Implementation of a General Treatment of Photoelectric-Related Phenomena for Compounds or Mixtures in EGS4 (Revised version, May 21, 2002)

H. Hirayama and Y. Namito

High Energy Accelerator Research Organization

Implementation of a
General Treatment of Photoelectric-Related Phenomena
for Compounds or Mixtures in EGS4
(Revised version, May 21, 2002)

Hideo Hirayama and Yoshihito Namito

High Energy Accelerator Research Organization
1-1 Oho, Tsukuba-shi, Ibaraki 305-0801, Japan

ABSTRACT

A general treatment of photoelectric-related phenomena for compounds or mixtures in EGS4 was modified using sub-shell photoelectric cross sections in PHOTX.

Sub-shell photoelectric cross sections for an each element were fitted to a quadratic function in a log-log plot. Thus obtained parameters were prepared as the `BLOCK DATA` in EGS4. It becomes possible to calculate branching ratios of each elements in EGS4 by this modification and ,therefore, it is not necessary to use piece-wise linear-fitted data calculated by PEGS4.

`SUBROUTINE PHOTO` became more simple and logical by this modification.

Contents

1. Introduction

We recently published the new way for a general treatment of photoelectric-related phenomena for compounds or mixtures in EGS4[1]. The energy dependent branching ratio of each sub-shell was introduced in this improvement by fitting from the data provided for limited materials[2], Ag, Pb and U.

The information that the PHOTX data base[3] includes sub-shell photoelectric cross sections for all elements was brought by Sakamoto at JAERI[4].

K-, L1-, L2-, L3 and other sub-shell photoelectric cross sections are fitted to a quadratic function in a log-log plot and prepared in the form of the `BLOCK DATA` of EGS4. It becomes possible to calculate the branching ratio of each element inside EGS4 by this improvement. It becomes not necessary to use piece-wise linear-fitted data calculated by `PEGS4` and means that the general treatment for compounds or mixtures can be applied to the material data calculated defaults `PEGS4`.

`SUBROUTINE PHOTO` becomes more simple and logical than the previous way using thus obtained sub-shell cross section data.

1.1. Energy Dependence Sub-Shell Photoelectric Effect Cross Sections

K-, L1-, L2, L3 and other photoelectric effect cross sections were fitted to a quadratic function in a log-log plot:

$$\ln(\sigma) = M_0 + M_1 \ln(k_0) + M_2 \ln(k_0)^2 + M_3 \ln(k_0)^3, \tag{1}$$

where k_0 denotes photon energy. The differences between original data and fitted results are less than 20% for element below Z=22 (Ti), 16% below Z=43 (Tc), 10% below Z=57 (La), 5% below Z=76 (Os) and 3% above Z=77 (Ir) except other cross section data for Na. As shown Fig. 1, coefficients $M_0.M_1, M_2$ and M_3 are almost smooth functions for atomic number.
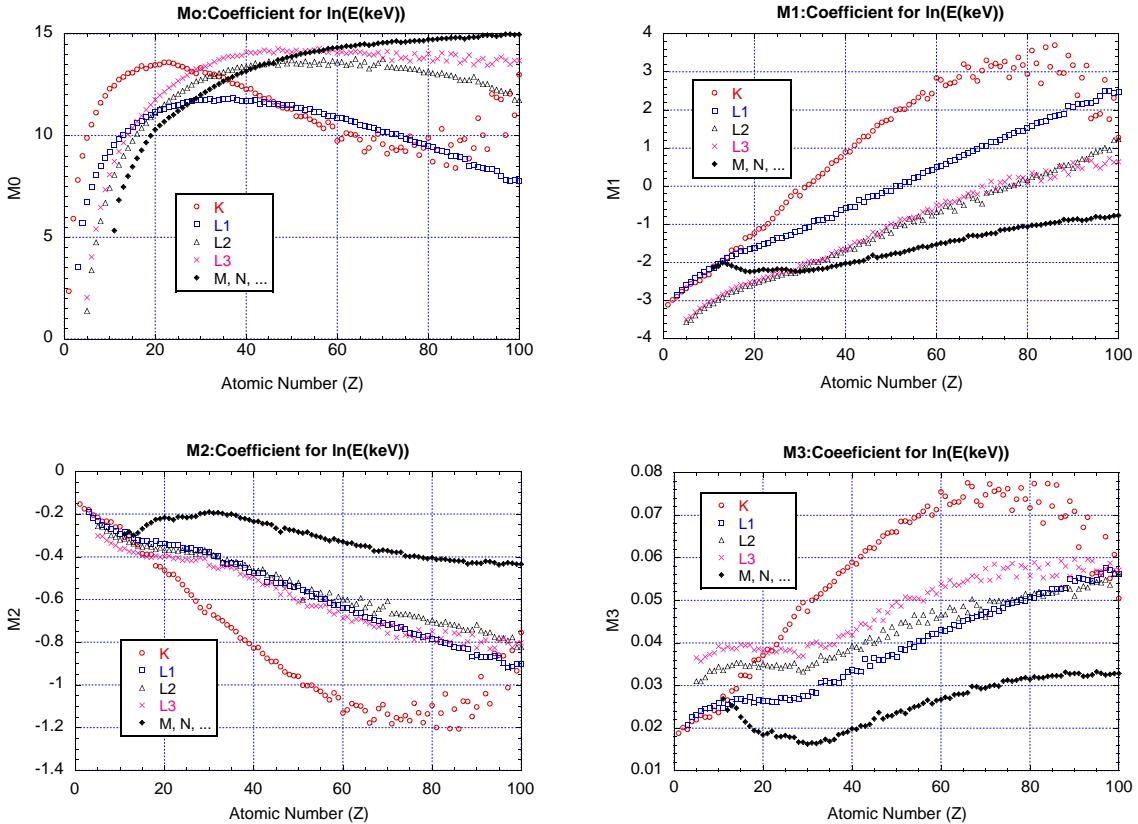
Figure 1: M_0, M_1, M_2 and M_3 coefficients.

