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Table of Contents

List of Figures

List of Tables

Introduction

The Monte-Carlo program BSIMUL was designed to simulate the interactions between gamma-rays and detectors. BSIMUL follows the path of a gamma-ray through a detector and can also be used to simulate spectra generated by a detector. Several improvements have been made to the program within the past year. The menu has been modified to allow the operator to use an input data file containing the simulation parameters. This enables the operator to set up a series of runs easily. Major portions of the program were rewritten to expand the possible detector configurations, and include tapered cylinders. Isotope and absorption coefficient libraries have been created, and the coefficients of compounds not in the coefficient library can be calculated if the density is known.

The photopeaks generated by BSIMUL are one channel wide, sufficient for peak-to-Compton ratio calculations, but not sufficient for predicting the true shape of a spectrum. Standard peak shapes are available for several detector materials and can be used to add a true peak shape to BSIMUL's output. BSIMUL now writes the files necessary to perform an efficiency calibration with the spectrum fitting program ROBFIT.

This report details the progress made in simulating gamma-ray spectra for a variety of user-specified detector designs. Several simulations were performed with the NEAR detector configuration. This report also includes a short discussion of work done in the related areas of spectral analysis and shield design. This work was required through contract F08650-94-C-0006, for the Advanced Research Projects Agency and the U.S. Air Force. The work on shield design is presented here as an illustration of the capabilities of the program.

The Simulation Program

A random number generator is used to simulate the behavior of gamma-rays as they pass through a detector. 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

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

[Ref 1], while the energy of the gamma-ray is calculated using the Klein- Nishina formula

$$\frac{d\sigma}{d\omega} = Zr_o^2\left(\frac{1}{1+\alpha(1-\cos\theta)}\right)^2\left(\frac{1+\cos^2\theta}{2}\right)\left(1+\frac{\alpha^2(1-\cos\theta)^2}{(1+\cos^2\theta)[1+\alpha(1-\cos\theta)]}\right). \qquad 2$$

BSIMUL was originally written with the assumption that the detector and shield would be cylindrically symmetric, and have constant radii. Removing the latter assumption created a substantial modification of the program, i.e., the subroutine used to calculate the time to a boundary between materials has been rewritten to enable the operator to model detectors with tapered parts. Rectangular parts can also be modeled by a slight modification to the collimator subroutines.

Since the program was originally written to model Germanium detectors, it was assumed that there would be a cold finger, dead layer, aluminum case, and possibly a shield. The detector material was assumed to be germanium, and changing it required editing the program. One array was used to specify both material and part, so that placing the shield inside the case, for instance, also required the program to be edited. The new version of the code separates the material from the part, and gives the operator complete freedom to use any design that contains fewer than 20 parts. One possible detector configuration is shown in Figure 1. The collimator subroutines that were discussed in the last annual report have now been fully tested.

In preparing to use the program with a graphical interface, the menu system has been replaced by an input file, shown in Table I. The first several lines (Table I-A) contain the number of events to be simulated, the isotopes and their relative strengths, and the source location. If the operator wants to simulate the spectrum of a source with a known strength,

it may be entered in nCi, muCi, or mCi. The program will calculate the number of gamma-rays that will be emitted in the direction of the detector. 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 5 is ignored.

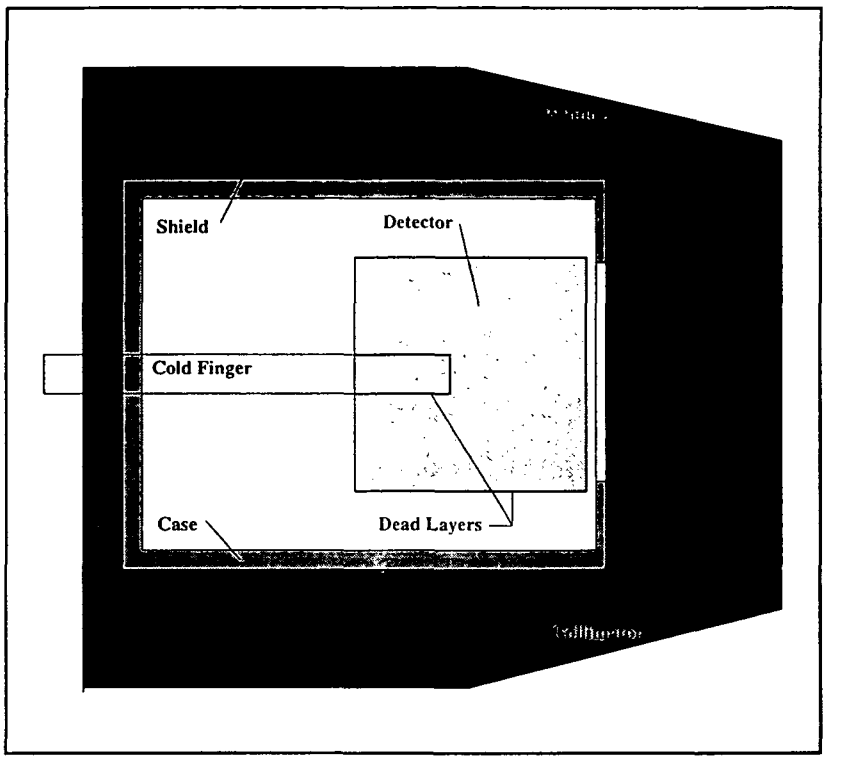

Figure 1: A sample detector and shield configuration.

The x and y source position parameters given in Table I-A are perpendicular to the axis of the detector shown in Figure 1. z is along the axis. The program is now capable of modelling rectangular or circular sources, which results in a more accurate simulation of a source that is close to the detector (or widespread). This can be particularly important in studying the effects of collimation on a spectrum. To model a point source, set the maximum and minimum radius values to zero and the program will run as before.

Table I-B shows the input and output files required to run BSIMUL. The isotope data files contain the energy and emission probability of each gamma-ray emitted with greater than 0.1% probability. Up to twenty isotopes may be used, and the number may easily be increased. The isotopes whose energies and emission probabilities are available are listed in Table II. In order to produce a realistic spectrum, the simulation must include elements that form a part of the natural background. Terrestrial background elements that form a prominent part of any spectrum are ^{40}K, ^{214}Bi, ^{212}Pb, and ^{228}Ac. The ratios of the activities

Table I-A. Input Parameters to BSIMUL.

