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IMPLEMENTATION OF THE ELECTRON IMPACT IONIZATION INTO THE EGS4 CODE

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Abstract A modification to the general-purpose Monte-Carlo electron-photon transport code EGS4 [1] was made in order to include K-shell electron-impact ionization. Gryziński's formula of electron-impact ionization is employed for the calculation along with a relativistic correction for the formula. The ratio of electron impact ionization cross section to the Møller scattering cross section is prepared by the PEGS4 program, and is used in the EGS4 calculation. A simulation of the photon emission from a Sn target for an incident 100 keV electron was performed using the improved EGS4 code; the calculated K-X ray and bremsstrahlung photon spectra agreed well with the measurements.

1 Introduction

When an electron beam hits a target, bremsstrahlung photons and characteristic X rays are generated. The characteristic X rays are emitted after the production of vacancies in the inner shells. Two major channels exist for the production of vacancies in the inner shells i.e.:

1. A vacancy is created in a photoelectric effect by bremsstrahlung photons.
2. The incident electron scatters an inner-shell electron (electron impact ionization:EII) and creates a vacancy in the inner shell.

In the case that the electron kinetic energy is less than a few 100 keV, channel 1 is narrow since the bremsstrahlung cross section is small and the contribution of channel 2 is compatible to the former one.

The authors calculated the photon spectra from targets irradiated by electrons with an energy less than a few MeV using the EGS4 code, and obtained agreement with a measurement in the part of bremsstrahlung [2, 3]. However the EGS4 calculation and measurement differed apparently concerning the part of the characteristic X ray; also, ignorance about the electron-impact ionization in the EGS4 calculation was supposed to be the reason of the discrepancy (See Fig.1).

In this study, a modification to the EGS4 was made in order to include the electron-impact ionization. The immediate purpose of the modification is to determine the reason for the discrepancy concerning the characteristic X ray. Electron-impact ionization makes a substantial contribution in a simulation of an ordinary-type X ray generator which uses an electron beam of the energy up to a few 100 keV. A simulation of this kind of X-ray generator using EGS4 thus becomes possible.

2 Electron impact ionization cross section

Powell has reviewed measurement data and formula concerning the electron-impact ionization cross section.[4] The following authors have developed EII formulas. Gryziński

developed the EII formula from classical theory [6, 7, 8]. Gryziński's formula agrees reasonably well with a measurement in the case that a relativistic correction is applied to the formula. Without a relativistic correction, Gryziński's formula apparently differs from measurements in the case that the incident electron kinetic energy (E_K) is greater than a few hundred keV. Kolbenstvedt made a EII cross section formula for a K-shell electron by adding the contribution due to ionization by a virtual photoeffect and a contribution due to close collisions [9]. Kolbenstvedt's formula apparently differs from Gryziński's formula in the case $E_K < \sim 4$ times the binding energy of the orbit electron (E_B); the former's cross section is about 0.7-0.8 times the peak value of the the cross section; the latter's cross section approaches 0 when E_K approaches E_B . Seltzer made a numerical evaluation of the EII cross section, and obtained good agreement with measurements over a wide range of incident electron energies [10].

Deiwiks et al measured the positron and electron impact ionization cross section[5]. Deiwiks et al have indicated that the positron impact-ionization cross section is apparently smaller than the electron-impact ionization in the case that the positron kinetic energy is less than $\sim 5 \times E_B$.

The SANDYL code [11] treats the electron impact ionization using Gryziński's formula in a nonrelativistic version. The ETRAN code treats K-shell ionization by electron impact using Kolbenstvedt's cross section.[12, 13]

3 Method of calculation

Gryziński's formula for the electron-impact ionization [7, 8] is used together with a relativistic correction, because this formula agrees well with measurements, and its value near to E_B is close to Seltzer's numerical evaluation.

$$\sigma_{EII} = \frac{0.0656 N_e f_V^{(0)rel}}{E_B^2} \frac{1}{f_V^{(0)}} \frac{1}{x} \left(\frac{x-1}{x+1} \right)^{3/2} \left[1 + \frac{2}{3} \left(1 - \frac{1}{2x} \right) \ln \left\{ 2.7 + (x-1)^{1/2} \right\} \right], \quad (1)$$

$$f_V^{(0)} = f_V|_{\theta=\pi/2} = \left(\frac{v_1}{v_2} \right)^2 \left(\frac{v_2^2}{v_2^2 + v_1^2} \right) = \frac{E_K}{E_B} \left(\frac{E_K}{E_K + E_B} \right)^{3/2}, \quad (2)$$

$$f_V^{(0)rel} = \frac{\kappa_1}{\kappa_2} \frac{2 + \kappa_1}{2 + \kappa_2} \left(\frac{1 + \kappa_2}{1 + \kappa_1} \right)^2 \times \left\{ \frac{(1 + \kappa_2)^2}{(1 + \kappa_2)^2 + (\kappa_1 \kappa_2) ((2 + \kappa_1)/(2 + \kappa_2)) ((1 + \kappa_2)/(1 + \kappa_1))^2} \right\}, \quad (3)$$

$$\kappa_1 = \frac{E_B}{m_0 c^2}, \quad \kappa_2 = \frac{E_K}{m_0 c^2}, \quad x = \frac{E_K}{E_B}. \quad (4)$$