Fig. 2 shows the comparisons between sub-shell photoelectric effect cross section data in PHOTX and in Matese and Johnson[2] for Ag, Pb and U, respectively. Both results agree well for these three elements.

The M_0, M_1, M_2 values of each sub-shell for all elements are also included in `BLOCK DATA ATOM`.
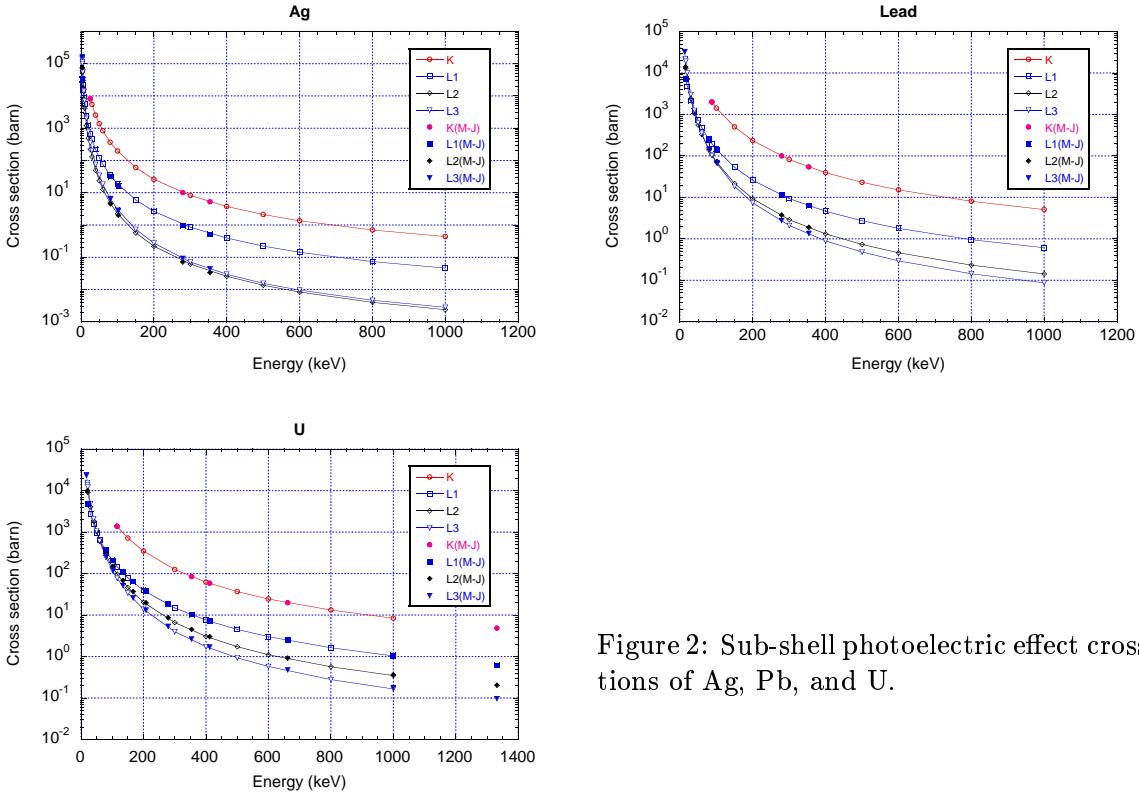
Figure 2: Sub-shell photoelectric effect cross sections of Ag, Pb, and U.

2. Modifications of PEGS4

The parts which are introduced to produce the branching ratio of each element a are deleted from `PEGS4`.

3. BLOCK DATA ATOM

Coefficients $M_0.M_1, M_2$ and M_3 are added to `BLOCK DATA ATOM` and `PHOTK`, `BKPHOT`, `RSCL1`, `RSCL2 and RSCL3` are deleted. These data become not necessary by introducing sub-shell photoelectric effect cross sections.

Table 1 Atomic data included in `BLICK DATA ATOM`.

Kind of data	Explanation
K edge energy	Table 2 of Table of Isotopes, Eighth Edition[5]
Probability of X-ray emission at K- and L-Shell absorption	Table 3 of Table of Isotopes, Eighth Edition
K X-ray energy	Table 7 Table of Isotopes, Eighth Edition
K X-ray emission probability	Table 7 Table of Isotopes, Eighth Edition Adjusted to experimental data by Salem et al.[6]
L1, L2, and L3 edge energy	Table 2 of Table of Isotopes, Eighth Edition
L X-ray energy	Table 7b of Table of Isotopes, Eighth Edition
Probability of Coster-Kronig L1- and L2-Shell absorption	Table 3 of Table of Isotopes, Eighth Edition
L X-ray emission probability	Theoretical data by J.M. Scofield[7] Adjusted to experimental data by Salem et al.
Average M edge energy	Calculated sub-shell binding energy in Table 2 of Table of Isotopes, Eighth Edition
Auger electron energy	Calculated neglecting correction term by using Atomic-Electron Binding Energy in Table 2 of Table of Isotopes, Eighth Edition
K-Auger Intensity	Z=12-17 Table 1 of Asaad[8] Z>17 Table 8 of Table of Isotopes, Eighth Edition
L-Auger Intensity	Table 2 from McGuire[9]
Coefficients M_0, M_1, M_2 and M_3	PHOTX[3]

