MEDIA` are listed in Tables 7 and 8, respectively. The variables for bound Compton scattering in `COMMON BCOMP` are listed in Table 9. The variables for EII in `COMMON EIICOM` are listed in Table 10. The important local variables in the EGS4 subroutines which are related to LSCAT are listed in Table 11. The variables in the shell-wise Compton profile input are listed in Table 12.

The variables in `COMMON SFCOM` and `COMMON CPCOM` in `pegs4nb.mor` are listed in Table 13 and Table 14, respectively.

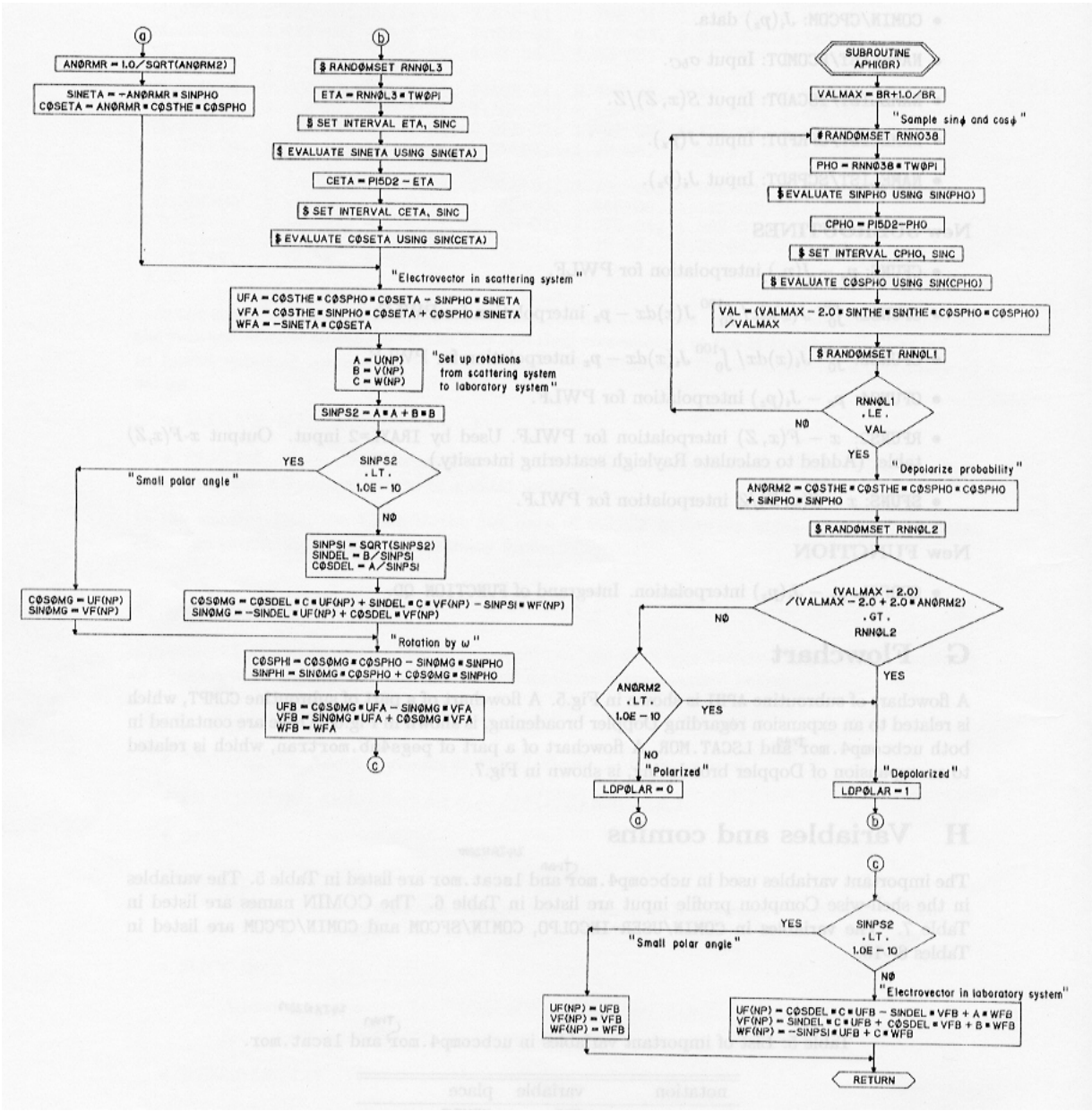

Figure 8: Flowchart of `SUBROUTINE APHI`.

