SLAC-PUB-7620
20 August 1997

EGS4 CALCULATIONS FOR A Cd-Zn-Te DETECTOR TO MEASURE SYNCHROTRON RADIATION AT PEP-II[⋆†]

W. R. Nelson

Stanford Linear Accelerator Center
Stanford University, Stanford, CA 94309

T. Borak, R. Malchow and W. Toki

Colorado State University
Fort Collins, CO 80523

J. Kadyk

Lawrence Berkeley Laboratory
Berkeley, CA 94720

ABSTRACT

Calculations have been performed with the EGS4 Code System for a CdZnTe semiconductor detector to be used in background studies of synchrotron radiation at PEP-II. The simulations take into account K-shell fluorescent-photon production in a CdZnTe mixture, electron-hole pair collection and electronic-noise broadening. The results are compared with measurements made with encapsulated ^{241}Am, ^{133}Ba and ^{109}Cd sources.

⋆ Submitted for presentation at the First International Workshop on EGS4 to be held at KEK, Tsukuba, Japan (26-29 August 1997).

† Work supported in part by the Department of Energy contract DE-AC03-76SF00515

1. Introduction

A well-collimated X-ray detector, with a CdZnTe semiconductor sensitive element, will be used for the study of synchrotron radiation backgrounds at PEP-II.‡ The EGS4 Code System[1] has been used in the design and characterization of the detector. Future EGS4 calculations using synchrotron-radiation spectra are expected to provide information concerning its response in the PEP-II radiation environment. In this paper we compare CZT calculations with measurements made using encapsulated ^{241}Am, ^{133}Ba and ^{109}Cd sources.

EGS4 is a Monte Carlo code that simulates the transport of electrons, positrons and photons in any element, compound or mixture. The following processes now come standard with EGS4: photoelectric effect (with angular sampling from the Sauter formula), coherent (Rayleigh) and Compton scattering (unbound), discrete Møller and Bhabha interactions, positron annihilation (in-flight and at-rest), continuous energy loss, Molière multiple scattering applied to charged-particle tracks and pair production/bremsstrahlung (with angular sampling). In addition to these processes, the simulations presented in this paper specifically take into account

- production of K-shell fluorescence from a CZT mixture, using an improvement to a method developed for EGS4 by Del Guerra *et al*[2],
- collection of electron-hole pairs (the signal) using the Hecht equation[3],
- broadening of the signal due to electronic-noise.

The CZT crystal that we are using is 3×3 mm^2 with a thickness of 2 mm. It is mounted inside a BNC-type connector with a 0.25-mm Be window on its face. For convenience, and without too much loss in generality, our EGS4 User Code (`ucczt3.mortran`) utilizes a standard cylinder-slab geometry package, with the cylindrical radius of the CZT crystal chosen to be 1.7-mm to provide an equivalent cross-sectional area of 9-mm^2.

2. Details of the EGS4 Simulation

2.1 Detector Material and Energy Cutoffs

The CZT material data was created with the `MIXT` option of PEGS4 using a density of 5.78 g/cm^3 and `RHOZ` values of 50.58, 3.27 and 63.80 for Cd, Zn and Te, respectively (corresponding to atomic percentages of 45, 5 and 50%). The PEGS4 energy limits were chosen to be `(AP=0.001,UP=10.0) and (AE=0.521,UE=10.511)` MeV for photons and electrons, respectively. Also, the Rayleigh scattering option was turned on (`IRAYL=1`) and the switch to make radiative stopping powers compliant with ICRU-37 was invoked (`IAPRIM=1`).

‡ Throughout the paper we will simply refer to this as the CZT detector.

In order to save computer time during the EGS4 runs the electron cutoff energy, `ECUT`, was set at 1.0 MeV (total energy), forcing the kinetic energy of the electrons to be deposited at their points of creation. The rationalization for doing this is based on the fact that the CSDA range of an electron having a kinetic energy of 100 keV is about 0.05 mm in CZT, which is much smaller than the dimensions of the CZT crystal. In any case, a check was made with `ECUT=AE=0.521` MeV (*i.e.*, 10 keV kinetic energy) and the results were essentially the same as with `ECUT=1.0` MeV. Since we did not transport electrons in these calculations, it was also not necessary to implement PRESTA[4].