4. Over-ride Macros (see kek4macn3.mor)

The following over-ride macros are used in EGS4.
Various names of variables are changed to reflect their meanings.

```
"THIS EXTENSION IS NEEDED FOR THE PHOTOELECTRON ANGLE SELECTION"
REPLACE {$COMIN-PHOTO;} WITH {;COMIN/BOUNDS,BREMPR,DEBUG,EDGE,
   EPCONT,MEDIA,MISC,PHOTIN,STACK,UPHIOT,USEFUL,USER,RANDOM/;}
"        ====        Added by H. Hirayama 12/29/97        "
" BREMPR Added by H. Hirayama 8/24/2000                   "
```

```
"Introduce energy dependent sub-shell photoelectric cross section"
"from PHOTX.  PHOTK, BKPHOT, RSCL1, RSCL2, RSCL3 are removed.    "
"PM0, PM1, PM2 and PM3 are defined for K, L1, L2, L2 and M,N... "
"                                         8/22/2000 H.H        "
REPLACE {;COMIN/EDGE/;} WITH
{;COMMON/EDGE/NAUGER,IEDGFL($MXREG),IAUGER($MXREG),$LGN(EKALPH,EKBETA,
OMEGAK,EMBIND,OMEGAL1,OMEGAL2,OMEGAL3,F12,F13,F23(100)),
EEDGE(4,100),EKX(10,100),DFKX(9,100),ELX1(8,100),
ELX2(5,100),ELX3(7,100),DFLX1(7,100),DFLX2(4,100),DFLX3(6,100),
PM0(5,100),PM1(5,100),PM2(5,100),PM3(5,100),
EKAUG(14,100),DFKAUG(13,100),EL1AUG(6,100),EL2AUG(6,100),
EL3AUG(6,100),DFL1AUG(5,100),DFL2AUG(5,100),DFL3AUG(5,100),
LEDGB(80,$MXMED),NGX($MXMED),UPE($MXMED),
$LGN(PHO($MXEPERMED)/0,1/),$LGN(PHOTBR($MXGE,$MXEPERMED,$MXMED)/0,1/),
EDGB(80,$MXMED),EXRAY(10),EAUGER(10),NEPM($MXEPERMED),NEDGB($MXMED),
NXRAY,NPHOTO,NAL1,NAL2,NBE1,NBE2,NBLK,NNOK,IZ,IEXTP,EBIND;}
```

5. Modification of SUBROUTINE HATCH (see kek4n3.mor)

The parts related to read IXRAY option are deleted from SUBROUTINE HATCH.

6. Modification of SUBROUTINE PHOTO (see kek4n3.mor)

The SUBROUTINE PHOTO was modified to calculate sub-shell photoelectric effect cross sections for each element included. The branching ratio of each element is calculated using these cross sections and used to determine the element that an incident photon interacts. Following statements at the top of the SUBROUTINE are used for these functions.

```
"Following statements are added by H. Hirayama to determine "
"element interact.   12/29/97                               "
IRL=IR(NP);
PEIG=E(NP);
MEDIUM=MED(IRL);

"Calculate energy dependent sub-shell ratio.      3/31/99 Y.N. & H.H."
"Revised to include K and M+N+....               8/22/2000  H.H"
PEIGK=PEIG*1000.0; "Energy of incident photon, in keV"
PHOLK=ALOG(PEIGK);  "ln(E), E in keV"
PHOLK2=PHOLK*PHOLK;
PHOLK3=PHOLK2*PHOLK;

TOTAL=0.0;
DO I=1,NNE(MEDIUM) [
IZ=ZELEM(MEDIUM,I);
IF(PEIGK.LE.EEDGE(1,IZ)) [CROSK(I)=0.0;]
ELSE [CROSK(I)=EXP(PM0(1,IZ)+PM1(1,IZ)*PHOLK+PM2(1,IZ)*PHOLK2+
      PM3(1,IZ)*PHOLK3);]
IF(PM0(2,IZ).EQ.0.0.OR.PEIGK.LE.EEDGE(2,IZ)) [CROSL1(I)=0.0;]
ELSE [CROSL1(I)=EXP(PM0(2,IZ)+PM1(2,IZ)*PHOLK+PM2(2,IZ)*PHOLK2+
```

```
        PM3(2,IZ)*PHOLK3);]
IF(PM0(3,IZ).EQ.0.0.OR.PEIGK.LE.EEDGE(3,IZ)) [CROSL2(I)=0.0;]
ELSE [CROSL2(I)=EXP(PM0(3,IZ)+PM1(3,IZ)*PHOLK+PM2(3,IZ)*PHOLK2+
        PM3(3,IZ)*PHOLK3);]
IF(PM0(4,IZ).EQ.0.0.OR.PEIGK.LE.EEDGE(4,IZ)) [CROSL3(I)=0.0;]
ELSE [CROSL3(I)=EXP(PM0(4,IZ)+PM1(4,IZ)*PHOLK+PM2(4,IZ)*PHOLK2+
        PM3(4,IZ)*PHOLK3);]
IF(PEIGK.LE.EMBIND(IZ)) ["below M-edge" TCROS(I)=0.0;]
ELSE [
  IF(PM0(5,IZ).EQ.0.0) [CROSM(I)=0.0;]
  ELSE [CROSM(I)=EXP(PM0(5,IZ)+PM1(5,IZ)*PHOLK+PM2(5,IZ)*PHOLK2+
    PM3(5,IZ)*PHOLK3);]
  TCROS(I)=CROSK(I)+CROSL1(I)+CROSL2(I)+CROSL3(I)+CROSM(I);
  BSHK(I)=CROSK(I)/TCROS(I);
  BSHL1(I)=(CROSK(I)+CROSL1(I))/TCROS(I);
  BSHL2(I)=(CROSK(I)+CROSL1(I)+CROSL2(I))/TCROS(I);
  BSHL3(I)=(TCROS(I)-CROSM(I))/TCROS(I);]
TCROS(I)=TCROS(I)*PZ(MEDIUM,I);
TOTAL=TOTAL+TCROS(I);
] "End of shell-wise photoelectric calculation"

IF(TOTAL.EQ.0.0) ["below M-edge for all elements included"
  EDEP=PEIG; $AUSCALL($PHOTXAUS);
  E(NP)=PZERO; RETURN;]

IF(NNE(MEDIUM).EQ.1) [IZ=ZELEM(MEDIUM,1); NOEL=1; GO TO :SHELL:;]

DO I=1,NNE(MEDIUM)-1 [
IF(I.EQ.1) [PBRAN(I)=TCROS(I)/TOTAL;]
ELSE [PBRAN(I)=PBRAN(I-1)+TCROS(I)/TOTAL;]

]

$RANDOMSET PBRAT;

DO I=1,NNE(MEDIUM)-1 [
IF(PBRAT.LE.PBRAN(I)) [IZ=ZELEM(MEDIUM,I);NOEL=I;GO TO :SHELL:;]
]

IZ=ZELEM(MEDIUM,NNE(MEDIUM));
NOEL=NNE(MEDIUM);
```