Table 7: List of LSCAT related variables in COMMON MISC.

Variable	Contents
`LPOLAR(I)`	Turn on/off linearly polarized photon scattering in region I.
`INCOHR(I)`	Turn on/off S/Z rejection in region I.
`IPROFR(I)`	Turn on/off Doppler broadening in region I.
`IMPACR(I)`	Turn on/off EII in region I.

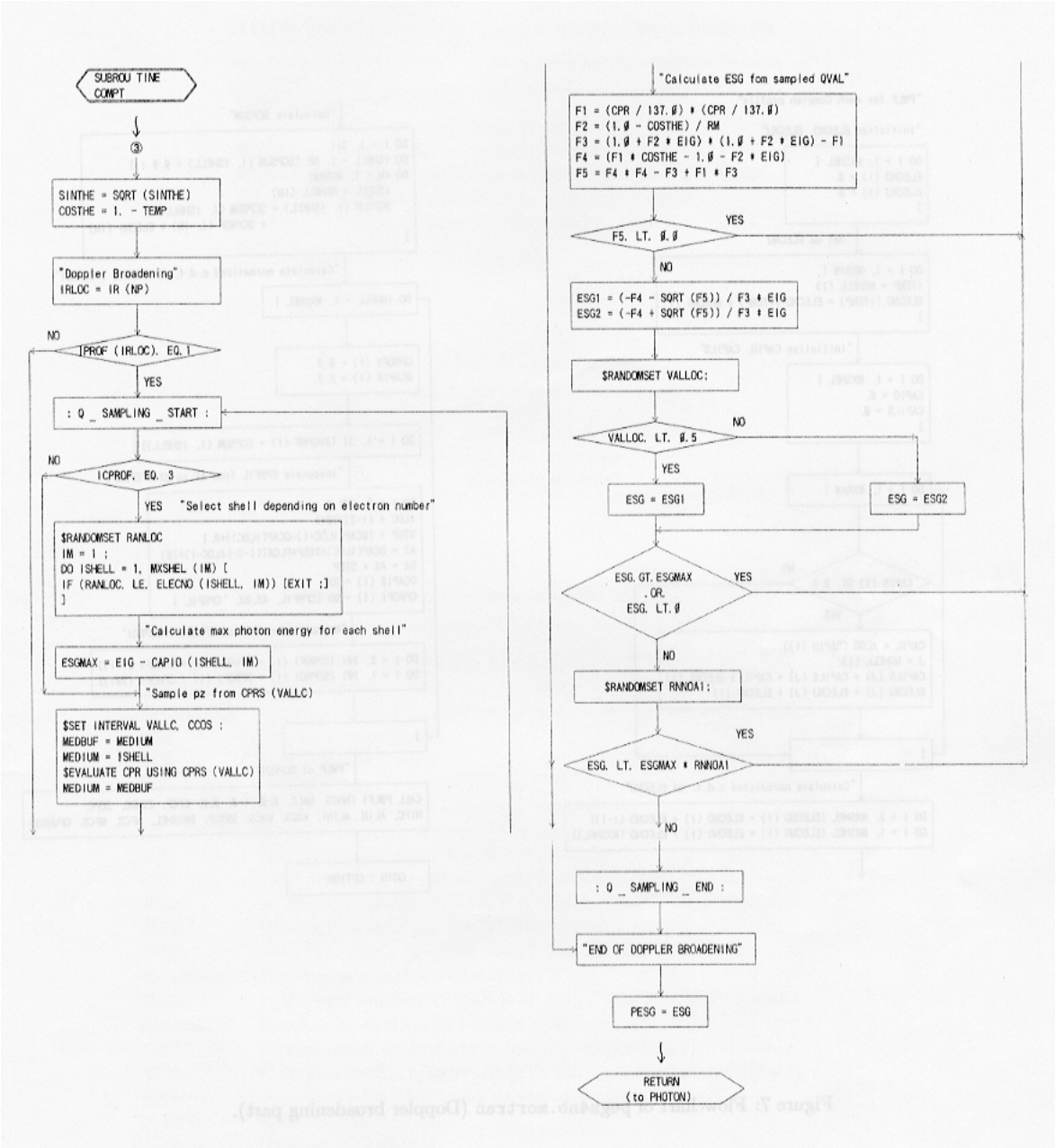

Figure 9: Flowchart of `SUBROUTINE COMPT` (Doppler broadening part).