2.2 Cylinder-Slab Geometry

As mentioned in the introduction `ucczt3.mortran` uses a standard cylinder-slab geometry package, with the cylindrical radius of the CZT crystal chosen to be 1.7-mm, as shown in Figure 1a.

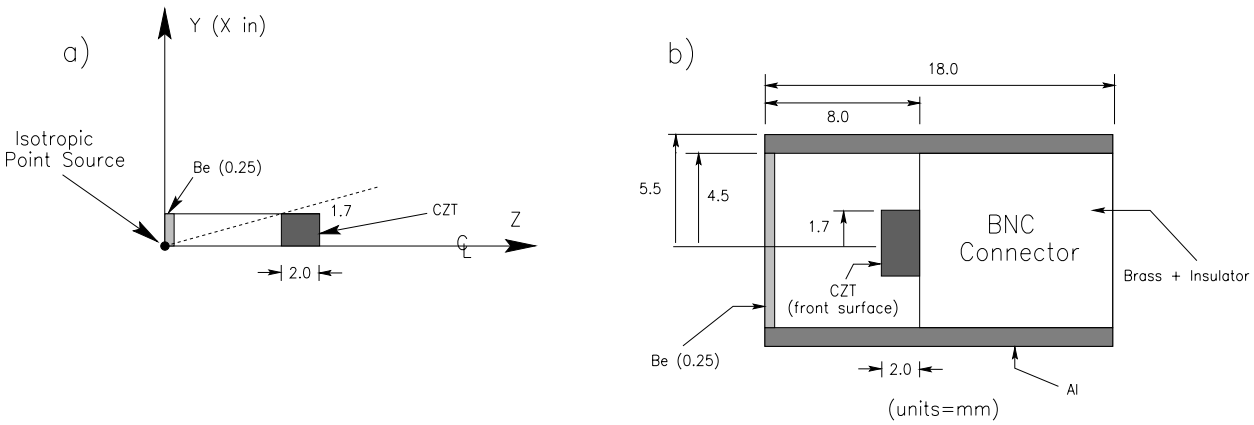

Fig. 1 a) Cylinder–slab geometry used in EGS4 simulations.
b) Sketch of detector (i.e., CZT mounted on a BNC connector).

The actual geometry of the "detector"—*i.e.*, a CZT crystal mounted inside a BNC connector—is slightly more complicated (see Figure 1b) and will be described in more detail in the measurements section of this paper. A radioactive source is also depicted in Figure 1a emitting particles isotropically. However, for efficiency reasons we only sampled isotropically within the angle subtended by the CZT crystal, indicated by the dotted line in Figure 1a.

2.3 Sampling K-shell Fluorescence in a CZT Mixture

The capability of producing K-shell fluorescent photons is a standard feature in EGS4, but in the default version of the code it is only applicable to regions in the geometry that are defined as pure elements. To overcome this limitation for this CZT mixture we employed a special sampling technique[2], that is described as follows.

In addition to the CZT-material data described above, data is also created for the Cd, Zn and Te elements themselves, and they are assigned to *"fictitious"* regions—*i.e.*, regions that are not actually part of the problem geometry. EGS4 is then instructed to make additional calls to the `AUSGAB` scoring routine before (`IARG=19`) and after (`IARG=20`) each photoelectric interaction*. Upon recognition in `AUSGAB` that a PE interaction is about to take place in a region defined as a CZT mixture, a temporary variable, `MedSav`, is set equal to the current medium of that region, `MEDIUM`, which frees up the latter so that it can be temporarily assigned to one of the fictitious regions. A random number is then drawn and, by means of the mean-free-path and branching-ratio data now made available in these fictitious regions for Cd, Zn or Te, the appropriate element is chosen.

To be more specific, the EGS4 variable, `MEDIUM`, is assigned to the appropriate fictitious region and a `RETURN` is made from `AUSGAB` to the calling routine (`SUBROUTINE PHOTON`) so that a fluorescent photon can be added (or not) to the stack of particles that will ultimately be transported by EGS4. Once this has been established, a subsequent call is again made to `AUSGAB` to set `MEDIUM` back to its its original value for the current (CZT) region. A partial listing is given in Appendix 1 for the `AUSGAB` code used in `ucczt3.mortran`.