Input file line	Comment
N	Y/N to plot the path of the gamma-rays through the detector system
counts	Event units: counts, nCi, μCi or mCi
100	Number of events
5676654 9612341	Random number seeds
1000.	Energy (keV) - used if no isotopes are specified
Source Position Parameters	
39.68	Source position on the z axis
C	Source symmetry: Rectangular or Circular (R or C)
0. 2.	Min, max source x dimension if rectangular, Radius if circular
	Min, max source y dimension (unused if circular)
Energy Calibration Parameters	
1500.	Maximum energy
20.	Minimum energy
4096	Maximum channel number
50.	Lower limit for detection in the shield
5000.	Lowest energy for Bremstrahlung
70.	Effective charge for Bremstrahlung

of these elements relative to the activity of ^{214}Bi have been found to be:

Isotope	Activity relative to ^{214}Bi
^{40}K	4.748
^{214}Bi	1.0
^{212}Pb	0.5227
^{228}Ac	0.4998

The simulation program uses the relative activities in calculating the probability of a

background gamma-ray.

The first output file will contain the spectrum of events occuring in the detector, the second will contain the spectrum of events occuring in the detector and not vetoed by the shield. The third and fourth files are used only when a collimator is specified. They contain spectra of events not vetoed by the collimator, and events vetoed neither by the collimator nor by the shield.

Table I-C contains the detector configuration and materials of the Near Earth Asteroid Rendezvous (NEAR) detector. The detector part is specified with a D in the second column; the shield and collimator are specified with an S and a C, respectively. The next variable is the material. Except in the case of BGO, this is written using the chemical formula. While the collimator material and dimensions are entered here, the hole pattern must be entered in the program itself.

Table I-B. Input Isotope and Output Spectrum Files.

Input File Line	Comment
2	Number of isotopes
bi-214 0.5	Isotope and percent probability of emission from that isotope
ac-228 0.5	
0.	Percentage of background isotopes
testbg2.sp	File name of spectrum of all counts in detector
testbgs2.sp	File name of spectrum of all counts not vetoed by the shield
temp5.sp	File name of spectrum of all counts not vetoed by the collimator
temp6.sp	File name of spectrum of all counts not vetoed by the collimator or shield

Table I-C. Input Detector Material and Configuration Parameters. These Are the Parameters Used to Model the NEAR Detector.

part	material	inner radius at bottom	outer radius at bottom	bottom	inner radius at top	outer radius at top	top
D	NaI	0.0	1.26	3.93	0.0	1.26	12.36
	Al	1.26	1.57	3.10	1.26	1.57	12.36
	Al	0.0	1.26	12.36	0.0	1.26	12.67
	Al	0.0	1.26	3.62	0.0	1.26	3.93
S	BGO	1.91	4.45	3.10	1.91	4.45	10.68
S	BGO	1.91	4.45	10.68	1.91	4.17	14.68
S	BGO	0.0	4.45	0.0	0.0	4.45	3.10

Table II. Isotopes with Gamma-Rays Available to the Program.

K 40	Co 60	Se 85	Sr 85
Y 88	Zr 95	Zr 97	Rb 89
Nb 94	Nb 95	Nb 95m	Mo 99
Ru 103	Ru 106	Tc 105	Tc 108a
Tc 108b	Cd 119	In 119	In 127a
In 127b	Sn 126	Sn 127	Sn 130
Sn 132	Te 132	Te 133	Te 133m
I 129	I 131	I 132	Xd 133
Cs 134	Cs 136	Cs 137	Ba 140
Ba 142	Ce 143	La 146	Sm 151
Bi 212	Bi 214	Cd 119	Ir 192
Tl 208	Pb 210	Pb 211	Pb 212
Pb 214	Rn 219	Rn 226	Ra 226
Th 227	Th 228	Ac 228	Pa 231
Pa 233	U 235	U 238	U 239
Np 239	Am 241	Am 243	Am 244
Am 244m	Cf 252		

Absorption Coefficients

The simulation program uses linear absorption coefficients in calculating interaction probabilities. A commercial program, PhotCoef, provides the linear photoabsorption, Compton, and pair production coefficients for each element in a compound. BSIMUL can use this to calculate absorption coefficients of any compound as follows:

$$\frac{\mu}{\rho} = \sum_{i=1}^{N} \frac{\mu_i}{\rho_i} w_i \qquad 3$$

where μ_i may represent the coefficient for photoabsorption, Compton absorption, or pair production of element i. N is the number of elements in the compound. w_i is the fraction by weight of the element i in the absorber, ρ_i is the density of the element, and ρ is the density of the compound.

The absorption coefficients of compounds calculated by BSIMUL were found to be the same as the coefficients calculated with PhotCoef to five significant figures. The absorption constants for each material in the library, shown in Table III, cover an energy range of 10 keV to 10 MeV in intervals of 10 keV up to 100 keV, in intervals of 100 keV up to 1 MeV, and in intervals of 1 MeV up to 10 MeV. The library will be expanded to contain all of the elements, so that any material can be modeled.

Table III. Materials with Linear Absorption Coefficients Calculated Using PhotCoef.

Elements					
Li	Be	B	C	N	O
F	Ne	Na	Al	Si	P
S	Cl	K	Cu	Ge	Cd
Te	Xe	Hg	Pb	Bi	
Compounds					
NaI	CsI	HgI_2	CdTe	BGO	

Detector Efficiency

The relative efficiency of a detector configuration can now be calculated from BSIMUL output. At the end of a simulation, the program now calculates the peak strengths by subtracting the average of twenty background points from the peak count value. The error is set equal to the square root of the average background value. Three files are produced:

File	Contents
fn.xda	Energy calibration constants
fn.pk	Peak position and error, FWHM and error, strength and error, and peak type
fn.ca	Peak position and error, energy and error, peak strength and error, emission probability and error

These files are used as the input files to the calibration program XCALIBER, which calculates a fit to the efficiency using cubic splines. The efficiency curve produced in this way may be considered to be an upper limit to the actual detector efficiency, since the BSIMUL peaks are one channel wide, and no strength is lost in the long tail.

One warning must be issued here. Both ^{214}Bi and ^{228}Ac emit a 904 keV gamma-ray. When ^{214}Bi and ^{228}Ac were first used as the efficiency calibration elements, the whole strength of that peak was attributed to both elements, and the calibration results were wildly wrong. In writing the calibration file the program now omits peaks whose energies are close enough that their photopeaks are placed in the same channel.

