CR-189403

Project #194001

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IN-73-CR
OCIT
34029
P-32

SEMIANNUAL TECHNICAL REPORT
for

CONTRACT #NAS5-32586

Submitted December 15, 1994
for the Months of
March 1, 1994 - August 31, 1994

REPORT DOCUMENTATION PAGE

Form Approved
OMB
No 0704-0188

1. AGENCY USE ONLY (Leave Blank)	2. REPORT DATE December 1994	3. REPORT TYPE AND DATES COVERED: Semi-Annual Status for March-August, 1994

4. TITLE AND SUBTITLE Quarterly Technical Report for Contract #NAS5-32586	5. FUNDING NUMBERS
6. AUTHORS A. C. Rester, Jr.	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Constellation Technology Corporation 9887 Fourth St. N., Suite 100 St. Petersburg, FL 33702	8. PERFORMING ORGANIZATION REPORT NUMBER
9. SPONSORING MONITORING AGENCY NAME(S) AND ADDRESS(ES) National Aeronautics and Space Administration Goddard Space Flight Center Greenbelt Road Greenbelt, MD 20771	10. SPONSORING MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES

Contract Monitor: Jack Trombka

12a. DISTRIBUTION AVAILABILITY STATEMENT	12b. DISTRIBUTION CODE

13. ABSTRACT
Progress made during the months of 1994 for contract are discussed. Technical data compiled during this time is presented.

14. SUBJECT NAME Monte-Carlo Gamma-Ray Spectrum Simulation	15. NUMBER OF PAGES
	16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT Unclassified	18. SECURITY CLASSIFICATION OF THIS PAGE Unclassified	19. SECURITY CLASSIFICATION OF ABSTRACT Unclassified	20. LIMITATION OF ABSTRACT

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Introduction

The gamma-ray spectrum simulation program BSIMUL was designed to allow the operator to follow the path of a gamma-ray through a detector, shield and collimator whose dimensions are entered by the operator. It can also be used to simulate spectra that would be generated by a detector. Several improvements have been made to the program within the last few months. The detector, shield and collimator dimensions can now be entered through an interactive menu whose options are discussed below. In addition, spectra containing more than one gamma-ray energy can now be generated with the menu - for isotopes listed in the program. Adding isotopes to the main routine is also quite easy. Subroutines have been added to enable the operator to specify the material and dimensions of a collimator.

This report details the progress made in simulating gamma-ray spectra for a variety of user-specified detector designs. In addition, a short discussion of work done in the related areas of pulse shape analysis and the spectral analysis is included. The pulse shape analysis and spectral analysis work is being performed pursuant to the requirements of contract F-94-C-0006, for the Advanced Research Projects Agency and the U.S. Air Force.

The Simulation Program

A random number generator is used to simulate the behavior of gamma-rays as they pass through a detector. The absorption coefficients of the materials making up the detector, shield and collimator are used to calculate the reaction probability for: 1) photoabsorption, 2) Compton absorption, 3) pair production and 4) Bremstrahlung. The direction that the gamma-ray takes after a Compton interaction is calculated using the random number generator in conjunction with Equation 1 [Ref 1], while the energy of the gamma-ray is calculated using the Klein-Nishina

$$\cos\theta = 1 + 511 \; keV \left(\frac{1}{E} - \frac{1}{E_0} \right) \qquad\qquad 1$$

formula. BSIMUL was originally written with the assumption that the detector and shield would be cylindrically symmetric. Taking advantage of the symmetry increased the speed greatly. The program can now generate a spectrum resulting from one million gamma-rays entering the detector or shield on a SUN Sparc20 in 25 minutes, so speed is no longer critical. New subroutines have been added to model a collimator with a hole pattern specified by the operator. While the size and locations of the collimator holes must now be entered into a subroutine by the operator, in the future they will be entered through the menu. The collimator subroutines may be expanded to permit modeling of completely asymmetric detectors.

Materials with absorption constants written into the program are aluminum, tungsten, germanium, silicon, lead, sodium iodide, cesium iodide, BGO and beryllium. The absorption constants for each material are entered for an energy range of 20 keV to 10 MeV. Expanding the program to allow the operator to simulate detectors and shields made of any other material requires only a knowledge of the absorption constants of the material.
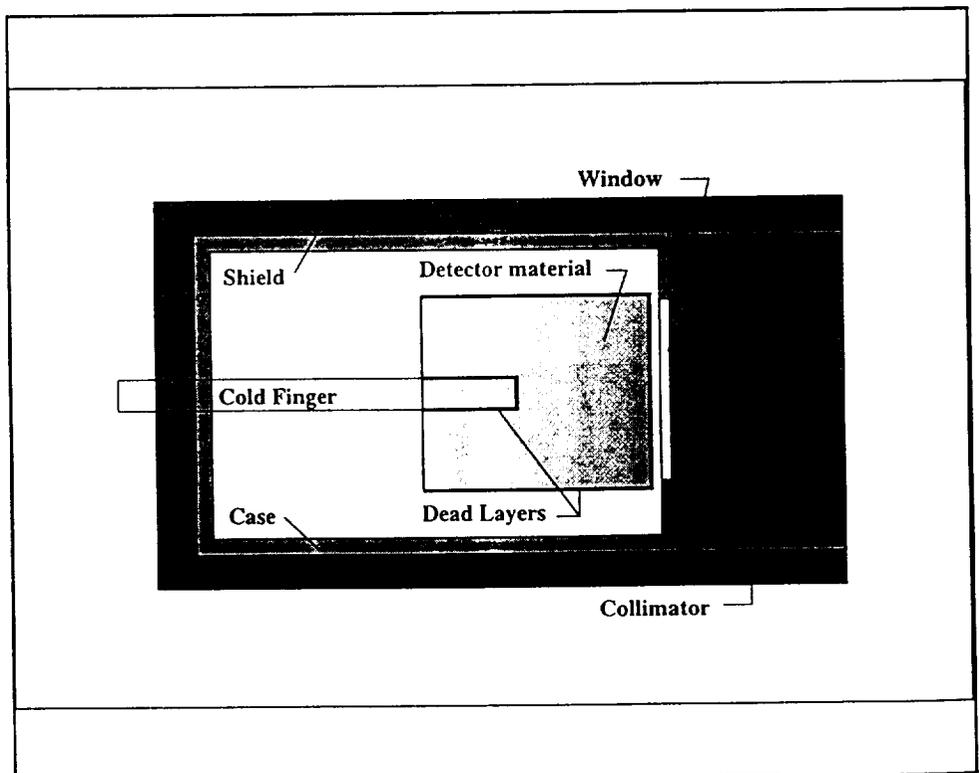

Figure 1 General detector and shield configuration.

SIMUL Menu

The first screen is a table of contents that allows the operator to enter the general information, graphics information, and detector and shield configuration screens listed below:

1 General information for the calculation
2 Graphics information
3 Detector geometry
4 Case and shield geometry
5 Cold finger geometry

The second screen, shown in Table 1, contains the number of events to be simulated, the isotopes and their relative strengths, and the source location. A typical spectrum contains between one million and five million gamma-rays, only a few of which deposit energy in the detector. A spectrum of one hundred thousand gamma-rays is useful only for studying the photopeaks. The energy entered in line three is used only if a single energy spectrum is desired. If isotopes are specified, the energy on line 3 is ignored. Up to ten isotopes may be entered in the menu. The x and y values are perpendicular to the axis of the detector shown in Figure 1. z is along the axis.

Table 1. General information for the simulation

Number of events	1000000
Random seeds	5676654, 9612341
Energy (keV)	1000.
Number of isotopes	2
List isotope and relative intensity	Co60, 0.5
	Cs137, 0.5
Initial x and y values	0.0, 0.0
Initial z value	100.0
Lower limit for BGO detection	50.00
Lowest energy for bremstrahlung	5000.0
Effective charge for bremstrahlung	70.0

Graphics information, shown in Table 2, is entered on the next screen. The graphics option on line 1 allowing the operator to have the path of each gamma-ray plotted as it passes through the shield and detector. In this case, the position, momentum, and energy of the gamma-ray are printed at each new reaction site. The type of reaction that occurs is also printed to standard output. Two histogram files are always generated, the first containing all counts and the second containing only counts that were not vetoed by the shield or collimator. Gamma-ray energies are converted to channel numbers with the calibration information on lines three and four before the histograms are written.

Table 2. Graphics information

Graph the events in the detector?	N
Histogram file names	test1.sp, test1s.sp
Energy range for histogram	20., 3020.
Size of histogram	4096

Table 3 shows the detector material and geometry. At the moment, the detector must be cylindrical and made of Ge, Si, NaI or CsI, although other materials can be added easily. The inner radius is always zero while the position of the bottom of the detector material is in relation to the bottom of the shield, which is always at z=0. The dead layers are only on the side and top of the material and may be set equal to zero. All of the lengths are in centimeters.

Table 3. Detector geometry

Detector material (Ge, Si)	Ge
Inner, outer radii of material	0.0, 2.95
Bottom, top of material	4.70, 10.14
Thickness of dead layer on side	0.00003
Thickness of dead layer on top	0.00003

Table 4 contains the case, shield and collimator information. Any of these can be omitted, but the bottom of the shield must always be at zero with the case above it. Also, the inner radius of the shield must be larger than the outer radius of the case. The shield can extend any distance beyond the detector. While the collimator material and dimensions

are entered here, the hole pattern must be entered in the program itself.

Table 4. Aluminum case and shield configurations. Collimator information.