2.4 Radioactive-Source Sampling

The input gamma and X-ray energies, and their corresponding intensities, were taken from ICRP Publication 38[5] for each of the three sources: ^{241}Am, ^{133}Ba and ^{109}Cd. Energy sampling was done by means of a simple cumulative distribution table. As an example, the 14 incident energies for ^{133}Ba (9 gamma-ray and 5 X-ray) are shown in Figure 2 (bold face and underlined). Also shown are the various escape peaks related to fluorescent X-rays produced in the CZT. However, the spectra are more complicated than the labels indicate. To illustrate, the peak labeled 53.150 in Figure 2 is actually composed of:

1. ΔE =53.150 keV — full energy absorption following PE interactions in Cd, Zn or Te of incident 53.150 keV gamma-rays,
2. ΔE =52.242 and 53.622 keV — PE interactions in Te by 79.620 and 81.000 keV incident gamma rays, respectively, followed by escape of 27.378 keV K_α X-rays,
3. ΔE =53.454 and 54.834 keV — PE interactions in Cd by 79.620 and 81.000 keV incident gamma rays, respectively, followed by escape of 26.166 keV K_β X-rays.

$\star$ Note: This is invoked by setting `IAUSFL(20)=1` and `IAUSFL(21)=1`, respectively, in the MAIN code.

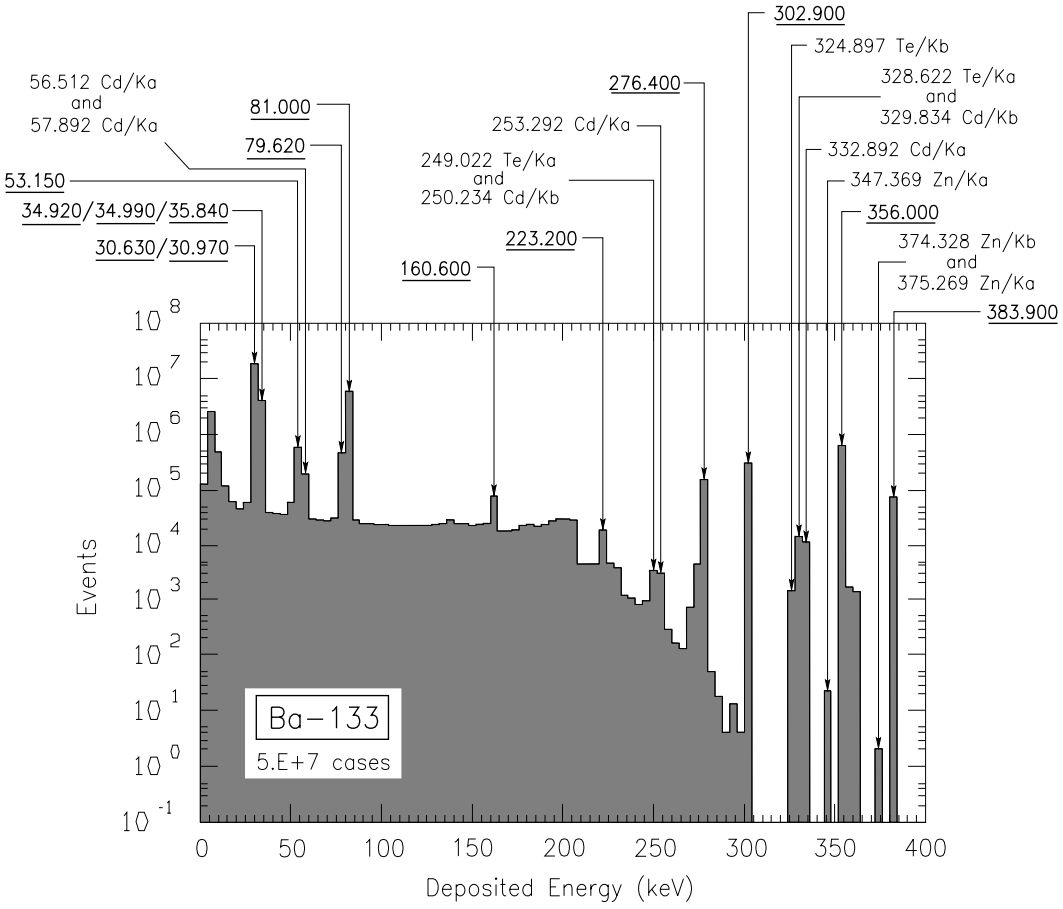

Fig.2 Energy deposited in CZT crystal for Ba−133 source.