Calculations

NEAR NaI Detector

The configuration of the NEAR detector is shown in Figure 2. Several simulations have been performed with this configuration. The spectra were convoluted with a NaI peak shape. The spectra shown in Figure 3 are the BSIMUL output and convolution of a Bi 214 and Ac 228 spectrum. The output from BSIMUL was used to calculate the efficiency of the detector as a function of energy. The shield does lower the Compton background significantly, as is shown in Figure 5. The efficiency, shown in Figure 6, is the same for both the nonvetoed spectrum and the spectrum of all counts. A fit to the convoluted spectrum of nonvetoed counts, shown in Figure 7, produced the peaks listed in Table IV.

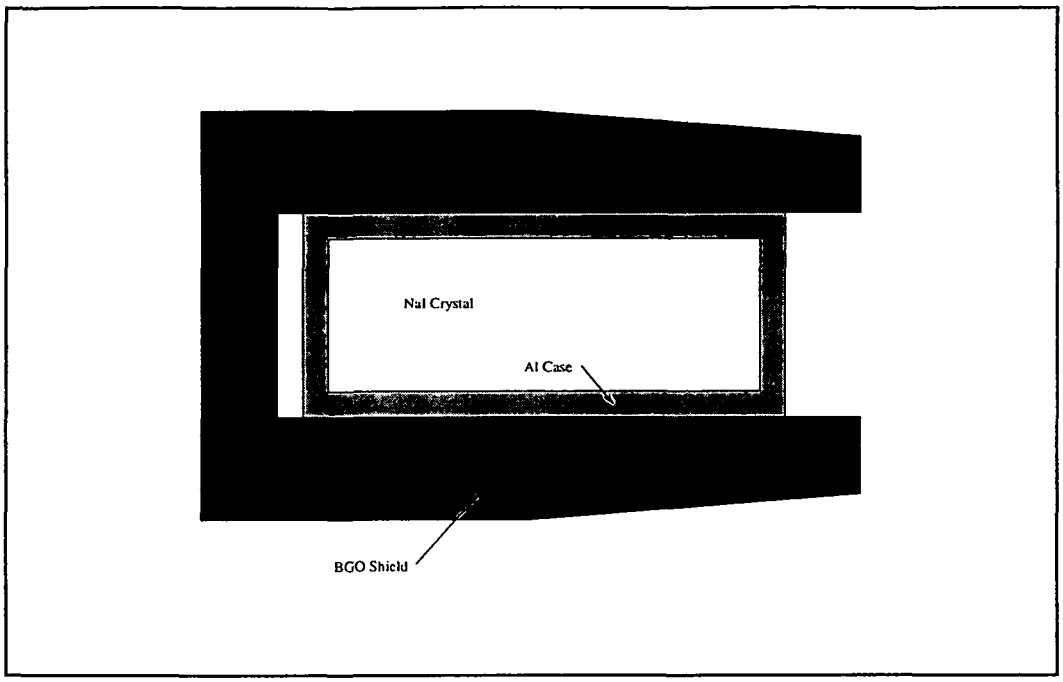

Figure 2. The NEAR Detector Configuration

A series of runs were performed to study the count rate as a function of the source position. Figures 7-9 show three of the spectra, which were calculated with Co and Cs sources. The peak and background count values in the 661 keV peak as a function of source position are listed in Table V. The sharp reduction in the peak count rate for all the energies that occurs at 11.5 degrees is due to the source being moved into the shadow of the shield. The increase in the peak count rate as the source is moved away from the vertical axis from 40 to 80 degrees has been seen experimentally in a Germanium detector. As Figure 9 shows, the shield is quite effective in preventing gamma-ray from entering through the side of the detector.