The sub-shell is determined using the sub-shell cross section of determined element.

```
"After this 'MEDIUM' is changed to 'IZ' to treat K , L X-rays"
"for each element.   H. Hirayama  12/29/97.                    "
:SHELL:

IF(PEIGK.LE.EEDGE(4,IZ)) ["below L3 edge and treat as "
"                                  M-absorption H. Hirayama 1/23/99."
  EBIND=EMBIND(IZ)*1.0E-3;EDEP=EBIND;
  GO TO :PHOTOELECTRON:; "below L3 edge"]


$RANDOMSET BR; "Sample to decide shell"

IF(BR.GT.BSHL3(NOEL)) ["M, N, ... absorption. Treat as M-absorption"
  EBIND=EMBIND(IZ)*1.0E-3;EDEP=EBIND;
  GO TO :PHOTOELECTRON:;]
ELSEIF(BR.LE.BSHK(NOEL)) [CALL KSHELL; "K absorption"
  "Set EBIND here for K-absorption"
  EBIND=EEDGE(1,IZ)*1.0E-3;]
ELSEIF(BR.LE.BSHL1(NOEL)) [CALL LSHELL(1); "L1 absorption" ]
ELSEIF(BR.LE.BSHL2(NOEL)) [CALL LSHELL(2); "L2 absorption" ]
ELSE [CALL LSHELL(3); "L3 absorption" ]
```

The full listings of SUBROUTINE PHOTO and other related SUBROUTINEs and the flow charts of these are given as Appendix 1 and 2, respectively.

References

[1] H. Hirayama and Y. Namito, "Implementation of a General Treatment of Photoelectric-Related Phenomena for Compounds or Mixtures in EGS4", *KEK Internal 2000-3*,(2000).

[2] J. J. Matese and W. R. Johnson, "Influence of Screening on the Atomic Photoeffect", *Phys. Rev.* **140**, A1-A7(1965).

[3] Radiation Shielding Information Center, "Photon Cross Section Data Base," *RSIC Data Package DLC-136/PHOTX*.

[4] Private communication.

[5] R. B. Firestone and V. S. Shirley edited., "Table of Isotopes, Eighth Edition", A Wiley-Interscience Publication, John Wiley & Sons, Inc. (1996).

[6] S. I. Salem, S. L. Panossian, and R. A. Krause, "Experimental K and L Relative X-Ray Emission Rates", *Atomic Data and Nuclear Data Tables* **14**, 91-109(1974).

[7] J. H. Scofield, "Relativistic Hartree-Slater Values for K and L X-Rays Emission Rates", *Atomic Data and Nuclear Data Tables* **14**, 121-137(1974).

[8] W. N. Asaad, "Intensities of the K-LL Auger Lines", *Nucl. Phys.* **44**, 399-414(1963).

[9] E. J. McGuire, "Atomic L-Shell Coster Kronig, Auger, and Radiative Rates and Fluorescence Yields for Na-Th", *Phys. Rev. A* **3**, 587-594(1971).