Is there an Al case? (Y/N)	Y
Inner, outer radii of Al	3.35, 3.51
Bottom, top of Al base	2.01, 2.51
Length of case	6.85
Is there a shield (Y/N)	Y
Shield material (BGO, Plastic, etc.)	BGO
Inner, outer radii of shield	4.00, 6.00
Bottom, top of shield base	0.0, 2.0
Length of shield	14.0
Collimator material (BGO, CsI)	NONE
Inner, outer radii of collimator	0.0, 3.515
Bottom, top of collimator	21.0, 31.0

The last screen, shown in Table 5, contains information on the cold finger and window. A thin beryllium window has been found to have very little effect on the spectra. The inner radius of the cold finger is always zero.

Table 5. Cold finger and window

Is there a Be window? (Y/N)	N
Inner, outer Be	0., 1.16
Bottom, top of Be	0., 0.001
Is there a cold finger? (Y/N)	Y
Inner, outer cf	0., 0.5
Bottom, top of cf	0., 6.70

Calculations

The program will now generate a spectrum with gamma-ray energies from up to ten isotopes, the identity and relative strengths of the isotopes being entered by the operator. For each isotope, the relative probability of a gamma-ray occurring at a particular energy is entered in the program. The energy of each gamma-ray in the simulation is chosen with a weighted random number. Isotopes that are not included in the program may be added easily in the main routine orsimul.f. The original method of running the program - with one gamma-ray energy - can still be used to generate spectra for peak-to-Compton ratio calculations. With a 30% HPGe detector as a model, several calculations with Co60 and Cs137 and BGO and CsI shielding were made. Figure A1 shows a comparison of real and simulated spectra with Cs 137 and Co 60 sources for the 30% HPGe detector with no shielding. The figures referred to in this section may be found in Appendix A. The simulated spectrum was normalized so that the 1173 keV peak has the same number of counts in both spectra. Co60 and Cs137 calibration sources were used for the real spectrum, which was taken with a 30% HPGe detector. The dimensions of the detector, shown in Table 1, were used in the simulations. The agreement between the two spectra is excellent in the region of 700 keV to 1200 keV. At low energies, the natural background and difference in number of Cs 137 gamma-rays causes the spectra differ. Small peaks seen in the simulated spectra are the 511 keV peak and the first and second escape peaks for the two gamma-rays of Co 60. The peaks in the simulated spectrum are at the moment one channel wide, but a cubic spline fit to a peak taken with the detector being simulated can be used to generate a more realistic peak shape.

Figures A2 through A5 show the effect of the shield material and thickness on Compton suppression. The configuration of the germanium detector used in the calculations is shown in Table 7. Figures A2 through A5 were generated by dividing the non-Compton suppressed counts by the total counts in each channel of the SIMUL output histograms. A CsI shield was used for the calculations shown in Figures A2 and A3. The shield was 1.5 cm thick in calculations shown in Figure A2 and 2.5 cm thick in the calculations shown in Figure A3. The shield material used to generate the next two figures was BGO, with 1.5 cm thick shield used in Figure A4 and a 2 cm thick shield used in Figure A5.

Also interesting is the ability of a shield to veto gamma-rays coming from the wrong direction. FigureA6 shows non-vetoed spectra arising from sources at two positions. The detector is the 30% germanium detector used above, with a cesium iodide shield 2.48 cm thick and extending 9.86 cm in front of the detector. The larger spectrum was generated with the gamma-rays at an initial position of x = 10 cm, y = 0 cm and z = 100 cm (the origin is at the base of the shield, so the top of the detector is at 10.14 cm and the top of the shield is at 20.00 cm). Gamma-rays entered at an angle of 5.7 degrees from the axis

Table 6: Dimensions of the 30% HPGe detector used in the experiments and simulations.

	Minimum value (cm)	Maximum value (cm)
Detector: inner and outer radii	0	2.95
Detector: bottom and top	4.7	10.14
Dead layer thickness		0.00003
Al case: inner and outer radii	3.35	3.51
Al case: bottom and top of the base	2.01	2.51
Al case: length		7.85
Shield: Bottom and top of the base	0	2
Shield: top		14
Cold finger: Inner and outer radii	0	0.5
Cold finger: Bottom and top	0	6.7

and reached the detector without entering the shield. In the second spectrum, the initial positions were x = 50 cm, y = 0 cm and z = 100 cm, so the gamma-rays entered the detector at an angle of 26.6 degrees from the axis and had to pass through the shield, which vetoed 80% of the total counts.

Figures A7 through A9 show the effect of the length of the shield on the spectra. Figures A7 and A8 show the total and non-vetoed spectra for the 30% HPGe detector and BGO shield configuration listed in the menu shown on pages two and three. In Figure A7, the shield extended four centimeters in front of the detector, while in Figure A8 it extended ten centimeters in front of the detector. The total spectra are nearly identical in the two figures, but the Compton edges of the non-vetoed spectra are much narrower in Figure A8 because the longer shield vetoes gamma-rays that are scattered. A gamma-ray entering the center of the detector can be vetoed by the shorter shield if it is scattered at an angle of less than 156 degrees, while the longer shield can veto a gamma-ray scattered at an angle of up to 170 degrees. The Co 60 Compton edges of the two non-vetoed spectra are compared in Figure A9.

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Plans

There remain four major improvements to be made to the program:

1) Include an option to allow the operator to use cubic splines to generate simulated histograms that have accurate peak shapes. At the moment the photopeak lines are one channel wide, which is adequate for the calculation of peak-to-Compton ratios and germanium spectra, but would not provide a useful simulation of a CsI scintillation spectrum, for instance. Several sample spectra have been taken with germanium, sodium iodide, and cesium iodide detectors that can be used to test the peak shape subroutines. Estimated time: 2 weeks

2) There are many places where the program could be greatly simplified. In addition, the speed may be increased significantly. This is a relatively low priority since it runs in 25 minutes on a SUN Sparc20 with an input of 1 million gamma-rays and a cylindrically symmetric configuration. Estimated time: 4 weeks

3) The range of materials whose behavior can be simulated can be expanded to include CdTe and HgI_2, for instance. The photo-absorption coefficients for these materials are available and the Compton (σ) and pair-production (κ) coefficients may be approximated from known coefficients as follows:

$$\frac{\kappa_1}{\rho_1} = \frac{\kappa_2}{\rho_2} \frac{A_2}{A_1} \left(\frac{Z_1}{Z_2} \right)^2 \qquad\qquad 1$$

$$\frac{\sigma_1}{\rho_1} = \frac{\sigma_2}{\rho_2} \frac{A_2}{A_1} \frac{Z_1}{Z_2} \qquad\qquad 3$$

where ρ is the density, A is the atomic weight and Z is the atomic number. The subscripts 1 and 2 refer to any two elements. For materials whose photoabsorption coefficients are not available, the interpolation formula

$$\frac{\tau_1}{\rho_1} = \frac{\tau_2}{\rho_2} \frac{A_2}{A_1} \left(\frac{Z_1}{Z_2} \right)^n \qquad\qquad 4$$

may be used. [Ref. 2] A study of the accuracy of the interpolation formulas will be performed, and the accuracy will be compared to the accuracy of the values of the absorption coefficients in use in the program. In addition, a commercially available program that calculates absorption coefficients may be used in conjunction with BSIMUL to allow the operator to simulate the behavior or any detector or shield material.

4) Finally, a graphical interface that allows the operator to draw the detector would be a great improvement over the current menu system. Popup menus would allow the operator to choose the material of each part and the exact dimensions would be entered through a text window.

In order to make further progress, we need the detector configurations for which spectra are desired. In addition, we need to know which materials are being considered for detectors and shielding. A list or sources and their probable strengths, or the environments that the detectors will be used in will enable us to perform realistic simulations.

Progress on Related Work

Pulse shape analysis

In a typical gamma-ray spectrum, one finds several undesirable features. In addition to the desired photopeaks, there are a Compton continuum background and Compton edge features. These features can be considered noise. As in any information bearing medium, one would benefit from increasing the signal to noise ratio. In a gamma-ray spectrum, this could be accomplished by reducing the Compton continuum and the Compton edges.

A newly developed method of doing this is pulse shape analysis. A pulse from a gamma-ray detector may contribute to the photopeak, the Compton continuum or the Compton edges. Rejecting pulses which contribute to the Compton continuum or Compton edges would eliminate the noise of the spectrum. By applying pulse shape analysis to each pulse coming from the detector, one may reject some of the undesired pulses and effectively improve the signal to noise ratio of a given spectrum.

Pulse shape analysis can be used to reduce the peak to noise ratio in a spectrum by vetoing those pulses that come from the edges of the detector. Gamma-rays that interact with the detector near the edge are much more likely to deposit only part of their energy in the detector than those that interact with the detector near the center. We have performed a series of experiments to optimize the criteria for determining the location of a pulse in a detector.

One criterion is the rise time. Pulses caused by interactions which occur near the outer edge of a detector (N-type cylindrical HPGe) tend to have a longer rise time than interactions occurring near the center of the detector. Therefore, rejecting pulses with long rise times will reject photons which have the greatest chance of scattering out of the detector. The method has been demonstrated to work quite well, with Peak to Compton ratios improving by a factor of 1.5. Other features of the pulses that we examined were the fall time and the widths of the pulse at 70% of the maximum and at 50% of the maximum. These criteria are almost completely energy independant. The ratio of the 70% pulse maximum to the 50% pulse maximum increases at the photopeaks and decreases at the Compton edges. The Compton features of a spectrum can be reduced by using these criteria to veto pulses. Figure 2 shows an unsuppressed spectrum and an unscaled suppressed spectrum. Figure 3 shows the same two spectra, only the suppressed spectrum has been scaled so that the 662 keV photopeaks of the two spectra are equal in height.