Here, σ_{EII} is the vacancy-creation cross section due to electron-impact ionization (barn/atom), N_e is the number of electrons in a shell (=2 in the case of the K shell), E_B and E_K are the binding energy of the orbit electron (MeV) and the incident-electron kinetic energy (MeV), respectively. $f_v^{(0)}$ and $f_v^{(0)rel}$ are velocity functions in the nonrelativistic and relativistic formula, respectively. $m_0 c^2$ is the electron rest mass.

After a vacancy is created in a K shell by EII, a K-X ray or Auger electron is sampled using the K-shell fluorescence yield. In the case of K-X-ray emission, K_{α_1} , K_{α_2} , K_{β_1} and K_{β_2} are sampled according to the intensity ratio. The calculation method to treat 4 kinds of K-X rays was taken from Hirayama's improvement of EGS4 [14]. Auger electron is not followed.

When a vacancy is created in the K shell by EII, K-shell binding energy is subtracted from the energy of either one of the two electrons related to the Møller scattering. This

energy subtraction is done in order to maintain energy conservation. The difference in the K-shell binding energy and K-X ray energy is deposited locally. In the case that EII occurs, and no K-X ray is generated (i.e. Auger electron emission), the K-shell binding energy is deposited locally.

In this study, only K-shell ionization by electron impact was treated; also, neither L, M and outer-shell ionization by electron impact nor any shell ionization by positron impact was treated.

4 Example of calculation result

Placious measured bremsstrahlung and the K-X ray from various targets [15, 16]. In Placious's measurement, 50 or 100 keV electrons are normally incident on the target, and those photons emitted toward 70° and 110° from the direction of the incident electron is measured. Among the various measured spectra, photons from a Sn target (target thickness, 21.6 mg/cm^2 ; incident electron kinetic energy, 100 keV) were simulated by the improved EGS4 code, since the K-X ray appears clearly in the spectra.

The EGS4 calculations were performed both with and without electron-impact ionization. The improvements of EGS4(PRESTA [17], use of ICRU-37/NBS radiative stopping powers [18] and improved angular distribution of bremsstrahlung photons [19]) were employed in all of the EGS4 calculations. As discussed in the appendix, the default EGS4 tend to underestimate the Møller scattering and bremsstrahlung in the case that the electron energy is less than about 5 MeV. Since the electron-impact ionization is calculated using the ratio of EII to the Møller scattering, an underestimation of the Møller scattering also causes an underestimation of EII. This underestimation of the bremsstrahlung and Møller scattering is corrected, as discussed in the appendix.

A comparison of the EGS4 calculation with measurements is shown in Fig. 1. The K-X ray intensity by EGS4 with EII agreed with the measurement within 10% in the spectra at both 70° and 110° , while the K-X ray intensity by EGS4 without EII was only about half of the measured intensity. The K-X rays generated in the photoelectric effect by the bremsstrahlung photons and the K-X rays generated in electron-impact ionization were of the same order. From this point, the reason for the under estimate of the K-X ray intensity in the previous EGS4 calculation [3] has been found to be an ignorance of the electron-impact ionization. Also, an EGS4 calculation with EII agreed well with ETRAN calculation (not shown), which also considers EII [16].

Appendix A. Modification of the program

The following subroutines and functions of PEGS4 were modified or added in order to implement electron-impact ionization:

- EIITM: Calculate the K-shell electron-impact ionization cross section.
- EFUNS: Calculate the ratio of the K-shell electron-impact ionization cross section (σ_{EII}) to the Møller-scattering cross section σ_M (σ_{EII}/σ_M).
- MAIN: Piecewise Linear Fit(PWLF) the ratio (σ_{EII}/σ_M) together with other electron cross sections and branching ratios.
- LAY: Output the PWLF result of the ratio (σ_{EII}/σ_M).

The following subroutines and functions of EGS4 were modified in order to implement the electron-impact ionization:

- HATCH: Read in the ratio (σ_{EII}/σ_M).
- EDGSET: Pass PHOTK to MOLLER. PHOTK is the ratio of the K-shell photoeffect cross section to the total photoeffect cross section.
- MOLLER: Sample the electron-impact ionization using the ratio (σ_{EII}/σ_M). Then, determine the K-X ray emission or the Auger-electron emission and sample the K-X ray energy.
- ELECTR: Return to SHOWER after calling of MOLLER if the particle at the top of the STACK is a photon.