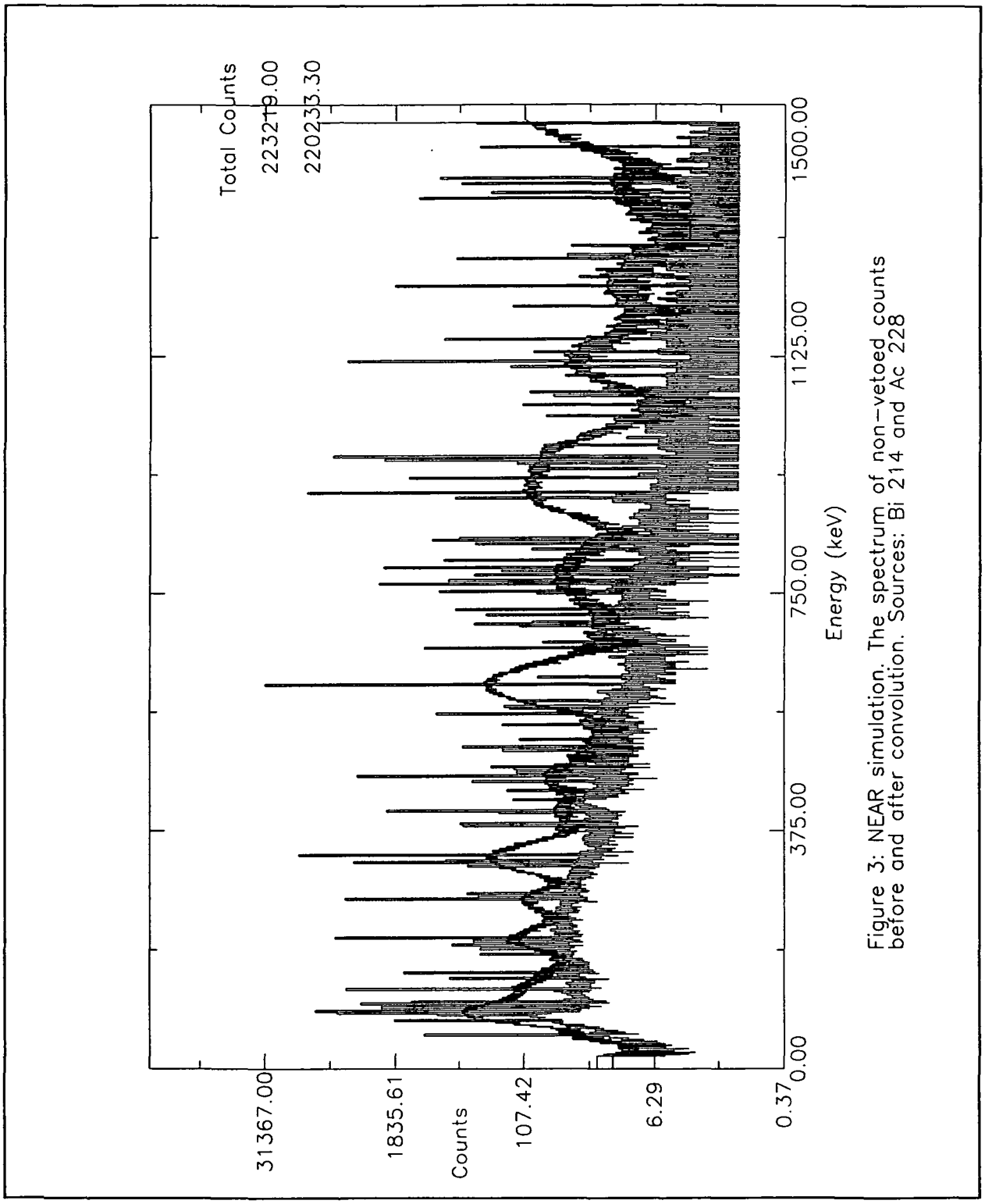

Figure 3: NEAR simulation. The spectrum of non-vetoed counts before and after convolution. Sources: Bi 214 and Ac 228

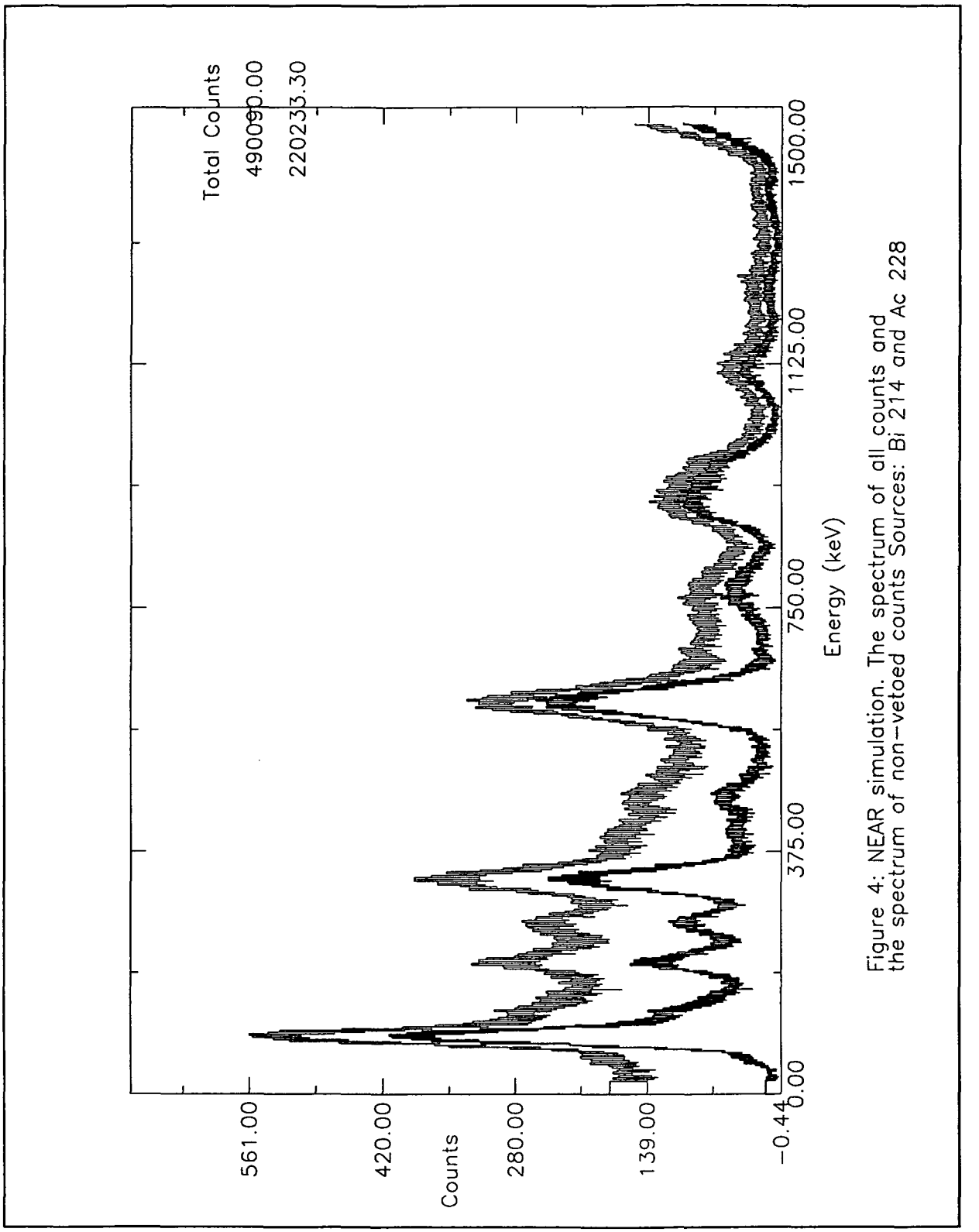

Figure 4: NEAR simulation. The spectrum of all counts and the spectrum of non-vetoed counts Sources: Bi 214 and Ac 228