2.5 Scoring of Electron-Hole Pair Collection

Electron-hole pairs are created whenever energy is deposited in a semiconductor. The output pulse is proportional to the charge that is collected which, in turn, is controlled primarily by the mobility-lifetime products, $\mu_e\tau_e$ and $\mu_h\tau_h$, for electrons and holes, respectively. The charge-collection efficiency is defined as the ratio of the number of charge carriers induced at the contacts to the total number of carriers generated by the photon interaction. If the effect of detrapping is neglected, the charge-collection efficiency in a crystal of thickness d can be determined by means of the Hecht equation[3]

$$\eta(z) = \frac{\lambda_e}{d}\left[1 - e^{-(d-z)/\lambda_e}\right] + \frac{\lambda_h}{d}\left[1 - e^{-z/\lambda_h}\right],$$

where $\lambda_e = \mu_e\tau_e E$ and $\lambda_h = \mu_h\tau_h E$ are the mean free paths for electrons and holes, respectively, z is the depth into the crystal from the negatively biased (V) front surface and

E is the electric field strength (V/d) in the detector. In Table 1 we give the values for the parameters that we have used in the calculations.

Table 1

Detector thickness, d	2 mm
Detector radius, r (effective)	1.7 mm
Detector density, ρ	5.78 g/cm^3
Electron-hole creation energy, w	5.0 eV
Mobility-lifetime (electrons), $\mu_e\tau_e$	7.0×10^{-3} cm^2/V
Mobility-lifetime (holes), $\mu_h\tau_h$	7.0×10^{-6} cm^2/V
Biasing potential, V	200 V
Fano factor, f	0.2
Electronic noise (broadening), σ_{enc}	150 e-h

2.6 Electronic-Noise Broadening

We have taken a relatively simple approach in order to arrive at detector response distributions that can be *visually* compared with our experimental results; that is, to account for such things as the Fano factor and to include broadening due to electronic noise, *etc.*[6] Namely, for each incident photon, we keep a running sum of the total number of electron-hole pairs that are created at the `EDEP` sites in the detector, each contribution multiplied by a charge-collection efficiency determined by the Hecht equation. To be more specific, we first determine

$$\begin{aligned} N &= \text{charge collected (unstraggled)} \\ &= \frac{1}{w} \sum \eta(z) E_{dep}(z) \ , \end{aligned}$$

where $\eta(z)E_{dep}(z)$ is the energy deposited at depth z from the front surface of the crystal and w is the average energy necessary to create an e-h pair in CZT. The total standard deviation is then determined from

$$\sigma = \sqrt{fN + \sigma_{enc}^2} \ ,$$

where f is the Fano factor for CZT and σ_{enc} is a standard deviation to account for the *equivalent noise charge* of the electronics[6]. At the present time we are using values for w, f and σ_{enc} similar to those reported by Bencivelli *et al.*[7] for Cd-Te (see Table 1).

Finally, the straggled (broadened) charge that is collected, N_s, is statistically determined by sampling from a Gaussian, centered about N with σ, and the corresponding energy, $E_s = wN_s$, is histogrammed for each incident photon event for comparison with experiment.

3. Description of Measurements

Measurements were taken with a CZT detector: $3 \times 3 \times 2$ mm^3 wafer of CZT crystal mounted directly on the center conductor of a BNC connector*. X-ray photographs were taken to verify the dimensions of the detector and Figure 1b is a sketch showing the important components.. An Al cylinder of 4.5-mm inner radius and 1-mm thickness surrounds the crystal. A 0.25-mm Be window, located 6-mm from the front face of the CZT crystal, serves as an end-cap for this cylinder.