Presently at Constellation Technology, other, more complex criteria are being developed which promise even higher peak-to-Compton ratios. Some of these have been demonstrated in digital experiments and have been implemented in analog hardware, allowing real time analysis.
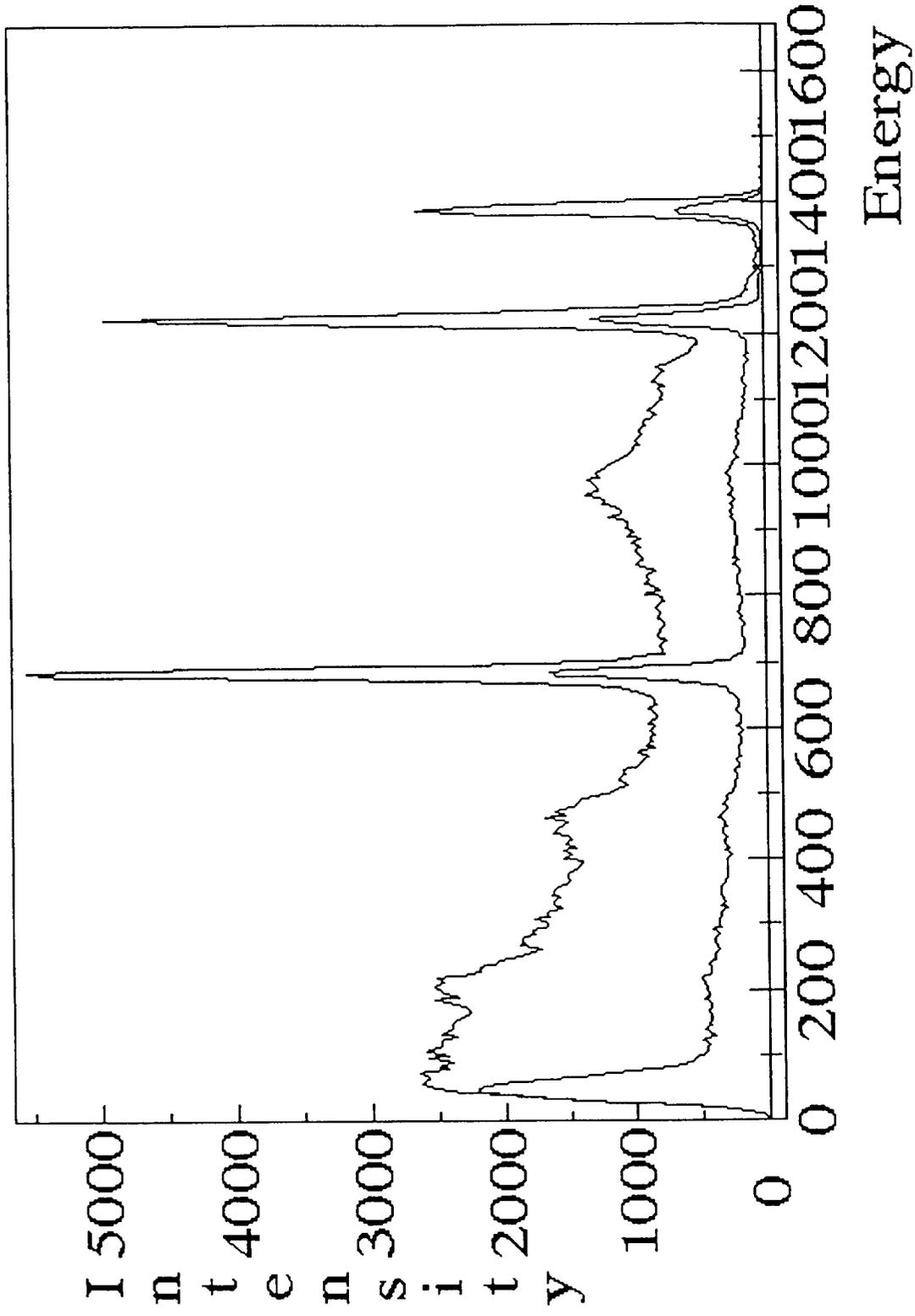
10

Figure 2. Upper Curve: Upsuppressed Spectrum
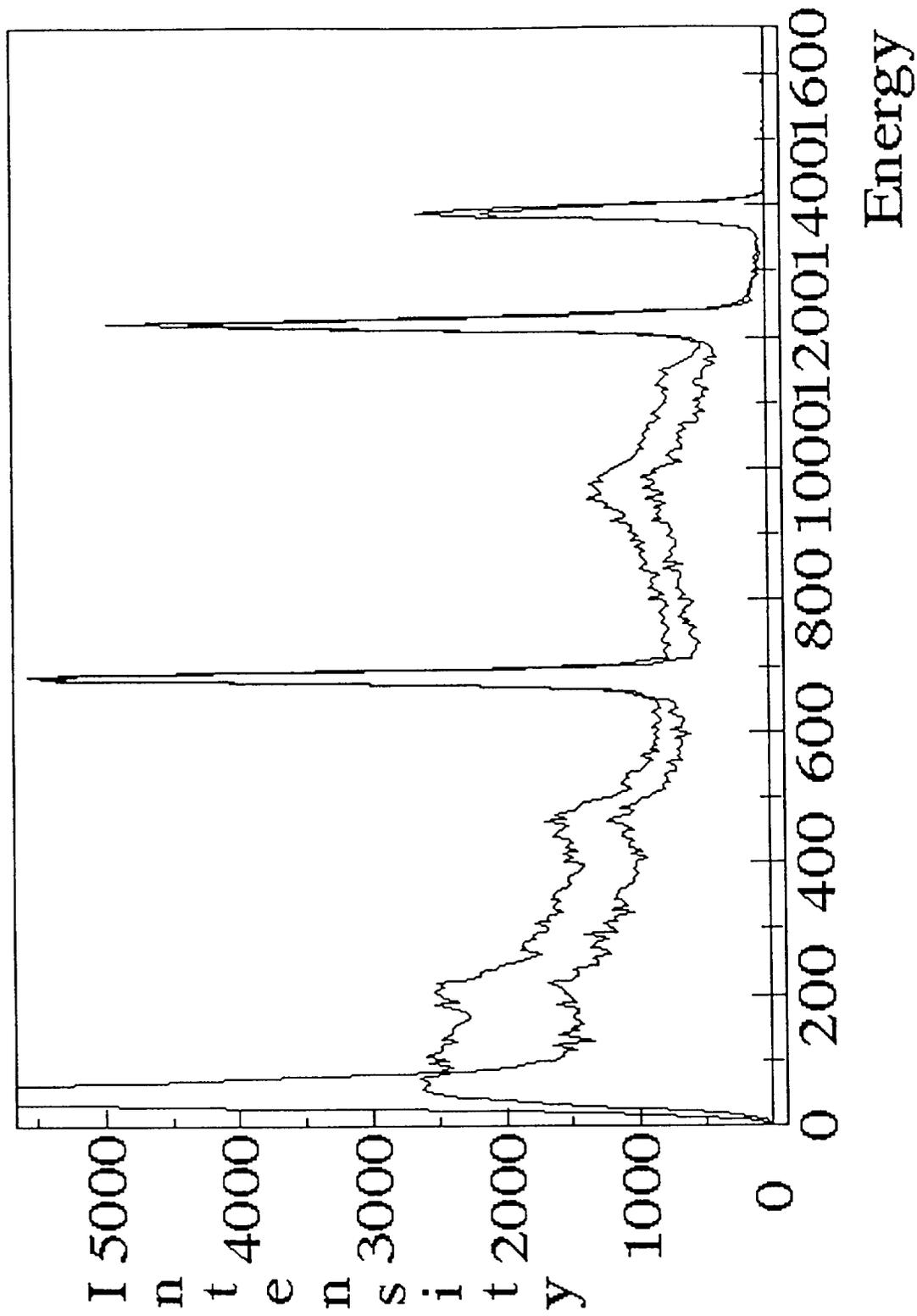Lower Curve: Suppressed Spectrum
Sources: Co60 and Cs137

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Figure 3. Upper Curve: Unsuppressed Spectrum
Lower Curve: Suppressed Spectrum scaled so that
the Cs137 Peaks are the Same Height.

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ROBFIT

The robust spectral fitting program ROBFIT uses cubic splines to fit gamma-ray spectra down to the noise level. The program is separated into two main routines: the background and peak fitting routines. Cubic splines are used to fit the background, while up to ten standard peak shapes are used to fit the peaks. The available peak shapes are Gaussian, Lorentzian, Voight and a computer-calculated peak shape that uses cubic splines to fit a peak in the spectrum that is specified by the user. The fits are performed as follows:

1) Calculate the standard peak shapes.
2) Fit the background with up to sixty constants that specify the cubic spline positions and magnitudes. The background function can be written [Ref 3].

$$S(x) = \sum_{i=0}^{3} c_i x^i + \sum_{j=1}^{M} d_j (k_j - x)^3 \qquad\qquad 4$$

where the number of splines, M, is specified by the user.
3) Subtract the background fit from the spectrum and fit the peaks with the standard peak shapes.
4) Subtract the fitted peaks from the spectrum and refit the background.
5) Repeat the last two steps until the error is within the limit set by the user.