Appendix 1 Full listings of SUBROUTINE PHOTO and related SUBROUTINEs (including in kek_improve.tar.Z or kek_improve.exe)

```
%E
"*********************************************************************"
"                                    STANFORD LINEAR ACCELERATOR CENTER"
SUBROUTINE PHOTO;
"     Photoelectron is not produced if photon energy less than        "
"     M-binding energy.                                 15 MAY 2002/1300"
"     Introduce energy dependent sub-shell cross section from PHOTX "
"                                                       22 AUG 2000/0900"
"                         Include Auger electrons --   6 FEB 1999/1600"
"                            SUBROUTINE Version --   5 SEP 1998/1500"
"             General COMPOUND/MIXTURE VERSION -- 29 DEC 1997/1600"
"                             L-EDGE VERSION -- 16 FEB 1996/1600"
"                             K-EDGE VERSION -- 27 JUL 1988/2300"
"*********************************************************************"
"****** SPECIAL VERSION FOR TREATING K-EDGE FLUORESCENCE *********"
"*********************************************************************"
" Programmers:  W. R. Nelson and T. M. Jenkins (SLAC)                 "
"               A.F. Bielajew (NRC) photoelectric angular distn       "
"               D.W.O. Rogers (NRC) document                          "
"               H. Hirayama (KEK) Produce photoelectrons below        "
"                         K-Edge together with L-X rays               "
"                         production.                                 "
"                         Modify to treat general treatment           "
"                         for a compound or a mixture.                "
"                         Include Auger electrons.                    "
"               Y. Namito (KEK) Modify sub-shell branching ratio      "
"                         from total level width to relative          "
"                         shell contribution.                         "
"*********************************************************************"
" SUBROUTINE EDGSET is not used to prepare information related to     "
" fluorescence photons.  The various atomic data related to photo-    "
" electric effect like K and L X-ray energies, their intensities,     "
" K, L, M and N Auger electron energies etc. are prepared as the      "
" BLOCK DATA ATOM for all elements.   Details are given in KEK        "
" Internal 2000-3.    May 2000, H. Hirayama and Y. Namito.            "
" The parts to determine Auger, fluorescence photon or Coster-Kronig"
" and those to decide fluorescence photon energy or Auger electron   "
" energy are changed to SUBROUTINEs by H. Hirayama (KEK).            "
" This is a special L-edge version of an EGS4 subroutine that is      "
" based on a special K-edge version by H. Hirayama (KEK).            "
"                                                                     "
" A special K-edge version of an EGS4 subroutine is patterned         "
" after a method developed in 1978 by A. Clark (LBL) with the         "
" help of W. R. Nelson (SLAC).  It requires subroutine                "
" EDGSET (or equivalent for setting up the branching ratios and       "
" fluorescent photon energies).                                       "
"                                                                     "
" Original one treat 2 fluorescence photons. Modified by H. Hirayama"
" (KEK) to treat 4 fluorescence photons.                              "
"                                                                     "
" This version adds selection of photo-electron angle                 "
"    see 'Photoelectron angle selection in the EGS4 code system'      "
"    A.F. Bielajew and D.W.O. Rogers, NRC Report PIRS-0052,Oct 86     "
"                                                                     "
"    This requires a redefinition of $COMIN-PHOTO which is done       "
"    in NRCC4MAC(P).MOR and definition of the macro                   "
"    $SELECT-PHOTOELECTRON-DIRECTION  (NRCC4MAC(P).MOR)               "
"    To select the A.D. in any region, one must set the variable      "
"    IPHTER(IR(NP))=1 passed in COMIN/USER;                           "
"                                                                     "
"    This version uses a simple model of K- and L-shell fluorescence."
"    To sample fluorescent x-rays from the K or L-shell in a given    "
"    region the flag IEDGFL(IR(NP)) (in COMIN/EDGE) must be set non- "
"    zero for each region; the value of IEDGFL is the value of Z used"
"    for that region - the model must treat the region as a single    "
"    element for the selection of the fluorescent x-ray.  IF IEDGFL   "
"    set to negative and its absolute value to Z, photoelectrons are  "
"    produced below K edge without the fluorescent x-ray.             "
"    The routine EDGSET(NREG) must be called if IEDGFL is set at any "
"    region.  Otherwise, photoelectron below K-edge is treated as an "
"    absorption and does not followed.          "                    "
"                                                                     "
"    The relevant arrays are all zeroed at the end of EGS4BLOK so     "
"    that if the user initializes nothing, the code is the same as    "
"    the EGS4 default system - i.e. no fluorescent x-rays and no      "
```

```
"   photo-electron A.D.                                                       "
"                                                                             "