In the PEGS4 and EGS4 calculation, the flag variable is used to enable EII, and a default calculation without EII is performed when the flag is turned off. In the PEGS4 calculation, IMPACT=2 enables an EII cross-section preparation; IMPACT=0 or no mention of IMPACT turns off the EII cross-section preparation. In the EGS4 user code, IMPACT(I)=1 specifies the inclusion of EII in region I, and IMPACT(I)=0 specifies the ignorance of EII in region I.

Appendix B. ESIG evaluation in USTEP loop

In a class-II simulation of charged-particle transport, Møller scattering, Bhabha scattering and bremsstrahlung production are treated as separate interactions only when the produced particle energy is beyond some threshold, on the other hand soft collisions are treated as continuous energy loss. In the EGS4 code, the interaction cross section (Σ) is defined as either (Møller scattering cross section + bremsstrahlung cross section) or (Bhabha cross section + bremsstrahlung cross section) for an electron and a positron, respectively. One problem concerning this treatment is that the interaction cross section is energy dependent, and the electron and positron energy changes continuously. EGS4 has a correction capability for this problem. This correction is effective when the interaction cross section is an increasing function of the energy, but is not effective when the interaction cross section is a decreasing function of the energy. For example, the interaction cross section of Sn has its minimum value at around 5 MeV. Thus, the interaction cross section of Sn is not adequately evaluated below 5 MeV. This causes an underestimation of both the Møller scattering and bremsstrahlung. Also, this causes an underestimation of

the electron-impact ionization, since the electron-impact ionization is sampled using the ratio of the electron-impact ionization to the Møller scattering in this study.

Two groups of the authors developed the methods to solve the underestimation of the Møller scattering and the bremsstrahlung. Ma and Nahum intensively studied the effect of this problem using their own algorithm [20]. Aarnio et al used maximum interaction cross section to determine interaction point in FLUKA [21].

In this study, following modification of the EGS4 algorithm was made to solve this problem. The number of electrons (N) which travel a distance x from the starting point without having any interaction is described by

$$\frac{dN}{dx} = -\Sigma(E(x))N. \quad (5)$$

Here, $E(x)$ is the electron energy at x and $\Sigma(E(x))$ is the electron interaction cross section for energy $E(x)$. Eq.(5) is solved as follows,

$$N(x = x_1) = N_0 \exp \left(- \int_{x_0}^{x_1} \Sigma(E(x)) dx \right) \quad (6)$$

$$\simeq N_0 \exp \left(- \sum_i \Sigma(E(x_i)) \Delta x \right) \quad (7)$$

Here, N_0 is the number of electrons at $x = x_0$. The derivation of Eq.(6) involves no approximation. Eq.(6) is rewritten as Eq.(7) in order to carry out an actual Monte-Carlo calculation. Δx corresponds to USTEP in the EGS4 code. Here, $\Sigma(E(x_i))$ is assumed to be a constant value in Δx , which this causes a minor step size dependence. The error in the Møller scattering and bremsstrahlung due to the finite step size is less than 0.2% in the energy range of this study (10 keV-100 keV) when the macro shown below is used.

The following macro is produced and used in the calculation to implement the modification described in this appendix.

```
"EVALUATE ESIG and PSIG in USTEP-loop(Before -DE)"
REPLACE {;SIG=SIG0*RHOF;};
  WITH {;SIG=RHOF*SIG0;
    IF(LELEC.LT.0)[$EVALUATE SIGB USING ESIG(ELKE);]
    ELSE[$EVALUATE SIGB USING PSIG(ELKE);]
    SIGBF=SIGB*RHOF;
  }
REPLACE {;DEMFP=AMAX1(0.,DEMFP-TVSTEP*SIG);};
  WITH {;DEMFP=AMAX1(0.,DEMFP-TVSTEP*SIGBF);
  }
REPLACE {;$RANDOMSET RFICT;}; WITH {;RFICT=0.0;};
```

In Fig.1, the difference of dashed line and dotted line indicates the effect of a correction of an underestimation of the bremsstrahlung.

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Figure 1: Spectra of the bremsstrahlung and K-X rays from a Sn target (21.6 mg/cm²). A 100 keV electron beam is normally incident on the target. Photons emitted toward (A) 70° and (B) 110° from the incident electron direction are shown, respectively. The closed circle is a measurement by Placious. The solid and dashes line show the EGS4 calculation with and without electron-impact ionization (Møller scattering and bremsstrahlung underestimation is corrected). The dotted line shows the EGS4 calculation in the condition that electron-impact ionization is not included and the Møller scattering and bremsstrahlung underestimation is not corrected. The dashed line and solid lines overlap many times.