ROBFIT has been used successfully in the analysis of gamma-ray data from the supernova SN 1987A [Ref 4]. The spectrum shown is Figures 4 and 5 show a typical spectrum and fit from the supernova [Ref 3].

Work on the spectral analysis program ROBFIT has proceeded along two lines. First, a new fitting program that compresses the data has increased the speed of the program by a factor of 10. Second, a new user interface has been written that makes the program much easier to use. Modifications to the data display routines now allow the operator to change scales with the arrow and page keys on both UNIX and DOS machines. It is now possible to use cubic splines to calculate the full width-half max of a peak while running the raw data display program.

The data compression routines are used by both the background and peak fitting portions of the program to increase both the speed and the accuracy of the fits. The original program compressed the background linearly to 1024 points, while the new routines perform a non-linear compression that places more points in areas where the background varies quickly and fewer points where the background is relatively constant. A new option added to the background fitting program is FBKG, which fits the background of a spectrum that is flat at large channel number. The spectrum shown in Figure 6 has been fitted with forty background constants and a cutoff of 100 by both versions of the background program. The
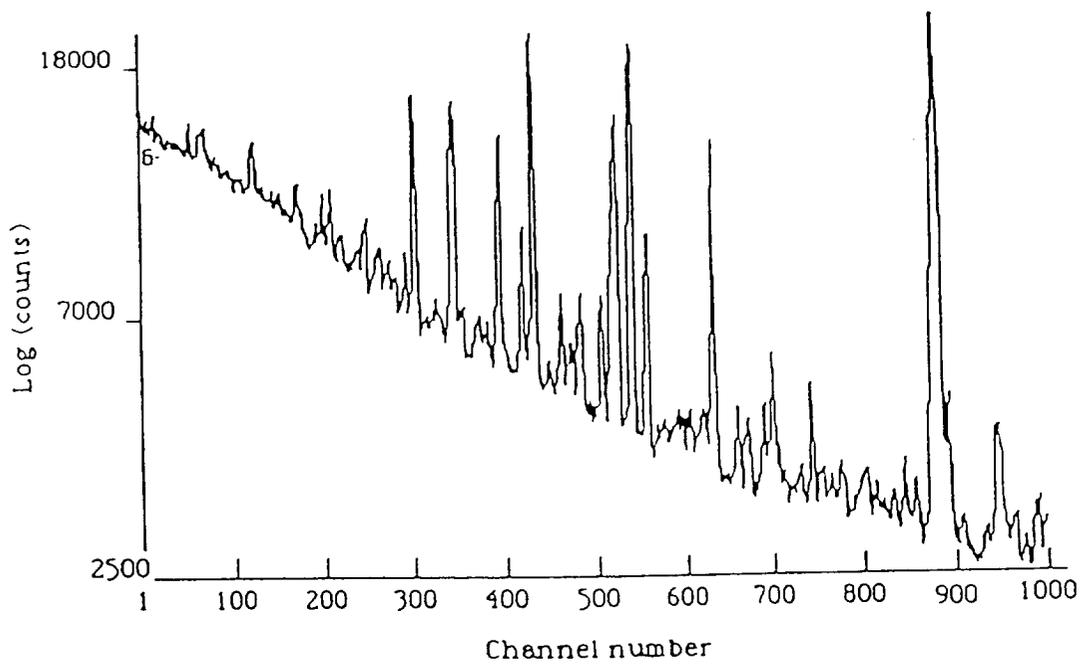
13

Figure 4. Gamma-Ray Spectrum From Supernova SN 1987A [REF 3]
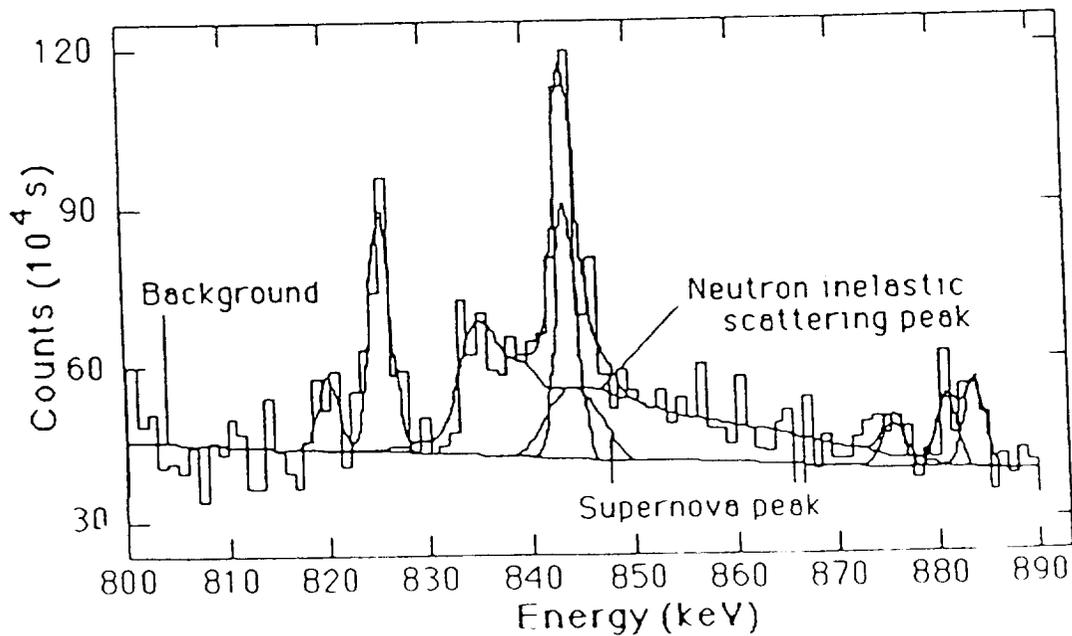

Figure 5. Fit Over a Small Range of the Supernova Spectrum [REF 3]

program ran in 13 minutes with non-linear data compression and in 26 minutes with linear compression. It has been found that compressing the peaks also results in an increase in speed without loss of accuracy. The compression factors for both the peak and background programs will be optimized.
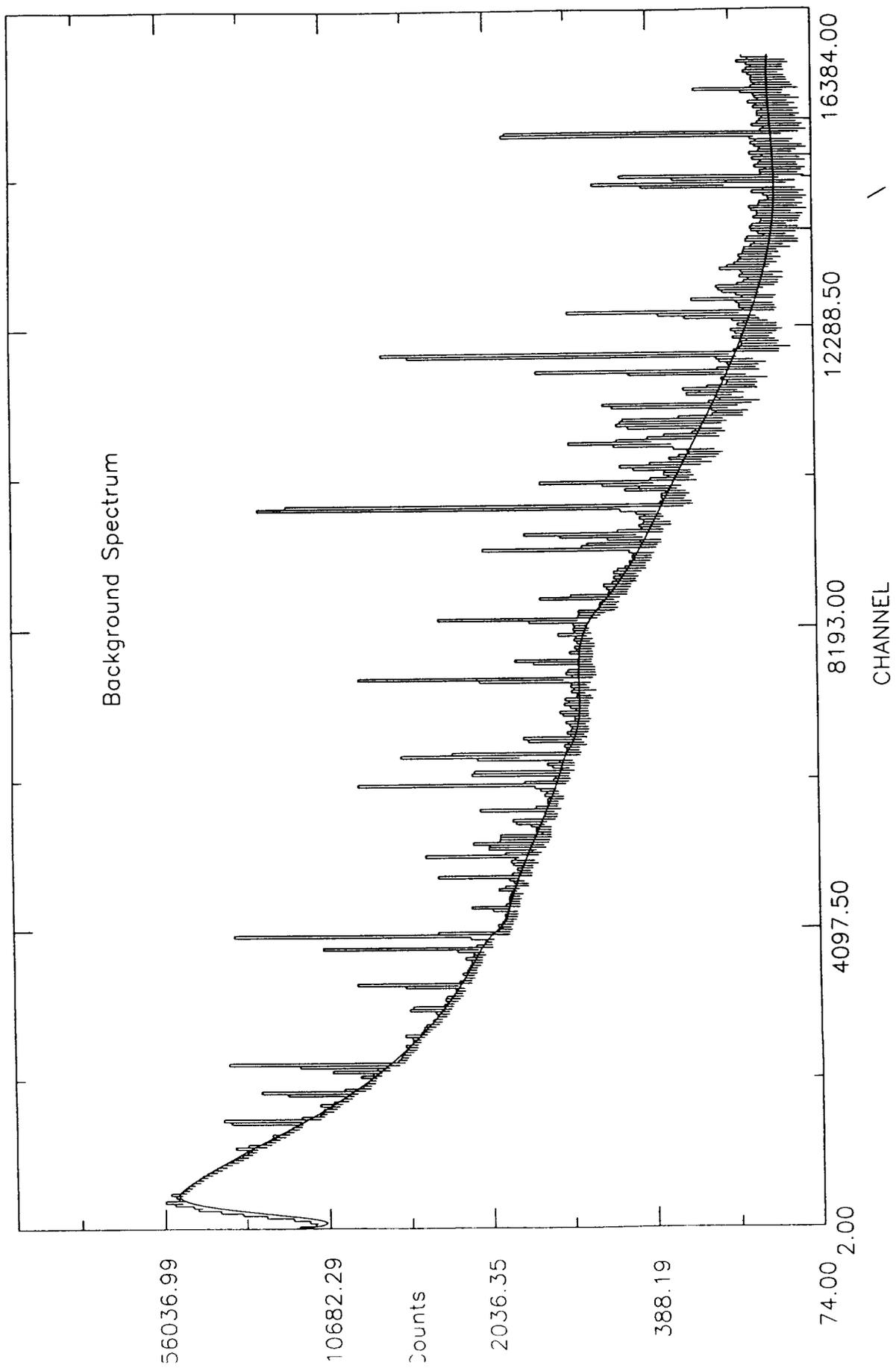
Figure 6. Background fit to the compressed data. 40 constants were used. The cutoff was 100.