The BNC-CZT unit was attached to a matching connector on an inverting low-noise, charge-sensitive preamplifier†. This direct connection reduces noise and resulted in a package that was approximately $2 \times 8 \times 10$ cm^3. A bias voltage of +200 V was supplied to the detector through the preamplifier, with the front surface of the crystal (see Figure 1b) negatively biased in order to maximize the collection of holes. Output pulses were processed with a pulse-shaping amplifier‡ having a 0.5 μsec shaping time and sent to a PC-based multi-channel analyzer§.

Random noise at room temperature from the detector assembly, including the shaping amplifier, was equivalent to approximately 200 mV. This corresponded to a detection threshold of approximately 6.5 keV.

The radiation sources were sealed in plastic discs, 25 mm in diameter and 2 to 5 mm thick. Analysis of the data using the 59.5 keV gamma-ray from ^{241}Am provided a yield of 55% in the total absorption peak for photons incident upon the surface of the CZT. The remaining photons produced signals that were registered at lower energies or were not detected. The manufacturer quoted a detection efficiency of $\sim$95% at 59.5 keV.

$\star$ eV Products, Model eV-180-3-3-2-S (375 Saxon Blvd., Saxonburg, PA 16056, USA).
$\dagger$ eV Products, Model eV-550.
$\ddagger$ Tennelec, Model 241 (601 Turnpike Ave., Oak Ridge, TN 37830, USA).
$\S$ The Nucleus Inc., Model PCA II (761 Emory Valley Rd., Oak Ridge, TN 37831, USA).

4. Calculations versus Experiment

Figure 3 compares the EGS4 simulation with experiment for the case of ^{241}Am. All of the photo and escape peaks appear at the correct energies, but the peak widths are not in perfect agreement with experiment. Also, an additional peak shows up at about 50 keV in the measurement data, but not in the simulation. We speculate that these are from Compton scattered photons from the plastic encapsulation of the source. It is difficult to make a comparison below 10 keV because of electronic noise.

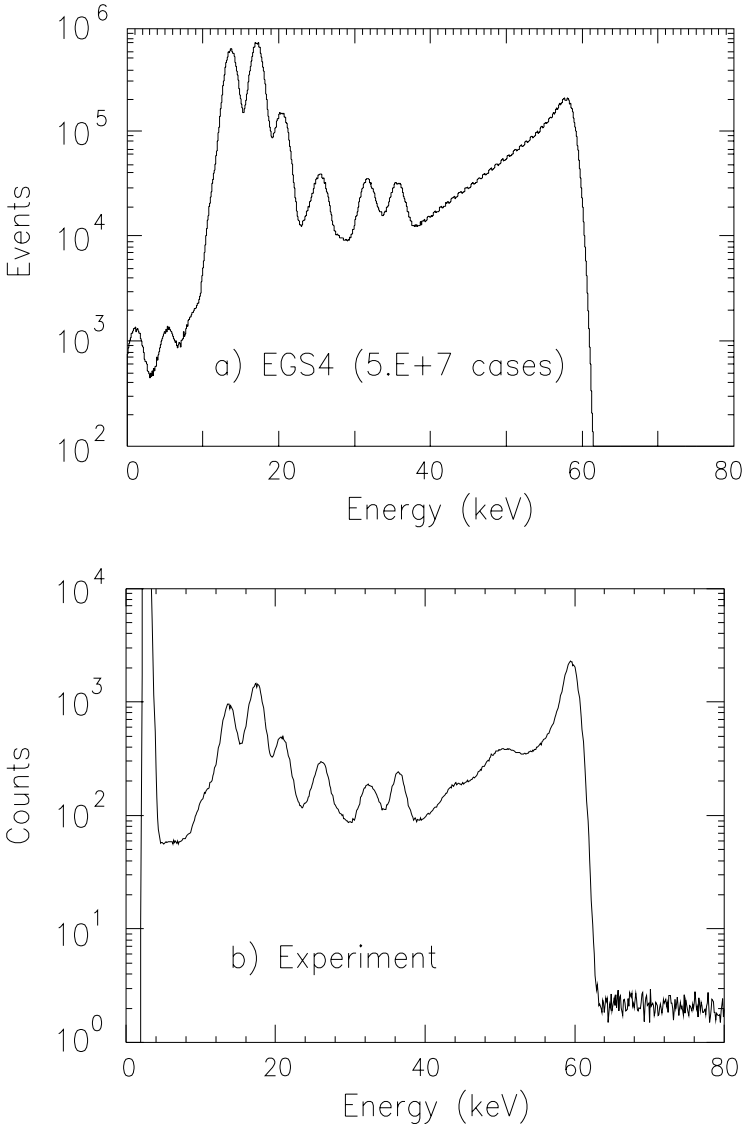

Fig. 3 Am−241 a) simulation, b) experiment.