Table 8: List of LSCAT related variables in COMMON MEDIA.

Variable	Contents
`INCOHM(J)`	Turn on/off S/Z rejection in medium J.
`IPROFM(J)`	Turn on/off Doppler broadening in medium J.
`IMPACM(J)`	Turn on/off EII in medium J.

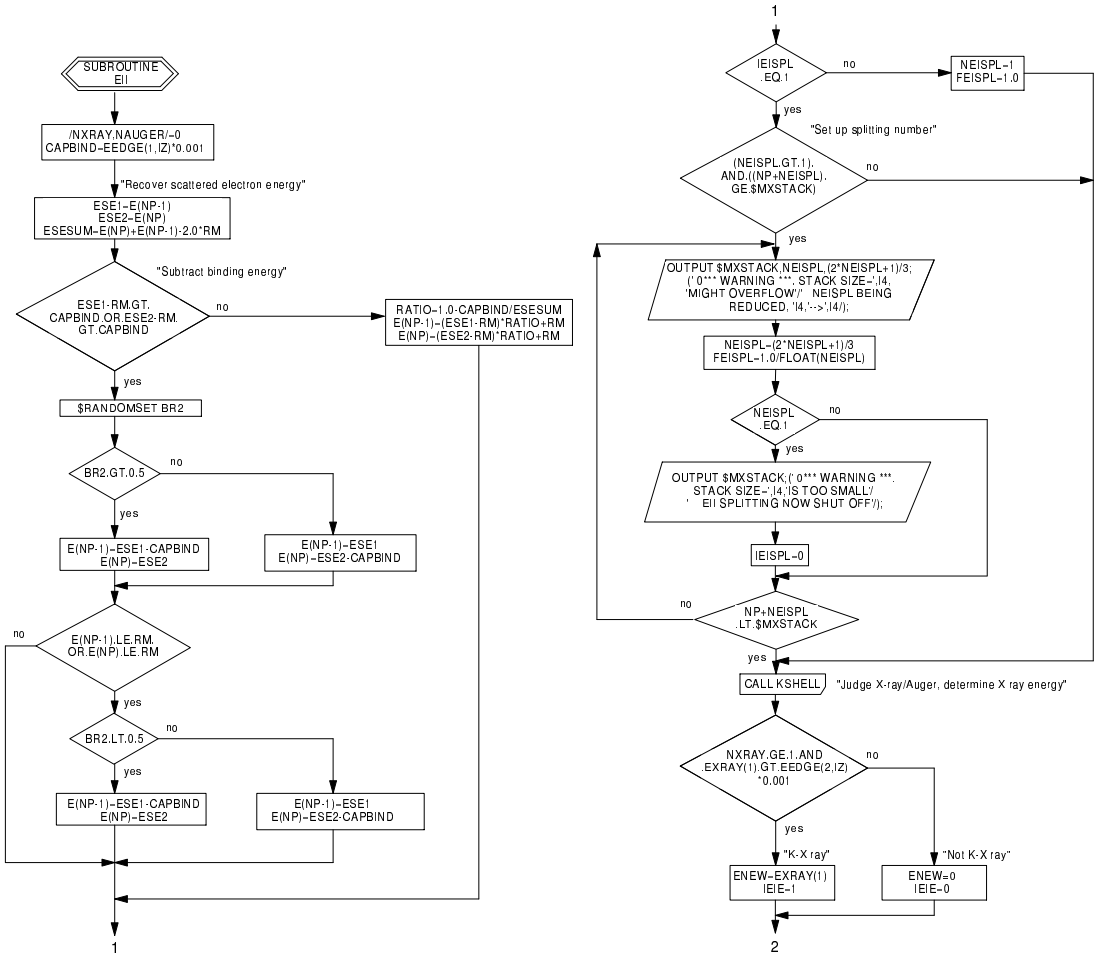

Figure 10: Flowchart of `SUBROUTINE EII`.

Table 9: List of variables in COMMON BCOMP.