"   The output from this routine is complex.      99/2/6 H.H. revised."
"   E < L-III-BE  => EDEP = EMBIND, Average M-binding energy               "
"   E > K-BE    no K-, L-shell          with K- or L-shell                 "
"               ENEW = PEIG-EBIND+RM ENEW = PEIG-EBIND+RM, and             "
"                                     K- or L-Xray and K-, or L-Auger "
"               EDEP = EBIND          EDEP = EBIND - ENEW                   "
"               E(NP) = EDEP          E(NP) = EDEP                         "
"               EBIND is one of K-BE, L-I-, L-II-, L-III- or M-BE.  "
"         If K-alpha1,  K-alpha2 or K-alpha3 is selected for K-shell,"
"         L-shell sampling follows after determination of K X-ray.  "
"         If L-shell electron related to K-Auger-electron, L-shell   "
"         sampling follows after determination of K-Auger.           "
"   L-I < E <K-BE                                                          "
"               no L-shell              with L-shell                       "
"               ENEW = PEIG-EBIND+RM ENEW = PEIG-EBIND+RM, and             "
"                                     L-Xray or L-Auger                    "
"               EDEP = EBIND          EDEP = EBIND - ENEW                   "
"               E(NP) = EDEP          E(NP) = EDEP                         "
"               EBIND is one of L-I-, L-II-, L-III- and M-BE.              "
"   L-II < E <L-I                                                          "
"               no L-shell              with L-shell                       "
"               ENEW = PEIG-EBIND+RM ENEW = PEIG-EBIND+RM, and             "
"                                     L-II- or L-III-X-ray or Auger        "
"               EDEP = EBIND          EDEP = EBIND - ENEW                   "
"               E(NP) = EDEP          E(NP) = EDEP                         "
"               EBIND is  one of L-II-, L-III- and M-BE.                   "
"   L-III < E <L-II                                                        "
"               no L-shell              with L-shell                       "
"               ENEW = PEIG-EBIND+RM ENEW = PEIG-EBIND+RM, and             "
"                                     L-III-X-ray or Auger                 "
"               EDEP = EBIND          EDEP = EBIND - ENEW                   "
"               E(NP) = EDEP          E(NP) = EDEP                         "
"               EDIND is  L-III- or M-BE.                                  "
"   In the case of L-I and L-II, L X-ray from L-II or L-III subshell"
"   is sampled due to Coster-Kronig effect.                               "
"                                                                         "
"       THEN IARG = 4 CALL IS MADE i.e. energy discarded in middle  "
"                                                                         "
" THEN                                                                    "
" E<M-BE  E(NP) = EBIND, EBIND is M-BE. E(NP)=Initial-EBIND+RM     "
" E>M-BE  IQ(NP) = -1, E(NP) = Initial - EBIND+RM                 "
"         and if flags on for Auger electron and/or fluorescence   "
"         and sampled, then NP => NP + 1 and electrons and/or gamma"
"         is set up                                                 "
"                                                                         "
" This version is modified from the original one for an element     "
" to a compound or a mixture for a general treatments of            "
" photoelectric effect.                                             "
"                                                                         "
" An element to cause photoelectric is determined using cross       "
" section data of each shell.       8/25/2000     H.H.              "
"*****************************************************************"
$ENERGY PRECISION PEIG;
$COMIN-PHOTO; "the next line is the default replacement for this"
";COMIN/DEBUG,EDGE,EPCONT,MEDIA,PHOTIN,STACK,UPHIOT,USEFUL/;"
"but for the photo-electron angle selection, see definition in "
"NRCC4MAC(P)"
DIMENSION CROSK($MXEL),CROSL1($MXEL),CROSL2($MXEL),CROSL3($MXEL),
          CROSM($MXEL),TCROS($MXEL),BSHK($MXEL),BSHL1($MXEL),
          BSHL2($MXEL),BSHL3($MXEL),PBRAN($MXEL);
/NXRAY,NAUGER/=0.0; "Set to 0 at first"

"Following statements are added by H. Hirayama to determine "
"element interact.   12/29/97                                "
IRL=IR(NP);
PEIG=E(NP);
MEDIUM=MED(IRL);

"Calculate energy dependent sub-shell ratio.      3/31/99 Y.N. & H.H."
"Revised to include K and M+N+....                8/22/2000  H.H"
PEIGK=PEIG*1000.0;  "Energy of incident photon, in keV"
PHOLK=ALOG(PEIGK);  "ln(E), E in keV"
PHOLK2=PHOLK*PHOLK;
PHOLK3=PHOLK2*PHOLK;

TOTAL=0.0;
DO I=1,NNE(MEDIUM) [
IZ=ZELEM(MEDIUM,I);
IF(PEIGK.LE.EEDGE(1,IZ)) [CROSK(I)=0.0;]
```

```
ELSE [CROSK(I)=EXP(PM0(1,IZ)+PM1(1,IZ)*PHOLK+PM2(1,IZ)*PHOLK2+
      PM3(1,IZ)*PHOLK3);]
IF(PM0(2,IZ).EQ.0.0.OR.PEIGK.LE.EEDGE(2,IZ)) [CROSL1(I)=0.0;]
ELSE [CROSL1(I)=EXP(PM0(2,IZ)+PM1(2,IZ)*PHOLK+PM2(2,IZ)*PHOLK2+
      PM3(2,IZ)*PHOLK3);]
IF(PM0(3,IZ).EQ.0.0.OR.PEIGK.LE.EEDGE(3,IZ)) [CROSL2(I)=0.0;]
ELSE [CROSL2(I)=EXP(PM0(3,IZ)+PM1(3,IZ)*PHOLK+PM2(3,IZ)*PHOLK2+
      PM3(3,IZ)*PHOLK3);]
IF(PM0(4,IZ).EQ.0.0.OR.PEIGK.LE.EEDGE(4,IZ)) [CROSL3(I)=0.0;]
ELSE [CROSL3(I)=EXP(PM0(4,IZ)+PM1(4,IZ)*PHOLK+PM2(4,IZ)*PHOLK2+
      PM3(4,IZ)*PHOLK3);]
IF(PEIGK.LE.EMBIND(IZ)) ["below M-edge" TCROS(I)=0.0;]
ELSE [
   IF(PM0(5,IZ).EQ.0.0) [CROSM(I)=0.0;]
   ELSE [CROSM(I)=EXP(PM0(5,IZ)+PM1(5,IZ)*PHOLK+PM2(5,IZ)*PHOLK2+