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[1] Glen F. Knoll, <u>Radiation Detection and Measurement</u>, John Wiley and Sons (1989).

[2] Dwight E. Gray, Coordinating Editor, <u>American Institute of Physics Handbook</u>, 3rd Ed., McGraw Hill (1972).

[3] R.L. Coldwell, G.J. Bamford, <u>The Theory and Operation of Spectral Analysis Using ROBFIT</u>, American Institute of Physics (1991).

[4] A.C. Rester, R.L. Coldwell, F.E. Dunnam, G. Eichhorn, J.I. Trombka, R. Starr, and G.P. Lasche, "Gamma-ray observations of SN 1987A from Antartica," Astrophys., J., 342, L71-3 (July 15, 1989).

Appendix A

Simulated Co 60 and Cs 137 Spectra
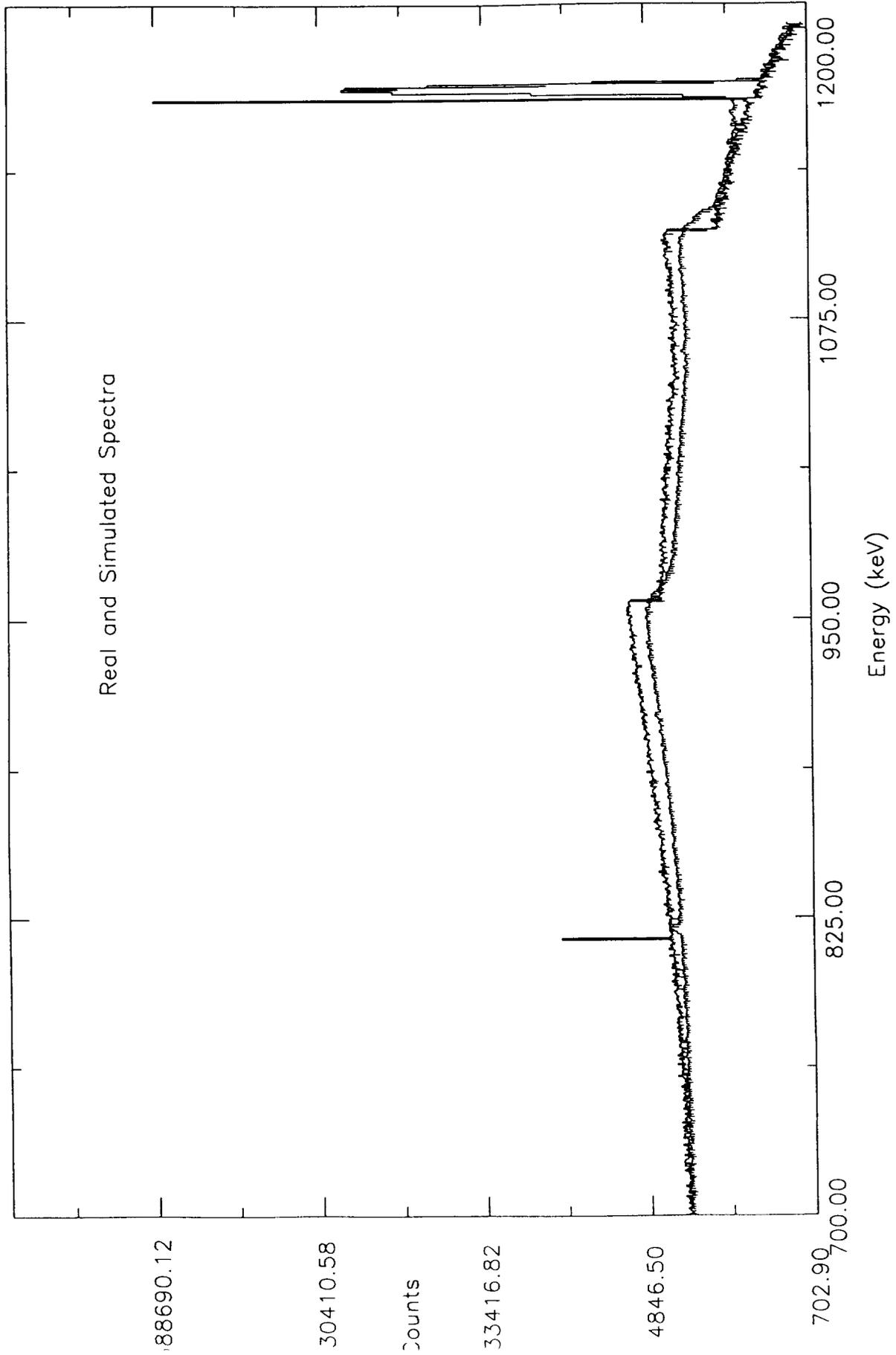
Figure A1. Curve 1: simulated spectrum normalized at the
1173 peak. Curve 2: real spectrum taken with 30% HPGe
detector. Sources: Co60, Cs137
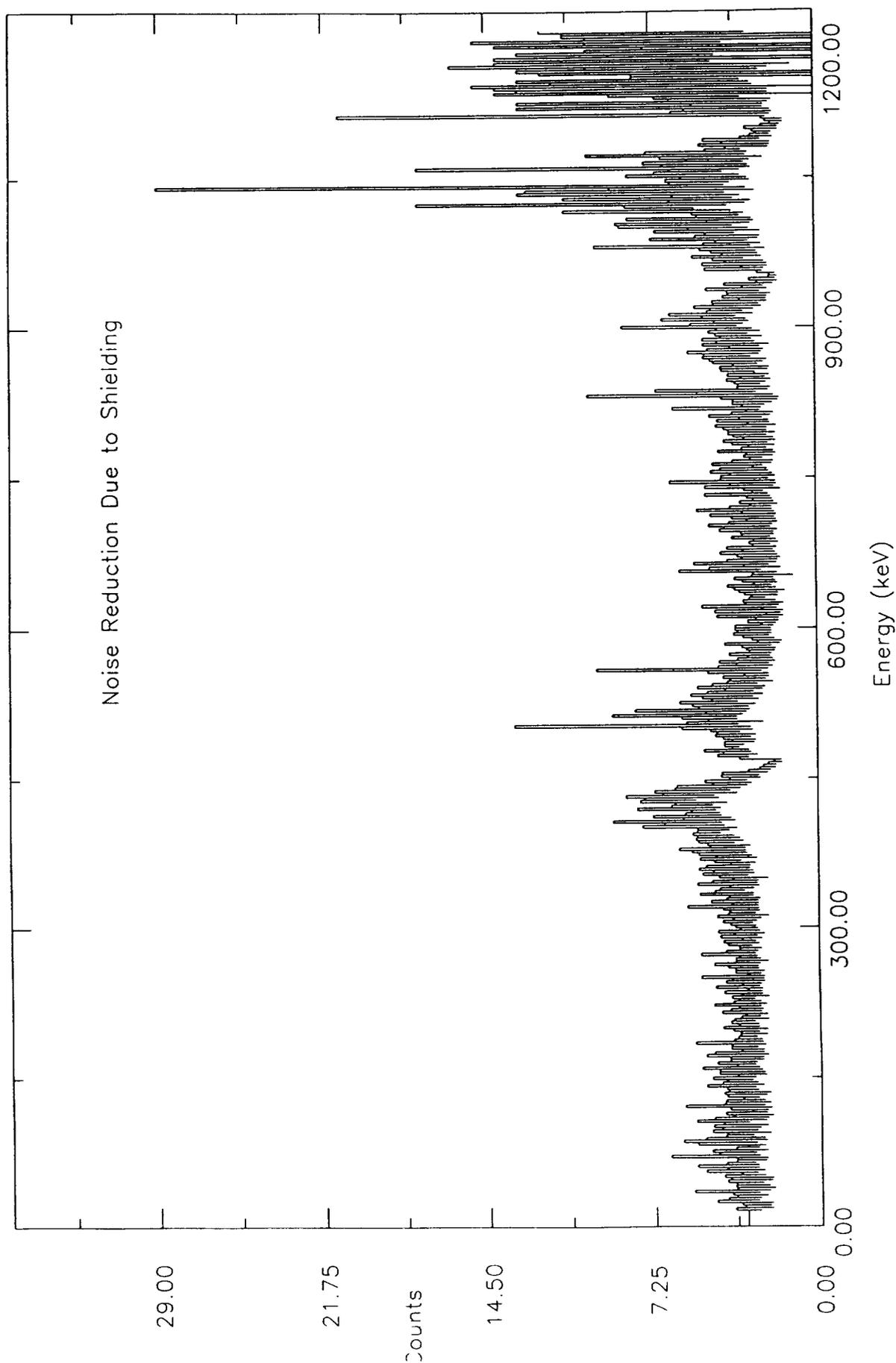
Figure A2. Simulation of a 30% HPGE detector with a 1.5 cm CsI shield. The curve is the ratio of total counts to non-vetoed counts.