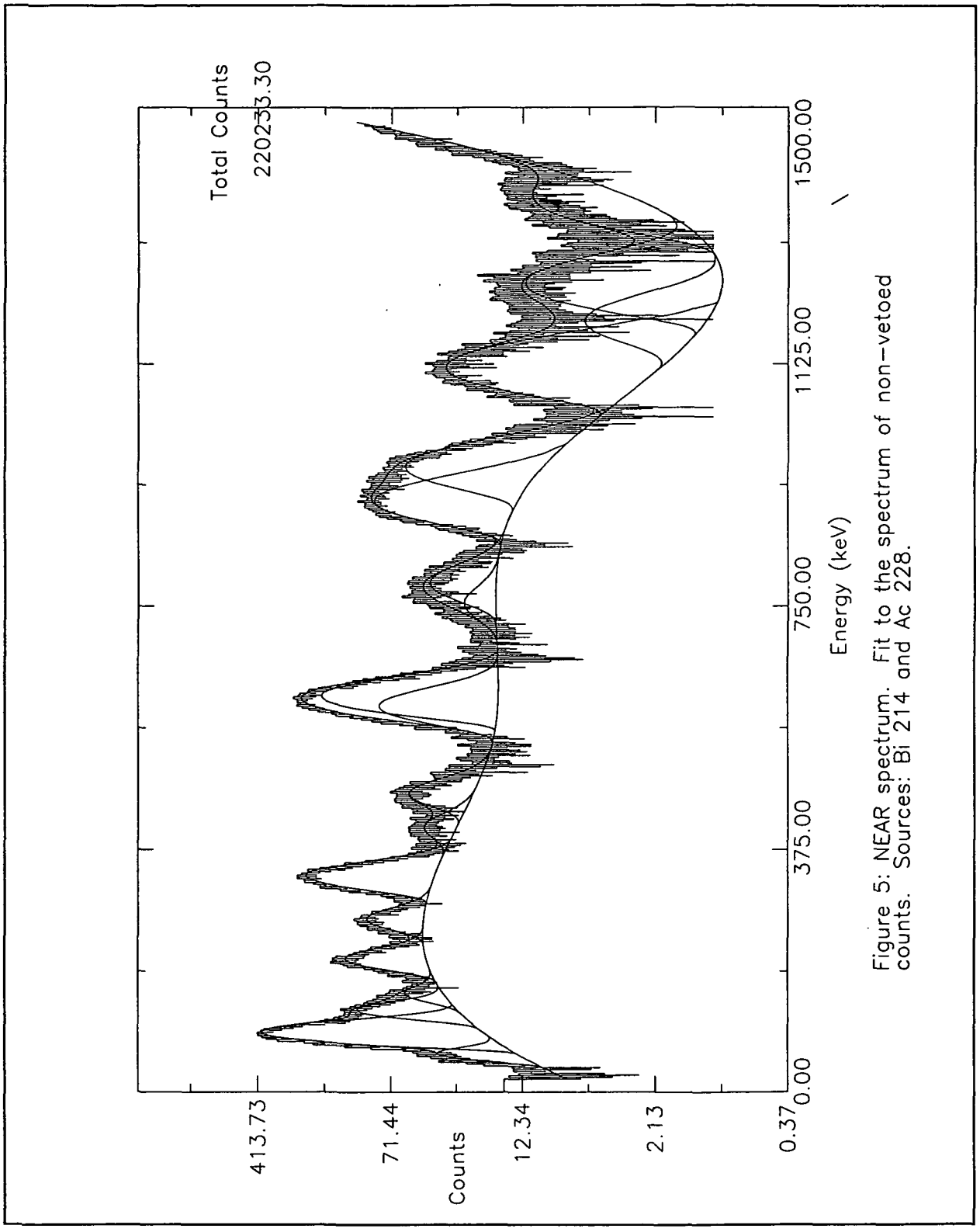

Figure 5: NEAR spectrum. Fit to the spectrum of non-vetoed counts. Sources: Bi 214 and Ac 228.

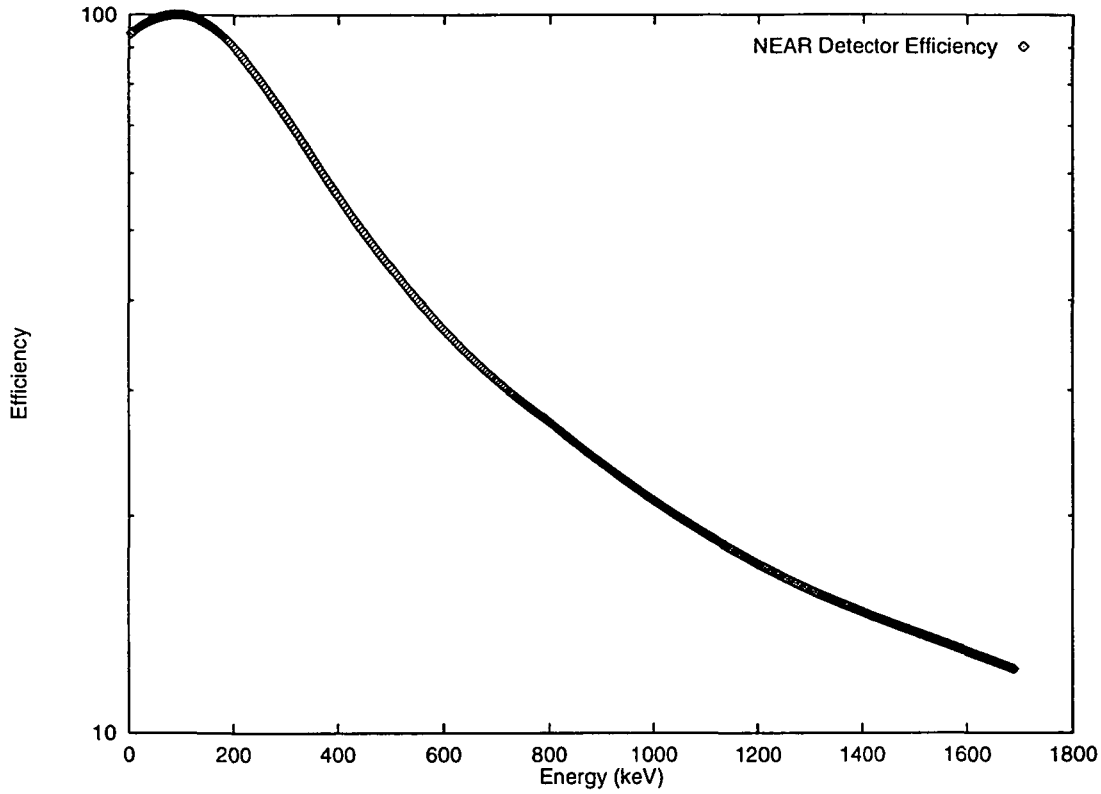

Figure 6: Simulated NEAR Efficiency.

Table IV. Peaks Found in the Convoluted NEAR Spectrum that was Simulated with Bi 214 and Ac 228 Isotopes.