Variable	Contents
`ICPROF(J)`	Compton profile is accompany in medium J in the cross section data(If $\neq 0$).
`SCO`	Bin coefficient for x.
`SXZ0,SXZ1`	PWLFed* S/Z value.
`CCO`	(Not use)
`CPIMEV`	(Not use)
`CPR0,CPR1`	(Not use)
`MXSHEL(N)`	Number of sub-shells of medium N.
`ELECNO(I)`	Number of electron in I-th sub-shell.
`CAPIO(I)`	I-th sub-shell orbit electron binding energy (MeV).
`CCOS`	Bin coefficient of p_z.
`CPRS0,CPRS1`	PWLFed* c.d.f.*2 of $J_i(p_z)$ or PWLFed* $J_i(p_z)$.

* Piece-Wise Linear Fitted. *2 Cumulative Density Function.

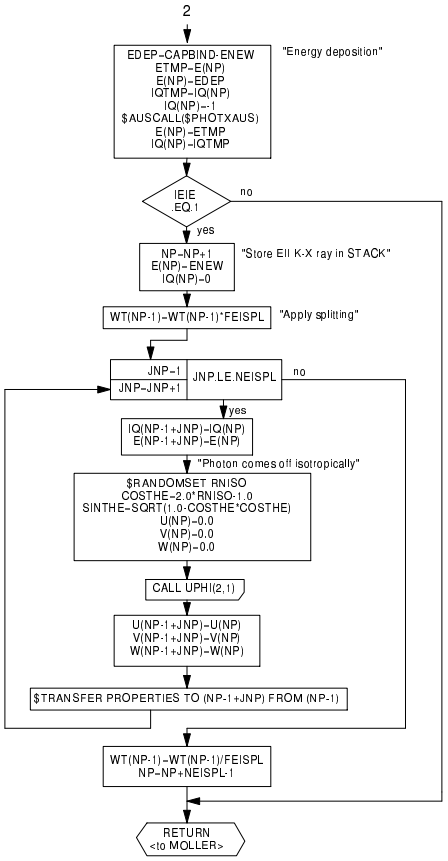

Figure 11: Flowchart of `SUBROUTINE EII` (Cont').

Table 10: List of variables in COMMON EIICOM

Variable	Contents
`IZEI`	Atomic number of an element in a material.
`EICO`	Bin coefficient of *R(E,J)*.
`EII0,EII1`	PWLFed *R(E,J)*.
`IEISPL`	Turn on/off splitting of EII K-X.
`NEISPL`	Number of splitting for EII K-X.
`FEISPL`	Inverse of `NEISPL`.