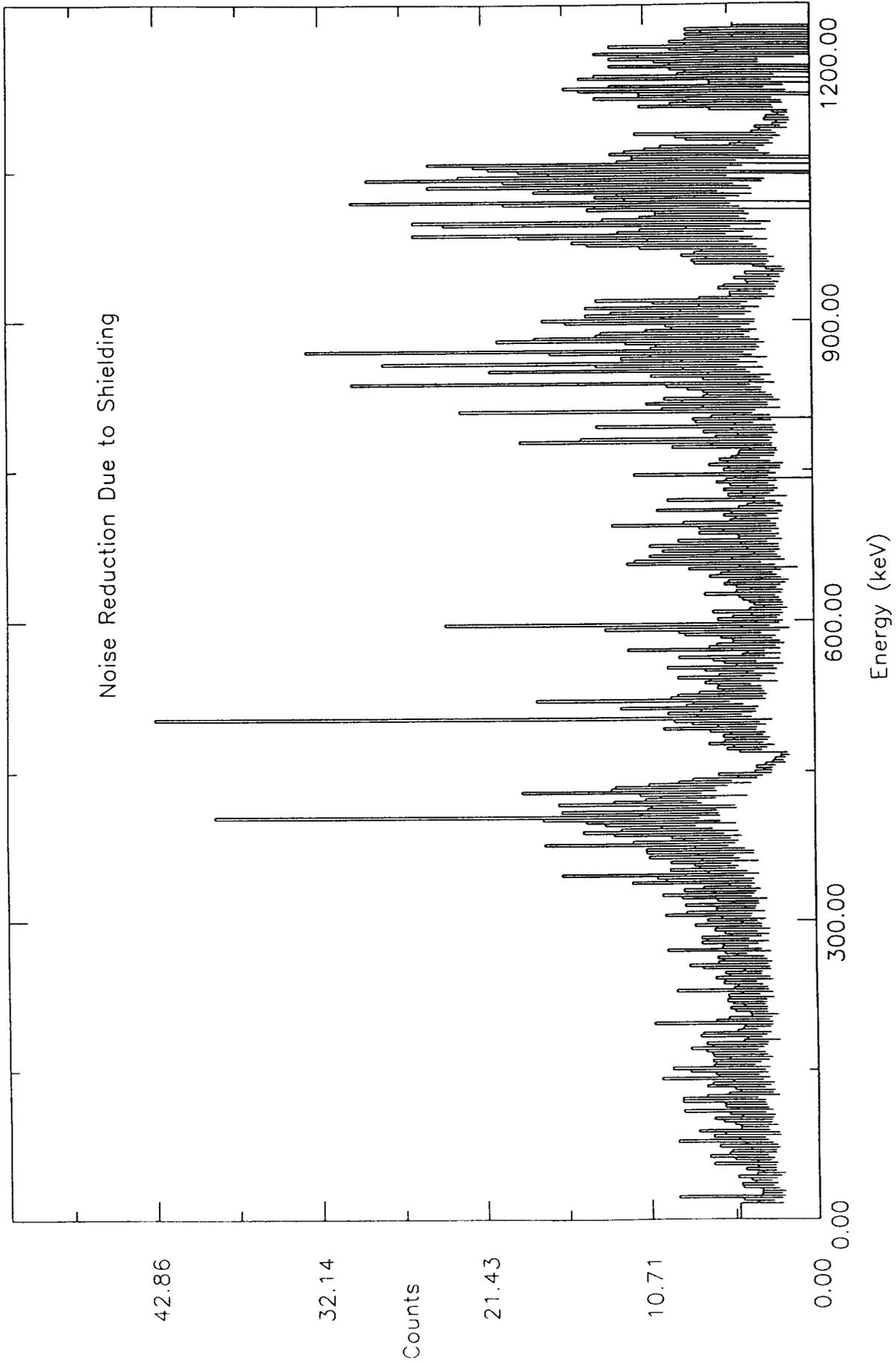
Figure A3. Simulation of a 30% HPGE detector with a 2.5 cm CsI shield. The curve is the ratio of total counts to non-vetoed counts.
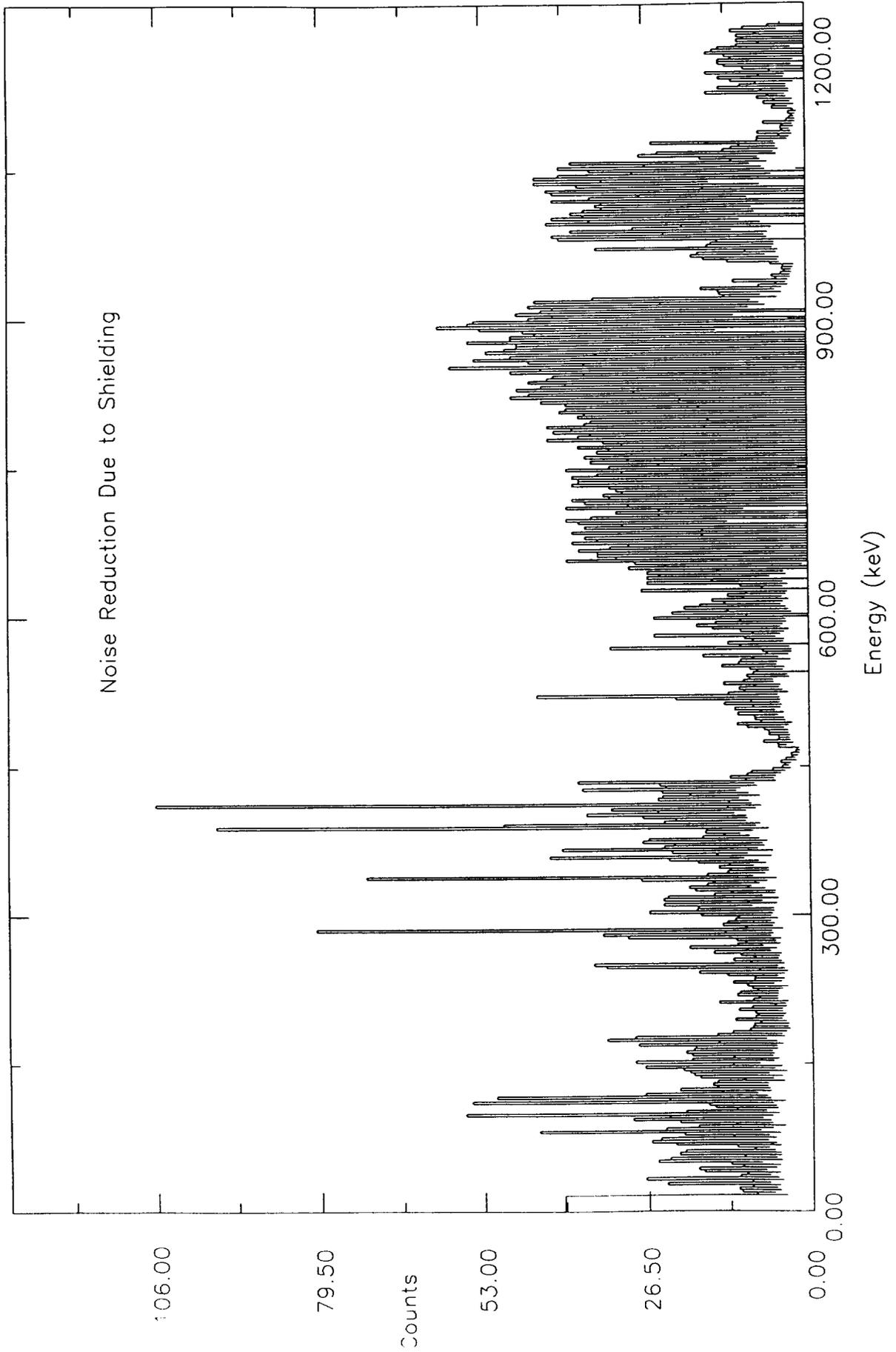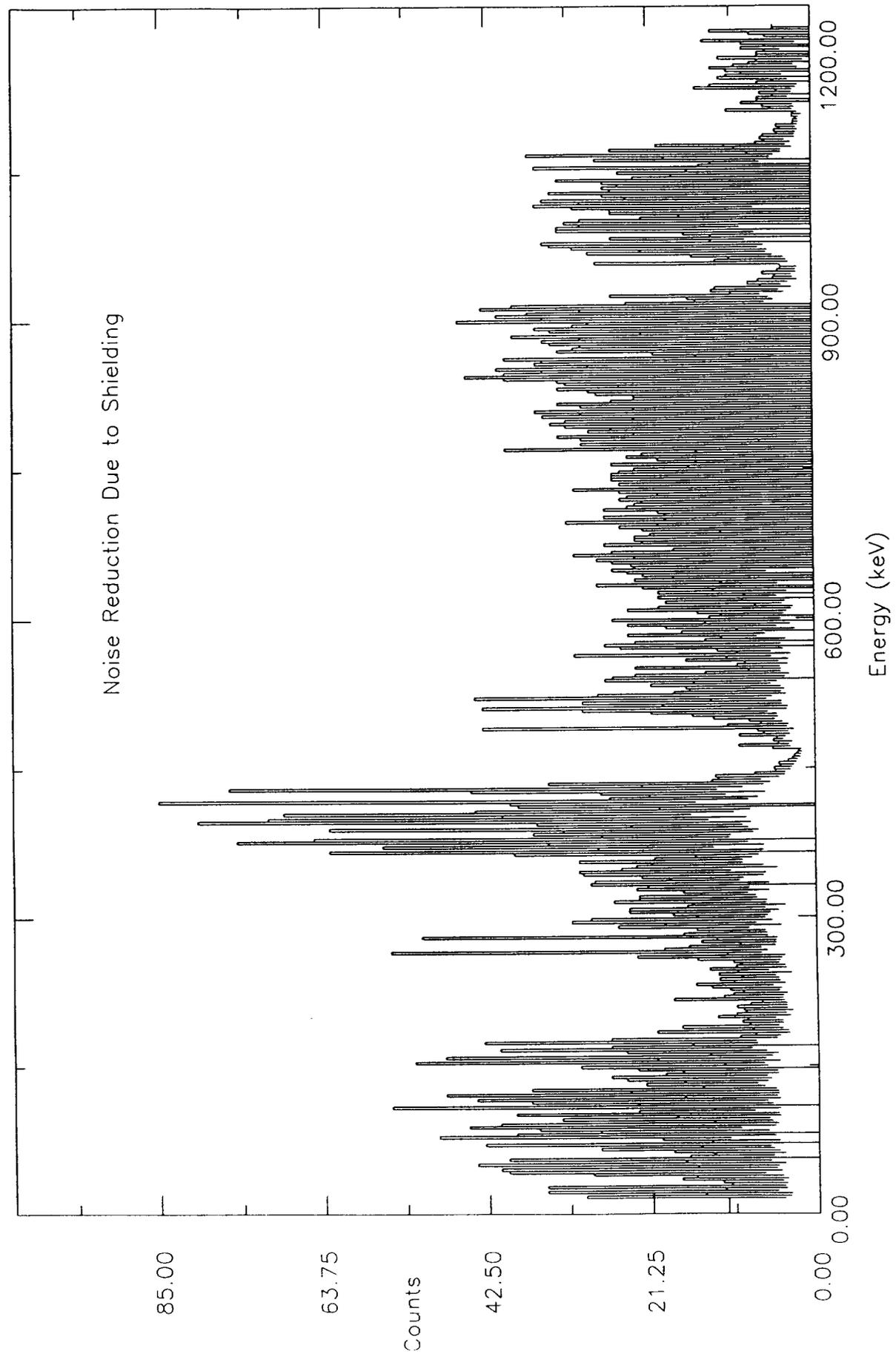
Figure A4. Simulation of a 30% HPGE detector with a 1.5 cm BGO shield. The curve is the ratio of total counts to non-vetoed counts.
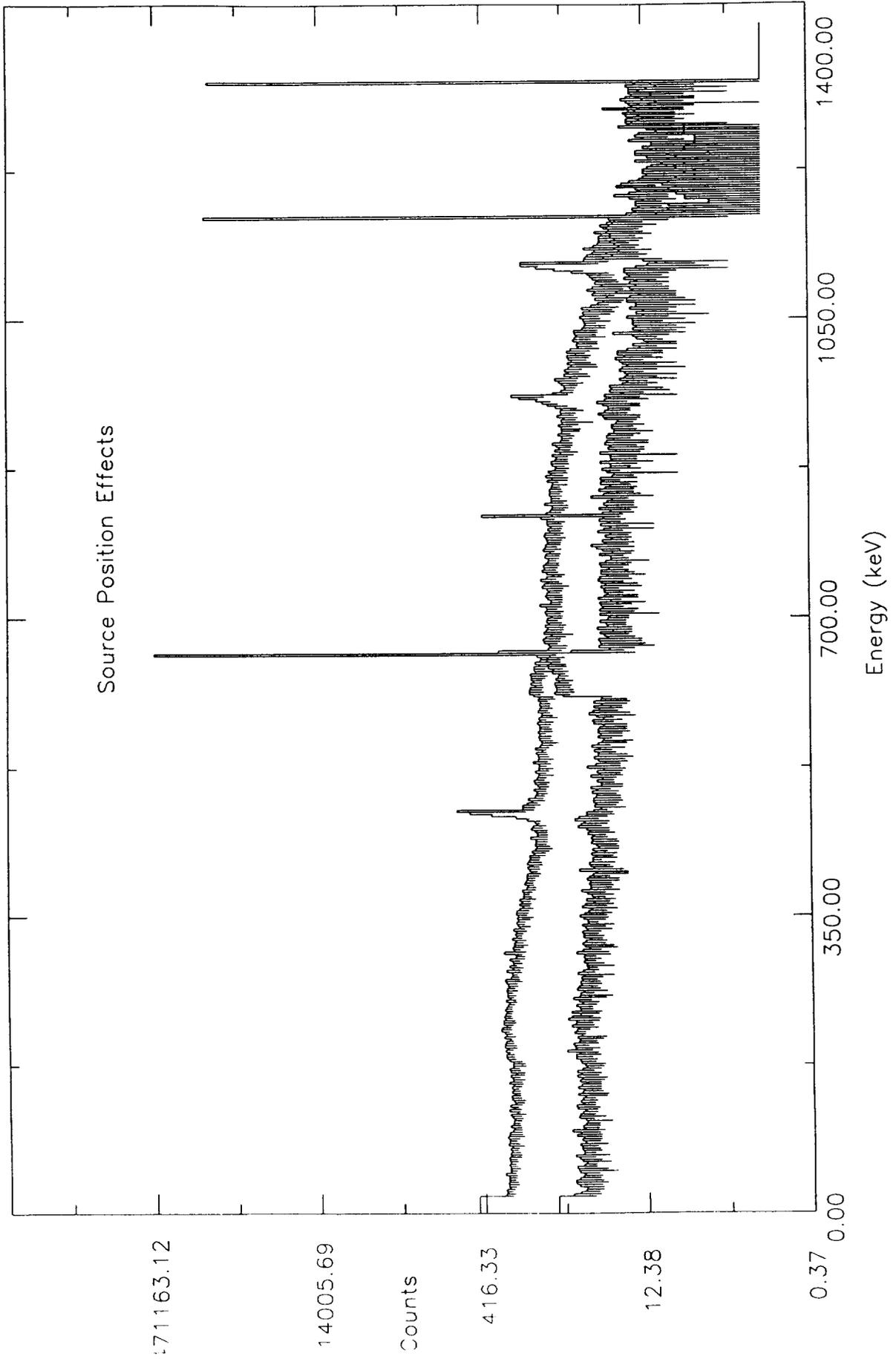
Noise Reduction Due to Shielding