Figure 4 compares the EGS4 simulation with experiment for the case of ^{133}Ba (only the peaks below 100 keV are of interest). Again, the peaks appear at the expected energies. For example, the peak between 52 and 55 keV is explained in Section 2.4. Also, the peak widths are in better agreement with experiment than for ^{241}Am. However, an unexpected peak appears at about 22 keV in the measurement data and not in the simulation.

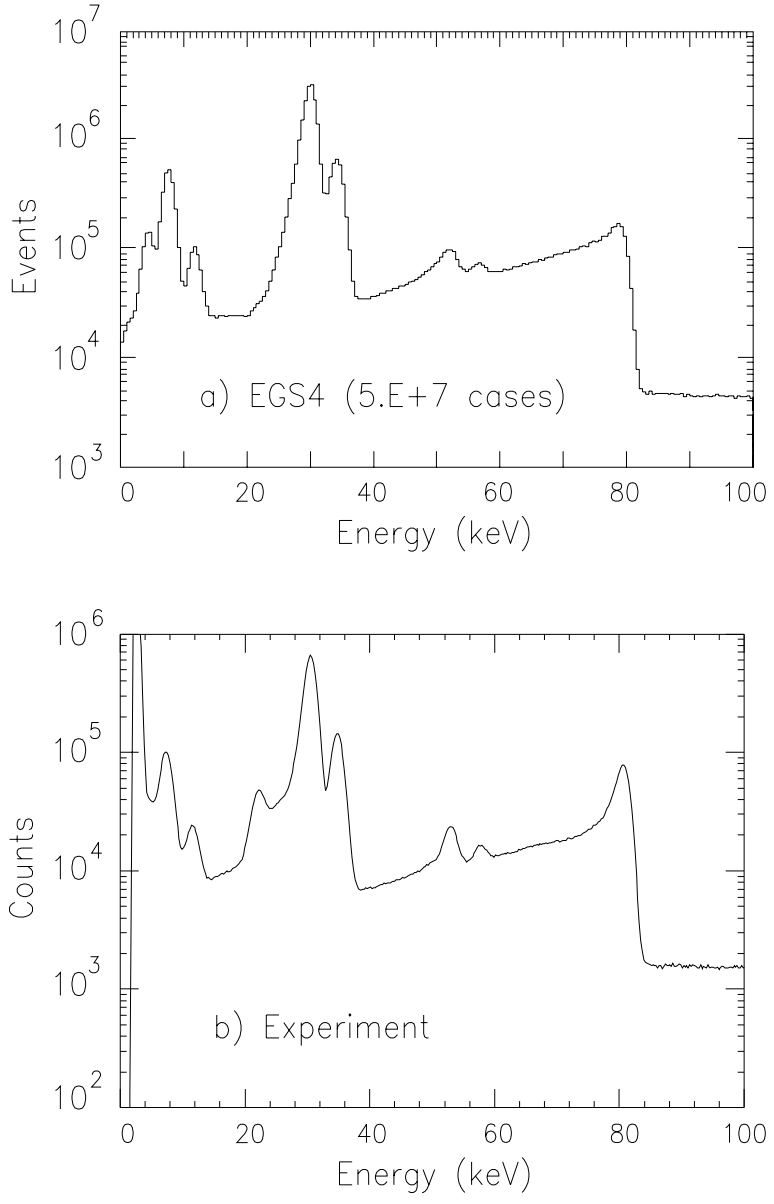

Fig. 4 Ba−133 a) simulation, b) experiment.

Figure 5 compares the EGS4 simulation with experiment for the case of ^{109}Cd. The peaks show up at the expected energies, but the two between 62 and 66 keV in the experimental data are unexpectedly narrow and are probably spurious. Also, the width of the peak near 88 keV is wider (and smaller) in the simulation than in the measurement, and another peak appears at about 16 keV in the measurement data, but not in the simulation.