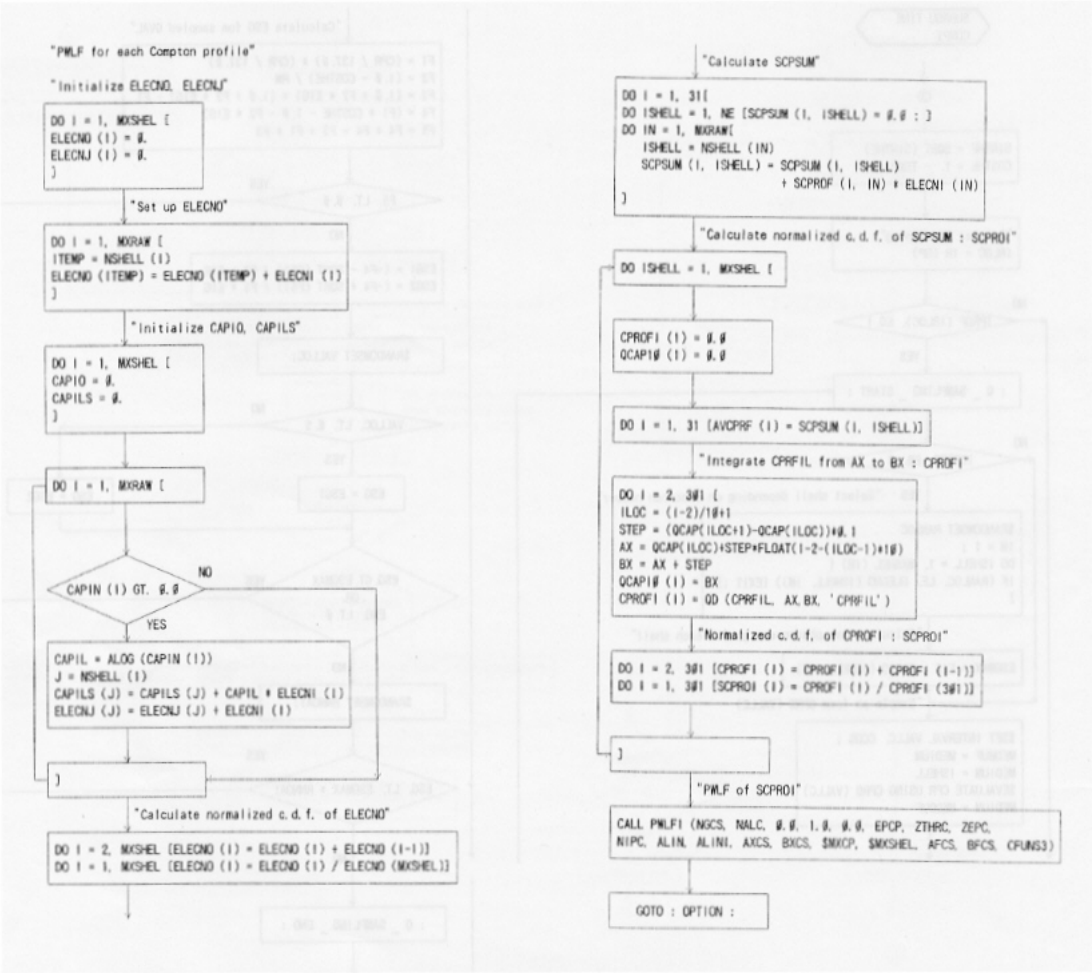

Figure 12: Flowchart of `pegs4nb.mor` (Doppler broadening part).

Table 11: List of important local variables in EGS4 subroutine of LSCAT.

notation	variable	place
p_z	CPR	COMPT
x	XVAL	COMPT
$S^{WH}(x,Z)/Z$	SXZ	COMPT
x interval number in PWLF of S/Z.	NGS	HATCH
p_z interval number in PWLF of $J(p_z)$.	NGC	HATCH
Number of intervals in PWLF of *R(E,J)*.	NEII	HATCH

Table 12: List of variables in `pegs4nb.mor` input (unit=15).

variable	contents
QCAP	Bin value of p_z.
MXRAW	Number of sub-shells in input.
MXSHEL	Number of sub-shells in output.
ELECNI	Number of electrons in each sub-shell in the input.
NSHELL	Relation of sub-shells in input and output.
CAPIN	Orbital electron binding energy in MeV.
SCPROF	Compton profile of each sub-shell.

Table 13: List of variables in COMMON SFCOM in `pegs4nb.mor`.

Variable	Contents
SCATF	S/Z value for each element. Namelist input.
SCATZ	Averaged S/Z for PWLF.
XSVAL	x bin value at S/Z input.
INCOH	Turn on S/Z output.

Table 14: List of variables in COMMON CPCOM in `pegs4nb.mor`.

Variable	Contents
`CPROF`	Input values of $J(p_z)$.
`CPROFI`	Integral of J_i in each interval.
`QCAP`	p_z bin value for $J(p_z)$ and $J_i(p_z)$ input.
`QCAP10`	10 times closer bin of QCAP. Used for integral of $J_i(p_z)$.
`SCPROF`	Namelist input of $J_i(p_z)$.
`SCPSUM`	Sum of `SCPROF` regarding i. Controlled by `NSHELL(I)`.
`SCPROI`	Normalized integral of $J_i(p_z)$.
`CAPIN`	Input `I`-th sub-shell orbit electron binding energy (MeV).
`CAPIO`	Output `I`-th sub-shell orbit electron binding energy (MeV).
`CAPILS`	logarithm of `CAPIN`. Used for calculate means of `CAPIN`.
`ELECNI(I)`	Number of electron in the `I`-th sub-shell (Input).
`ELECNJ(I)`	Number of electron in the `I`-th sub-shell. Used for mean `CAPIN`.
`ELECNO(I)`	Number of electron in the `I`-th sub-shell (Output).
`NSHELL(I)`	Subshell number (in output) for the `I`-th sub-shell electron (in input).
`CPIMEV`	Mean ionization energy (MeV). Not use as this is for IPROFR=1 only.
`ICPROF`	Doppler broadening is accompany in the cross section data (if not 0).
`MXSHEL`	Number of sub-shells in output.
`MXRAW`	Number of sub-shells in input.