Analysis Results		Isotope Data [Ref 2]		
Energy (keV)	Peak strength (counts)	Energy (keV)	Emission Probability (%)	Isotope
59.82 +/- .5	1398.12 +/- 69.41	57.81	.525	Ac-228
92.99 +/- 1.	29922.5 +/- 245.6	89.955 93.35	3.4 5.6	Ac-228 Ac-228
127.83 +/- .5	5929.66 +/- 182.2	129.03	2.9	Ac-228
153.06 +/- 1.2	1809.79 +/- 141.4	153.89	.84	Ac-228
207.17 +/- .28	7599.96 +/- 124.9	209.31	4.1	Ac-228
268.04 +/- .4	5016.51 +/- 113.4	270.26	3.8	Ac-228
333.92 +/- .16	18242.9 +/- 168.8	328.07 338.42	3.5 12.4	Ac-228 Ac-228
409.88 +/- 1.	1914.51 +/- 92.24	409.62	2.2	Ac-228
461.29 +/- .7	3960.20 +/- 101.6	463.1	4.6	Ac-228
594.92 +/- 4.	9288.07 +/- 4570.			
609.68 +/- 2.	21103.3 +/- 4595.	609.311	46.1	Bi 214
751.88 +/- 5.6	1429.28 +/- 422.4	755.28 768.35	1.32 4.88	Ac 228 Bi 214
783.20 +/- 2.4	3972.13 +/- 426.4	794.79	4.6	Ac-228
910.28 +/- .5	12872.1 +/- 221.6	911.16	29.	Ac-228
963.81 +/- .8	8690.42 +/- 211.5	964.64	5.8	Ac-228
1116.44 +/- .6	6118.90 +/- 108.0	1120.27	15.	Bi 214
1188.78 +/- 7.	838.668 +/- 83.50	1155.18	1.69	Bi 214
1246.04 +/- 1.8	2196.66 +/- 108.4	1238.11	5.9	Bi 214
1373.92 +/- 1.2	1634.47 +/- 54.26	1377.66	4.02	Bi 214

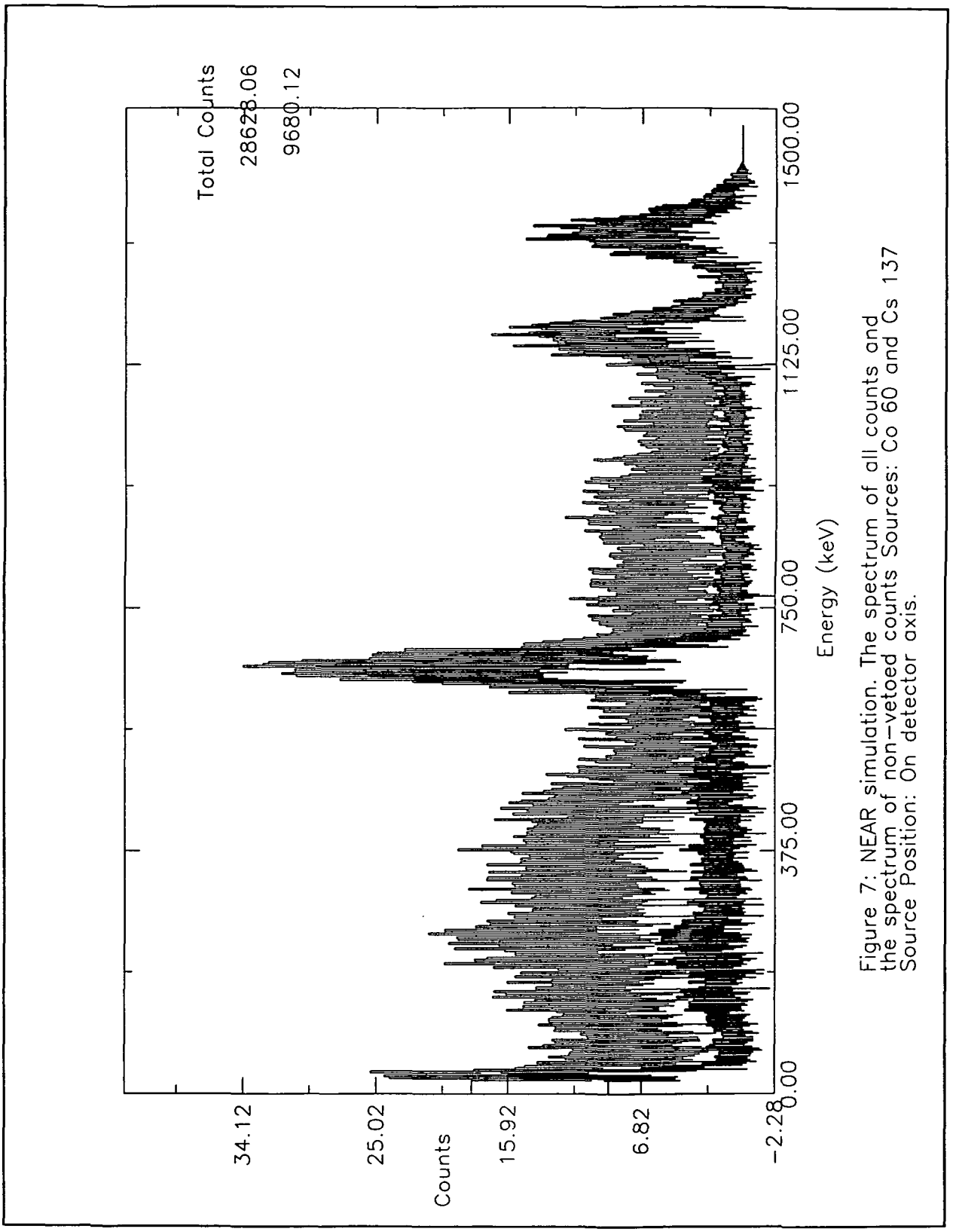

Figure 7: NEAR simulation. The spectrum of all counts and the spectrum of non-vetoed counts Sources: Co 60 and Cs 137 Source Position: On detector axis.