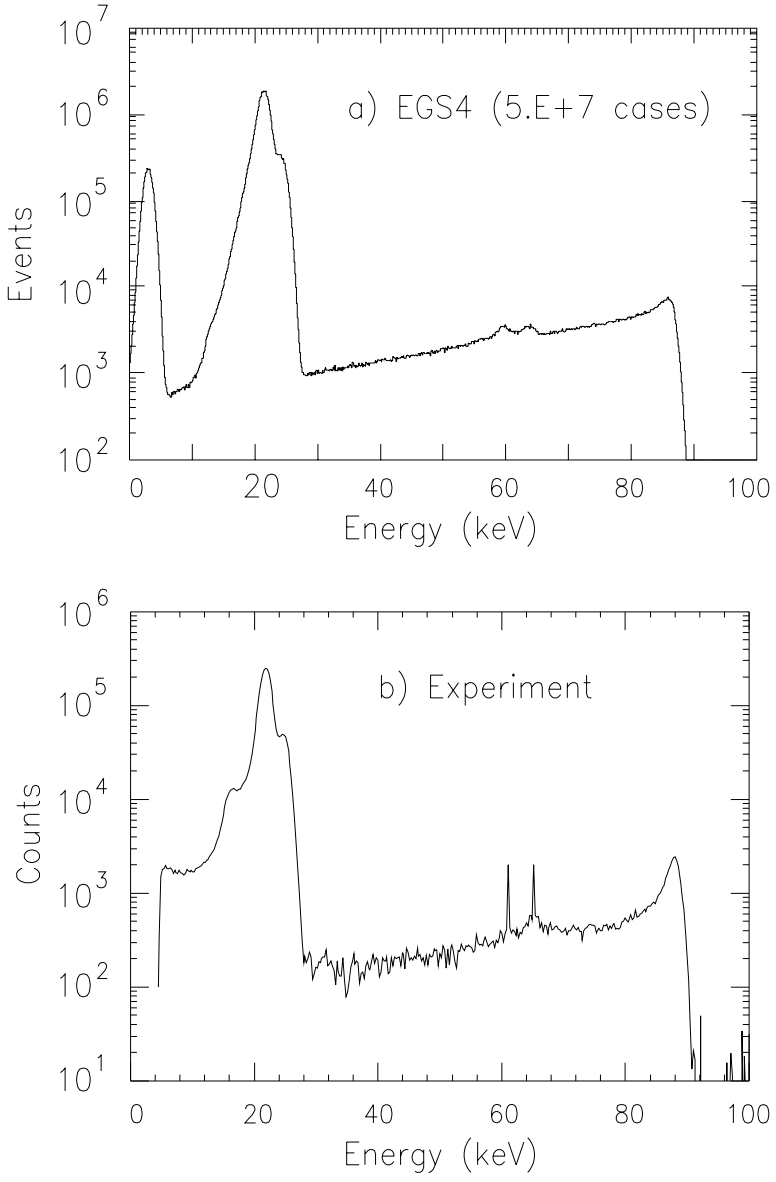

Fig. 5 Cd−109 a) simulation, b) experiment.

5. Concluding Remarks

We have used EGS4 to simulate the response of a CZT crystal, mounted within a BNC connector, taking into account the incomplete collection of charge by means of the Hecht equation, and also including the production of K-shell fluorescent photons. When compared with measurements, using three radioactive sources, all of the photo and escape peaks appear at their expected locations. However, a few anomalies remain to be understood. Specifically, a few peaks show up in the experimental data that are not observed in the EGS simulation.

In addition, the widths of the peaks in the simulation appear to be wider than in the experimental data. Possibly this can be explained by our incomplete knowledge of the many parameters involved—*e.g.*, the mobility-lifetime values for electrons and holes, the Fano factor for CZT, the electronic noise, and even the value of w, are not precisely known. Also, the Hecht model itself may be too simple.

Nevertheless, the simulations are in fair agreement with measurements, which gives us confidence that the CZT detector can be useful in studying synchrotron radiation backgrounds near the interaction point of PEP-II.