Energy (keV)

Counts

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Figure A5. Simulation of a 30% HPGE detector with a 2.5 cm BGO shield. The curve is the ratio of total counts to non-vetoed counts.

Figure A6. The upper curve is from a source 5.7 degrees from the axis. The lower curve is from a source 26.6 degrees from the axis. Sources: Co60, Cs137
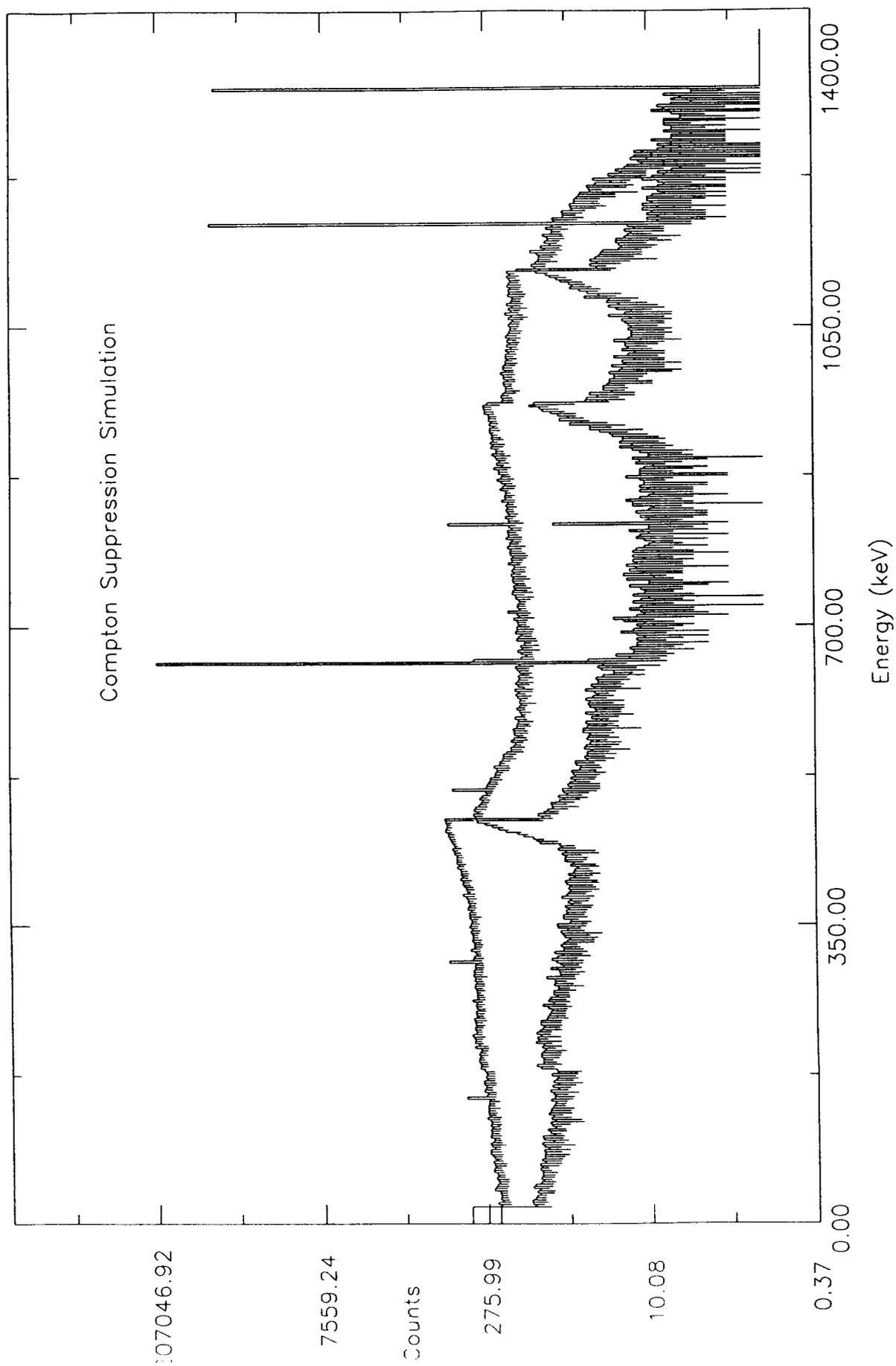
Figure A7. Total counts (upper curve) and non-vetoed counts (lower curve). The BGO shield extends 4 cm in front of the Ge. Sources: Co60, Cs137
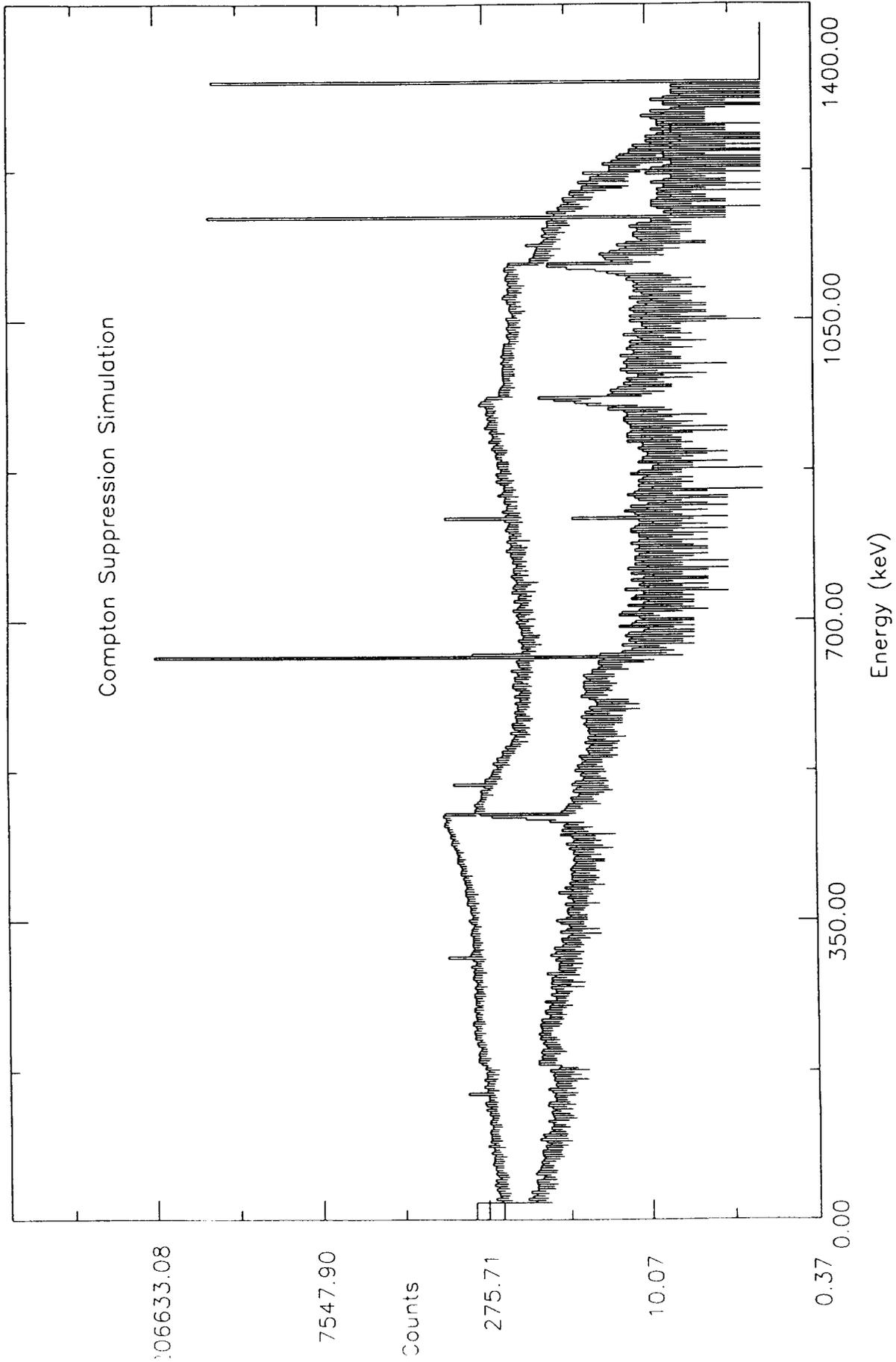
Figure A8. Total counts (upper curve) and non-vetoed counts (lower curve). The BGO shield extends 10 cm in front of the Ge. Sources: Co60, Cs137
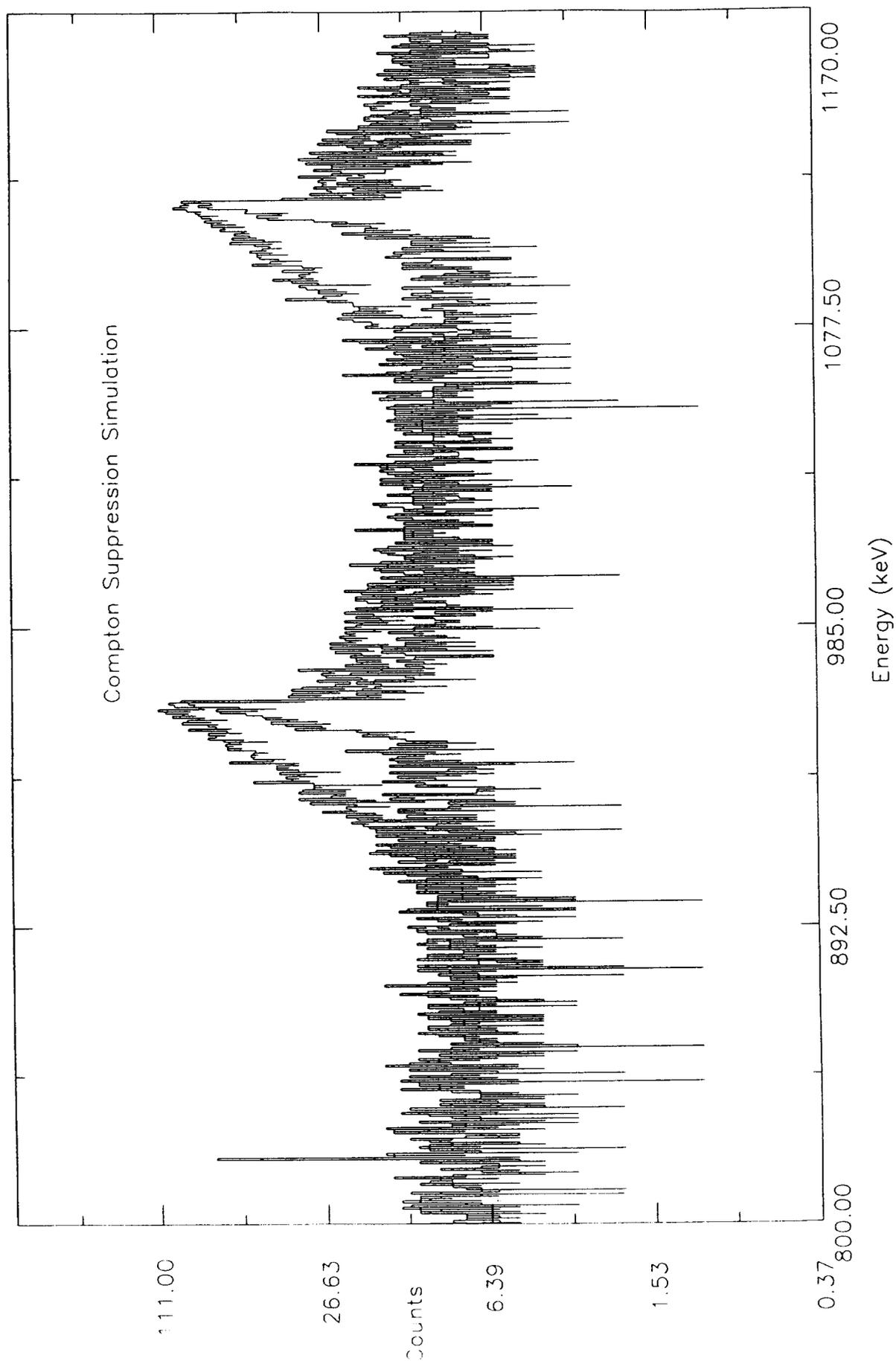
Figure A9. Upper curve: BGO shield extends 4 cm.
Lower curve: BGO shield extends 10 cm.
Sources: Co60, Cs137