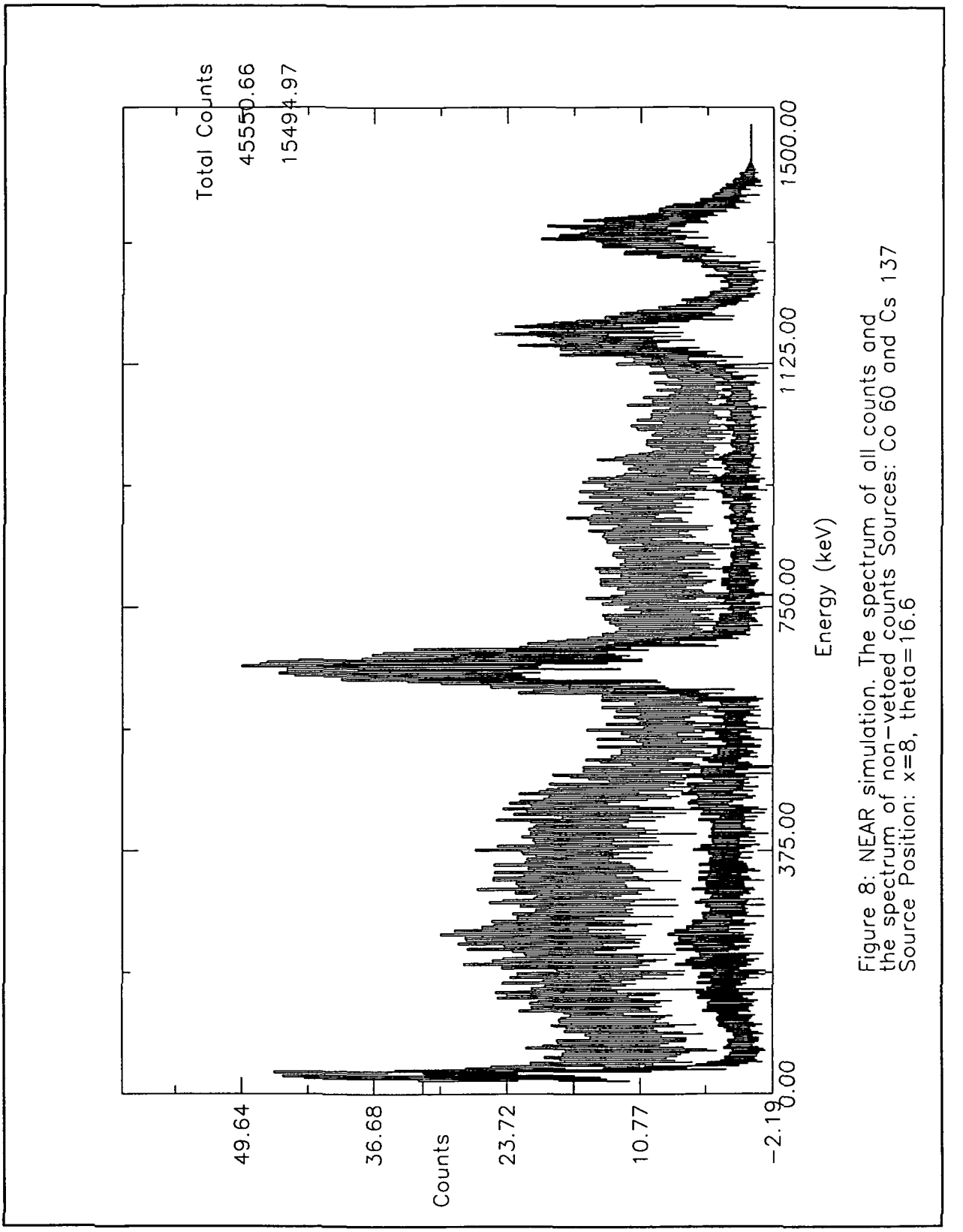

Figure 8: NEAR simulation. The spectrum of all counts and the spectrum of non-vetoed counts Sources: Co 60 and Cs 137 Source Position: x=8, theta=16.6

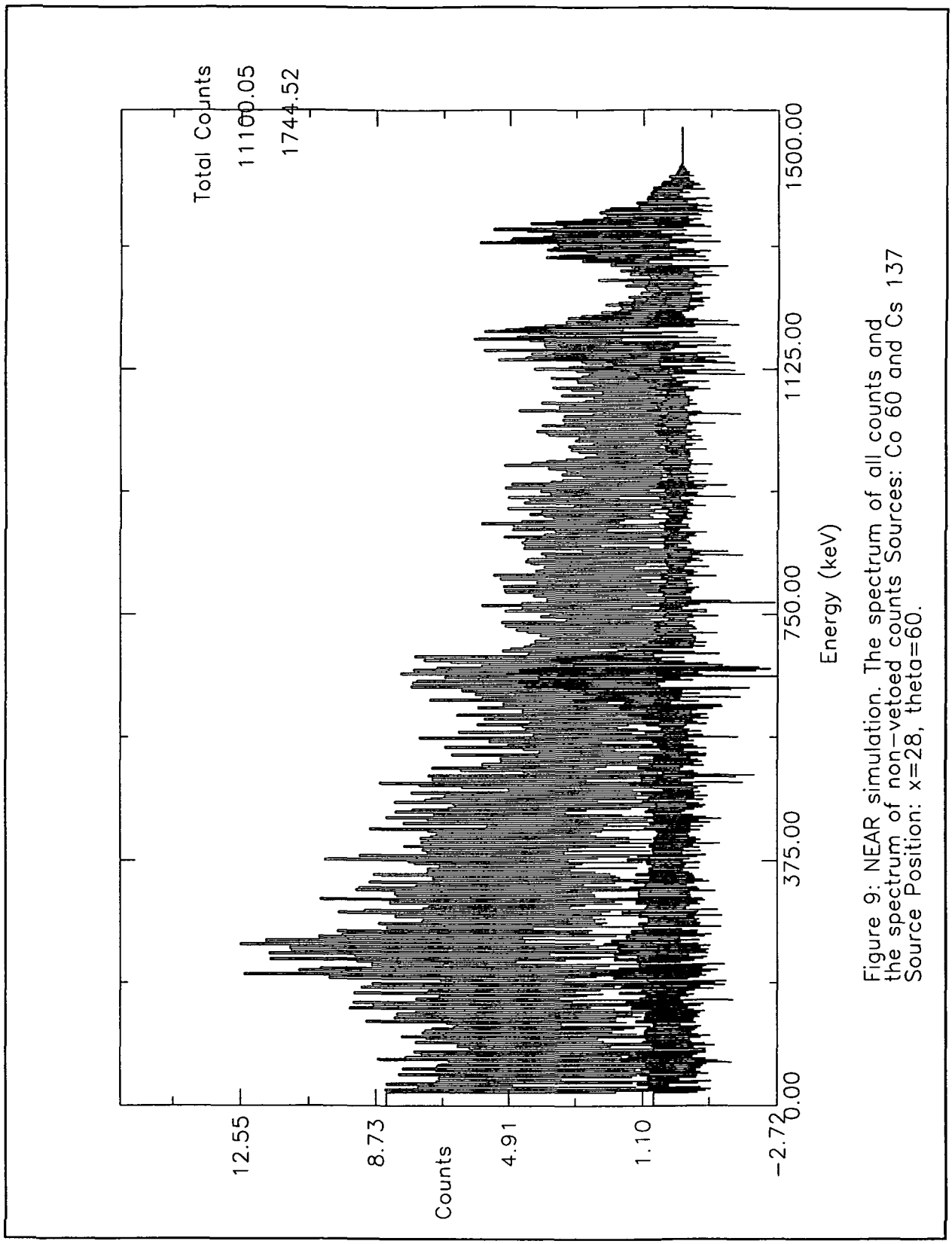

Figure 9: NEAR simulation. The spectrum of all counts and the spectrum of non-vetoed counts Sources: Co 60 and Cs 137 Source Position: x=28, theta=60.