     PM3(5,IZ)*PHOLK3);]
   TCROS(I)=CROSK(I)+CROSL1(I)+CROSL2(I)+CROSL3(I)+CROSM(I);
   BSHK(I)=CROSK(I)/TCROS(I);
   BSHL1(I)=(CROSK(I)+CROSL1(I))/TCROS(I);
   BSHL2(I)=(CROSK(I)+CROSL1(I)+CROSL2(I))/TCROS(I);
   BSHL3(I)=(TCROS(I)-CROSM(I))/TCROS(I);]
TCROS(I)=TCROS(I)*PZ(MEDIUM,I);
TOTAL=TOTAL+TCROS(I);
] "End of shell-wise photoelectric calculation"

IF(TOTAL.EQ.0.0) ["below M-edge for all elements included"
   EDEP=PEIG; $AUSCALL($PHOTXAUS);
   E(NP)=PZERO; RETURN;]

IF(NNE(MEDIUM).EQ.1) [IZ=ZELEM(MEDIUM,1); NOEL=1; GO TO :SHELL:;]

DO I=1,NNE(MEDIUM)-1 [
IF(I.EQ.1) [PBRAN(I)=TCROS(I)/TOTAL;]
ELSE [PBRAN(I)=PBRAN(I-1)+TCROS(I)/TOTAL;]

]

$RANDOMSET PBRAT;

DO I=1,NNE(MEDIUM)-1 [
IF(PBRAT.LE.PBRAN(I)) [IZ=ZELEM(MEDIUM,I);NOEL=I;GO TO :SHELL:;]
]

IZ=ZELEM(MEDIUM,NNE(MEDIUM));
NOEL=NNE(MEDIUM);

"After this 'MEDIUM' is changed to 'IZ' to treat K , L X-rays"
"for each element.   H. Hirayama 12/29/97.                   "
:SHELL:

IF(PEIGK.LE.EEDGE(4,IZ)) ["below L3 edge and treat as "
"                                   M-absorption H. Hirayama 1/23/99."
   EBIND=EMBIND(IZ)*1.0E-3;EDEP=EBIND;
   GO TO :PHOTOELECTRON:; "below L3 edge"]


$RANDOMSET BR; "Sample to decide shell"

IF(BR.GT.BSHL3(NOEL)) ["M, N, ... absorption. Treat as M-absorption"
   EBIND=EMBIND(IZ)*1.0E-3;EDEP=EBIND;
   GO TO :PHOTOELECTRON:;]
ELSEIF(BR.LE.BSHK(NOEL)) [CALL KSHELL; "K absorption"
   "Set EBIND here for K-absorption"
   EBIND=EEDGE(1,IZ)*1.0E-3;]
ELSEIF(BR.LE.BSHL1(NOEL)) [CALL LSHELL(1); "L1 absorption" ]
ELSEIF(BR.LE.BSHL2(NOEL)) [CALL LSHELL(2); "L2 absorption" ]
ELSE [CALL LSHELL(3); "L3 absorption" ]


IF(IEDGFL(IRL).LE.0) [NXRAY=0;]
IF(IAUGER(IRL).LE.0) [NAUGER=0;]

EDEP=EBIND;
IF(NXRAY.GE.1) [
   DO IPHOT=1,NXRAY [
     EDEP=EDEP-EXRAY(IPHOT);]]

IF(NAUGER.GE.1) [
   DO IELEC=1,NAUGER [
     EDEP=EDEP-EAUGER(IELEC);]]
```

```
"Following statement is necessary not to treat negative energy"
"photons due to numerical precision"
IF(EDEP.LT.0.0) [EDEP=0.0;]

:PHOTOELECTRON:
E(NP)=EDEP;

$AUSCALL($PHOTXAUS);


" 'SET UP PARTICLE(S) LOOP"
IQ(NP)=-1; "PHOTOELECTRON (ALWAYS SET UP)"
E(NP)=PEIG-EBIND+PRM;
$SELECT-PHOTOELECTRON-DIRECTION; "defined in NRCC4MAC(P).MOR"
IF(NAUGER.NE.0) ["Set up Auger electrons"
   DO IELEC=1,NAUGER [
      NP=NP+1; E(NP)=EAUGER(IELEC)+PRM; IQ(NP)=-1;
      "Auger electrons comes off isotropically"
      $RANDOMSET RNISO;
      COSTHE=2.0*RNISO-1.0;
      SINTHE=SQRT(1.0-COSTHE*COSTHE);
      U(NP)=0.0; V(NP)=0.0; W(NP)=1.0; "MAKES THINGS EASIER IN UPHI"
      CALL UPHI(2,1);
      $TRANSFER PROPERTIES TO (NP) FROM (NP-1);]]

IF(NXRAY.NE.0) ["Set up fluorescent photons"
   DO IPHOT=1,NXRAY [
      NP=NP+1;
      E(NP)=EXRAY(IPHOT);
      IQ(NP)=0;

      "PHOTON COMES OFF ISOTROPICALLY"
      $RANDOMSET RNISO;
      COSTHE=2.0*RNISO-1.0;
      SINTHE=SQRT(1.0-COSTHE*COSTHE);
      U(NP)=0.0; V(NP)=0.0; W(NP)=1.0; "MAKES THINGS EASIER IN UPHI"
      CALL UPHI(2,1);
      $TRANSFER PROPERTIES TO (NP) FROM (NP-1);]]
"END OF 'SET UP PARTICLE(S)' LOOP"

RETURN;
"END OF SUBROUTINE PHOTO" END;

%E
```

```
          ╔═══════════════╗
          ║  SUBROUTINE   ║
          ║     PHOTO     ║
          ╚═══════════════╝
                 │
                 ▼
    ┌──────────────────────────┐
    │ /NXRAY,NAUGER/=0          │
    │ IRL=IR(NP)                │
    │ PEIG=E(NP)                │
    │ MEDIUM=MED(IRL)           │
    │ PEIGK=PEIG*1000.0         │
    │ PHOLK=ALOG(PEIGK)         │
    │ PHOLK2=PHOLK*PHOLK        │
    │ PHOLK3=PHOLK2*PHOLK       │
    │ TOTAL=0.0                 │
    └──────────────────────────┘
                 │
                 ▼
        ┌─────┬──────────────┐
        │ I=1 │ I>NNE(MEDIUM)│ ────── yes ──────────────────────────────►  3
        │I=I+1│              │
        └─────┴──────────────┘
                 │
                 ▼
    ┌──────────────────────┐
    │ IZ=ZELEM(MEDIUM,I)   │
    └──────────────────────┘
                 │
                 ▼
           ╱ PEIGK ╲
          ╱  .LE.   ╲ ── yes ──►  ┌──────────────┐
          ╲EEDGE(1,IZ)╱           │ CROSK(I)=0.0 │
           ╲        ╱              └──────────────┘
             │ no
             ▼
    ┌────────────────────────────────────┐
    │ CROSK(I)=EXP(PM0(1,IZ)+PM1(1,IZ)*PHOLK+│
    │    PM2(1,IZ)*PHOLK2+PM3(1,IZ)*PHOLK3)  │
    └────────────────────────────────────┘
                 │
                 ▼
          ╱ PM0(2,IZ) ╲ ─ yes ─►  ╱ PEIGK ╲
          ╲  .EQ.    ╱            ╱  .LE.   ╲ ── yes ──► ┌───────────────┐
          ╲  0.0    ╱            ╲EEDGE(2,IZ)╱           │ CROSL1(I)=0.0 │
             │ no                   │ no                 └───────────────┘
             ▼                      ▼
    ┌────────────────────────────────────┐
    │ CROSL1(I)=EXP(PM0(2,IZ)+PM1(2,IZ)*PHOLK+│
    │    PM2(2,IZ)*PHOLK2+PM3(2,IZ)*PHOLK3)   │
    └────────────────────────────────────┘
                 │
                 ▼
          ╱ PM0(3,IZ) ╲ ─ yes ─►  ╱ PEIGK ╲
          ╲  .EQ.    ╱            ╱  .LE.   ╲ ── yes ──► ┌───────────────┐
          ╲  0.0    ╱            ╲EEDGE(3,IZ)╱           │ CROSL2(I)=0.0 │
             │ no                   │ no                 └───────────────┘
             ▼                      ▼
    ┌────────────────────────────────────┐
    │ CROSL2(I)=EXP(PM0(3,IZ)+PM1(3,IZ)*PHOLK+│
    │    PM2(3,IZ)*PHOLK2+PM3(3,IZ)*PHOLK3)   │
    └────────────────────────────────────┘
                 │
                 ▼
  1              2                                                         3
```