REFERENCES

1. W. R. Nelson, H. Hirayama and D. W. O. Rogers, "The EGS4 Code System", SLAC Report 265 (1985).
2. A. Del Guerra, W. R. Nelson and P. Russo, "A Simple Method to Introduce K-Edge Sampling for Compounds in the Code EGS4 for X-Ray Element Analysis", Nucl. Instr. Meth. A306 (1991) 378 [Erattum: Nucl. Instr. Meth. A359 (1995) 637].
3. G. Baldazzi, D. Bollini, F. Casali, P. Chirco, A. Donati, W. Dusi, G. Landini, M. Rossi and J. B. Stephen, "Timing Response of CdTe Detectors", Nucl. Instr. Meth. A326 (1993) 319.
4. A. F. Bielajew and D. W. O. Rogers, "PRESTA: The Parameter Reduced Electron-Step Transport Algorithm for Electron Monte Carlo Transport", Nucl. Instr. Meth. B18 (1987) 165; also NRC-PIRS-0042 (1986).
5. *Radioactive Transformations*, Publication 38, International Commission of Radiological Protection, Annals of the ICRP 11-13 (1983).
6. W. R. Leo, Techniques for Nuclear and Particle Physics Experiments (Springer-Verlag, Second Edition, 1994); see Chapter 10.
7. W. Bencivelli, E. Bertolucci, U. Bottigli, A. Del Guerra, A. Messineo, W. R. Nelson, P. Randaccio, V. Rosso, P. Russo and A. Stefanini, "Evaluation of Elemental and Compound Semiconductors for X-ray Digital Radiography", Nucl. Instr. Meth. A310 (1991) 210.

Appendix 1

Code section from SUBROUTINE AUSGAB of ucczt3.mortran (see text)

```
IF(IARG=19 & MED(IR(NP))=MEDdet) [  "Before PHOTO-call in detector reg."
  ESING=E(NP);                "Single precision (local) variable (MeV)"
  GLE=ALOG(ESING);
  MEDSAV=MEDIUM;  IRSAV=IR(NP);          "Save for future IARG=20 entry"

  IR(NP)=NREGp-2;  MEDIUM=MED(IR(NP));                    "Get Cd data"
  $SET INTERVAL GLE,GE;
  $EVALUATE GMFPCd USING GMFP(GLE);
  $EVALUATE GBR2Cd USING GBR2(GLE);

  IR(NP)=NREGp-1;  MEDIUM=MED(IR(NP));                    "Get Zn data"
  $SET INTERVAL GLE,GE;
  $EVALUATE GMFPZn USING GMFP(GLE);
  $EVALUATE GBR2Zn USING GBR2(GLE);

  IR(NP)=NREGp;  MEDIUM=MED(IR(NP));                      "Get Te data"
  $SET INTERVAL GLE,GE;
  $EVALUATE GMFPTe USING GMFP(GLE);
  $EVALUATE GBR2Te USING GBR2(GLE);

  G1=PZ(MEDdet,1)*WA(MED(NREGp-2),1)*(1.-GBR2Cd)/RHOR(NREGp-2)/GMFPCd;
  G2=PZ(MEDdet,2)*WA(MED(NREGp-1),1)*(1.-GBR2Zn)/RHOR(NREGp-1)/GMFPZn;
  G3=PZ(MEDdet,3)*WA(MED(NREGp  ),1)*(1.-GBR2Te)/RHOR(NREGp  )/GMFPTe;
  G123=G1 + G2 + G3;

  "Now.....(temporarily) set IR(NP) and MEDIUM variables"
  $RANDOMSET RNEDGE;
  IF    (RNEDGE<=G1/G123)      [IR(NP)=NREGp-2;]
  ELSEIF(RNEDGE<=(G1+G2)/G123) [IR(NP)=NREGp-1;]
  ELSE                         [IR(NP)=NREGp  ;]
  MEDIUM=MED(IR(NP));
  RETURN;
  ]                                              "End of IARG=19 loop"
ELSEIF(IARG=20 & MEDSAV=MEDdet) [    "After PHOTO-call in detector reg."
  MEDIUM=MEDSAV;  IR(NP)=IRSAV;             "and....reset the variables"
  IF(NP > 1)[IF(IR(NP-1)>=NREGp-2) [IR(NP-1)=IRSAV;]]
  RETURN;
  ]                                              "End of IARG=20 loop"
```