Appendix 2–1

1   2   3

```
PM0(4,IZ)
.EQ.
0.0
```
yes →
```
PEIGK
.LE.
EEDGE(4,IZ)
```
yes → CROSL3(I)=0.0

no

PEIGK .LE. EEDGE(4,IZ) → no

CROSL3(I)=EXP(PM0(4,IZ)+PM1(4,IZ)*PHOLK+
PM2(4,IZ)*PHOLK2+PM3(4,IZ)*PHOLK3)

```
PEIGK
.LE.
EMBIND(IZ)
```
yes →
```
PM0(5,IZ)
.LE.
0.0
```
yes → CROSM(I)=0.0

TCROS(I)=0.0

no   no

CROSM(I)=EXP(PM0(5,IZ)+PM1(5,IZ)*PHOLK+
PM2(5,IZ)*PHOLK2+PM3(5,IZ)*PHOLK3)

TCROS(I)=CROSK(I)+CROSL1(I)+CROSL2(I)+CROSL3(I)+CROSM(I)
BSHK(I)=CROSK(I)/TCROS(I)
BSHL1(I)=(CROSK(I)+CROSL1(I))/TCROS(I)
BSHL2(I)=(CROSK(I)+CROSL1(I)+CROSL2(I))/TCROS(I)
BSHL3(I)=(TCROS(I)-CROSM(I))/TCROS(I)

TCROS(I)=TCROS(I)*PZ(MEDIUM,I)
TOTAL=TOTAL+TCROS(I)

```
TOTAL
.EQ.
0.0
```
"below M-edge"
yes → EDEP=PEIG → $AUSCALL($PHOTXAUS) → E(NP)=PZERO

no

```
NNE(MEDIUM)
.EQ.
1
```
"element"
yes → IZ=ZELEM(MEDIUM,1)
NOEL=1

no   "compound
or
mixture"

I=1
I=I+1   I>NNE(MEDIUM)-1 → yes

no

```
I
.EQ.
1
```
yes → PBRAN(I)=TCROS(I)/TOTAL

no

PBRAN(I)=PBRAN(I-1)+TCROS(I)/TOTAL

4   5   6

Appendix 2–2

4 **5** **6**

$RANDONSET PBRAT

I=1
I=I+1
I>NNE(MEDIUM)-1 → yes

no

PBRAT .LE. PBRAN(I) → no

yes → IZ=ZELEM(MEDIUM,I)
NOEL=I

IZ=ZELEME(MEDIUM,NNE(MEDIUM))
NOEL=NNE(MEDIUM)

:SHELL:

$RANDOMSET BR

BR .GT. BSHL3(NOEL) — "M, N ..-absoption" yes → EBIND=EMBIND(IZ)*1.0E-3
EDEP=EBIND

no "K or L photoelectric"

BR .LT. BSHK (NOEL) — "K photoelectric" yes → CALL KSHELL

no

BR .LT. BSHL1(NOEL) — "L1 photoelectric" yes → CALL LSHELL(1)

no

BR .LT. BSHL2 (NOEL) — "L2 photoelectric" yes → CALL LSHELL(2)

no "L3 photoelectric"

CALL LSHELL(3)

IEDGFL(IRL) .LE. 0 — yes → NXRAY=0

no

IAUGER(IRL) .LE. 0 — yes → NAUGER=0

no

7 **8** **9**

Appendix 2–3

7 **8** **9**

EDEP=EBIND

NXRAY .GE. 1 — no →

yes

IPHOT=1
IPHOT=IPHOT+1 | IPHOT>NXRAY — yes →

no

EDEP=EDEP-EXRAY(IPHOT)

NAUGER .GE. 1 — no →

yes

IELEC=1
IELEC=IELEC+1 | IELEC>NAUGER — yes →

no

EDEP=EDEP-EAUGER(IELEC)

EDEP .LT. 0.0 — yes → EDEP=0.0

no

:PHOTOELECTRON:

E(NP)=EDEP

$AUSCALL($PHOTXAUS)

IQ(NP)=-1
E(NP)=PEIG-EBIND+PRM

$SELECT-PHOTOELECTRON-DIRECTION

NAUGER .NE. 0 — no →

yes

10 **11** **12**

Appendix 2–4

10　　　　　　　　　　　　　　　　　　　　　**11**　　**12**

↓ **yes**

| IELEC=1 |
| IELEC=IELEC+1 |　| IELEC>NAUGER |

　　　　　　　　　　　　　　　　yes →

no ↓

NP=NP+1
E(NP)=EAUGER(IELEC)+PRM
IQ(NP)=-1

$RANDOMSET RNISO

COSTHE=2.0*RNISO-1.0
SINTHE=SQRT(1.0-COSTHE*COSTHE)
U(NP)=0.0
V(NP)=0.0
W(NP)=1.0

CALL
UPHI(2,1)

$TRANSFER PROPERTIES TO (NP) FROM (NP-1)

```
       NXRAY
       .NE.          no  →
        0
```

↓ **yes**

| IPHOT=1 |
| IPHOT=IPHOT+1 |　| IPHOT>NXRAY |

　　　　　　　　　　　　　　yes →

no ↓

NP=NP+1
E(NP)=EXRAY(IPHOT)
IQ(NP)=0

$RANDOMSET RNISO

COSTHE=2.0*RNISO-1.0
SINTHE=SQRT(1.0-COSTHE*COSTHE)
U(NP)=0.0
V(NP)=0.0
W(NP)=1.0

CALL
UPHI(2,1)

$TRANSFER PROPERTIES TO (NP) FROM (NP-1)

RETURN TO
PHOTON

Appendix 2–5