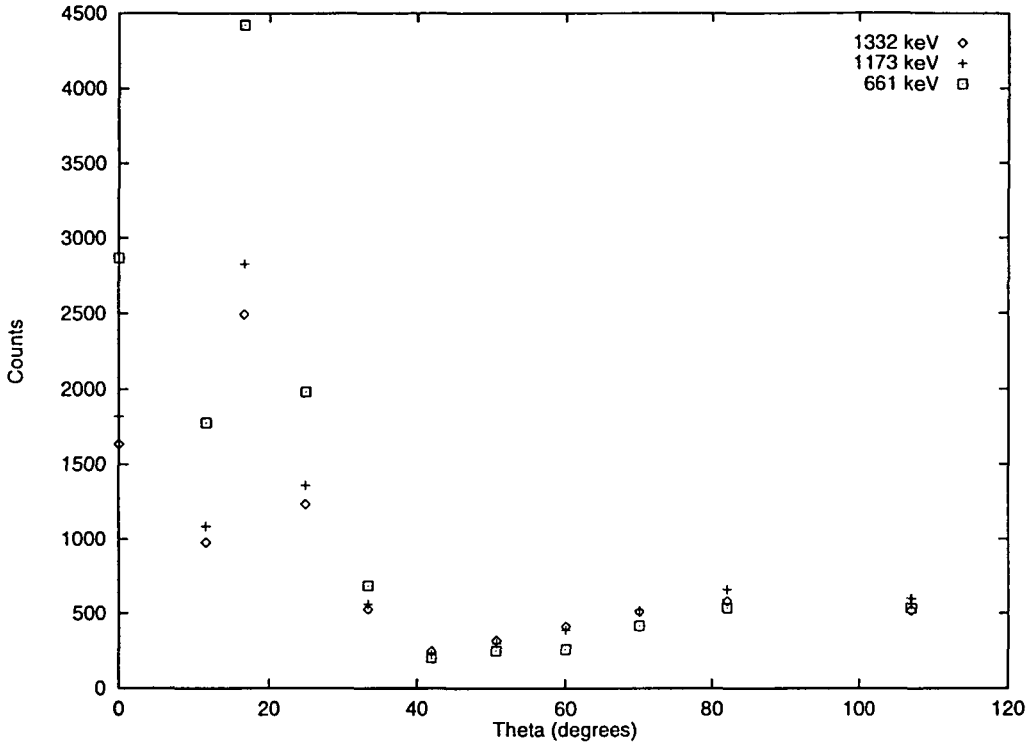

Figure 10: The peak count rates as a function of the angle between the source position and detector axis.

Table V. Source Position Dependance of the 661 keV Peak and Background Count Rate.

x	Theta (degrees)	Counts in 661 keV peak	Counts in background of nonvetoed spectrum at 661 keV	Counts in background of spectrum of all counts at 661 keV.
0.	0.	2870	13	91
4.	11.5	1774	9	49
8.	16.6	4422	25	144
12.	25	1980	16	81
16.	33.4	683	5	49
20.	42	202	3	36
24.	50.7	247	5	36
28.	60	259	3	40
32.	70	418	8	49
36.	82	536	5	45
40.	107	532	9	49

Ge Detectors

The work discussed in this section was performed pursuant to the requirements of contract F08650-94-C-0006, for the Advanced Research Projects Agency (ARPA) and the U.S. Air Force. It is included here as an illustration of the capabilities of the program. The work also proved to be useful as a full test of several of the modifications that have been made under the NASA contract.

The Germanium detector response was modeled with BSIMUL for various detector/shield geometries, and source/background conditions. Figure 10 shows an overlay of data taken

with a 30% Ge detector and a BGO shield. ^{137}Cs and ^{60}Co sources of roughly equal strength were used. A 1% background was assumed, and the shield shape was approximated, since the actual shield does not have cylindrical symmetry. The simulated spectrum was not given an accurate peak shape, since the interest was in the peak strengths only.

The simulations were done using the dimensions for a 100% Ge crystal unless otherwise specified; and a 2 mm thick aluminum case around the crystal was assumed. A minimum of one million gamma-rays were used for each spectrum, a study of the detector performance as a function of shield thickness was made. Figure 11 shows the peak-to-Compton ratios and Figures-of-Merit obtained using CsI and BGO shields. The background was 10 times the source strength. The shield extended 6 cm in front of the detector, so that the acceptance angle was about 69°. It was found that the optimum acceptance angle varies with the source strength and background count rate: if the shield extends far in front of the detector, the gamma-rays will Compton scatter from the shield to the detector.

Simulations were run to determine the difference in performance between N and P type Ge detectors as a function of detector efficiency. The detector and shield mass were varied to keep the total mass constant, so as the detector efficiency was increased, the shield thickness was decreased. The Figure-of-Merit (FOM)

$$F_2(E_1) = \frac{\epsilon(E_1)}{[R(E_1)\epsilon_{c2}(E_1)]^{1/2}} \qquad 4$$

is useful in evaluating the suitability of a detector for a particular task. $\epsilon(E)$ is the efficiency at energy E, $\epsilon_{c2}(E)$ is the Compton efficiency due to a second gamma-ray, and R is the resolution. A plot of the FOM relative to the FOM obtained using and un-shielded 100% N-type detector vs. the detector efficiency for both N and P type detectors is shown in Figure 12 for two low energy gamma-rays. At 129 keV the advantage of N over P type is evident, while at 375 keV there appears to be no significant difference.

A collimator with a 10° angle of acceptance was modeled using a range of gamma-ray energies. The peak count rate as a function of source position is shown in Figure 16. Because a point source was used, there is a reduction in peak counts occurring below 5°.

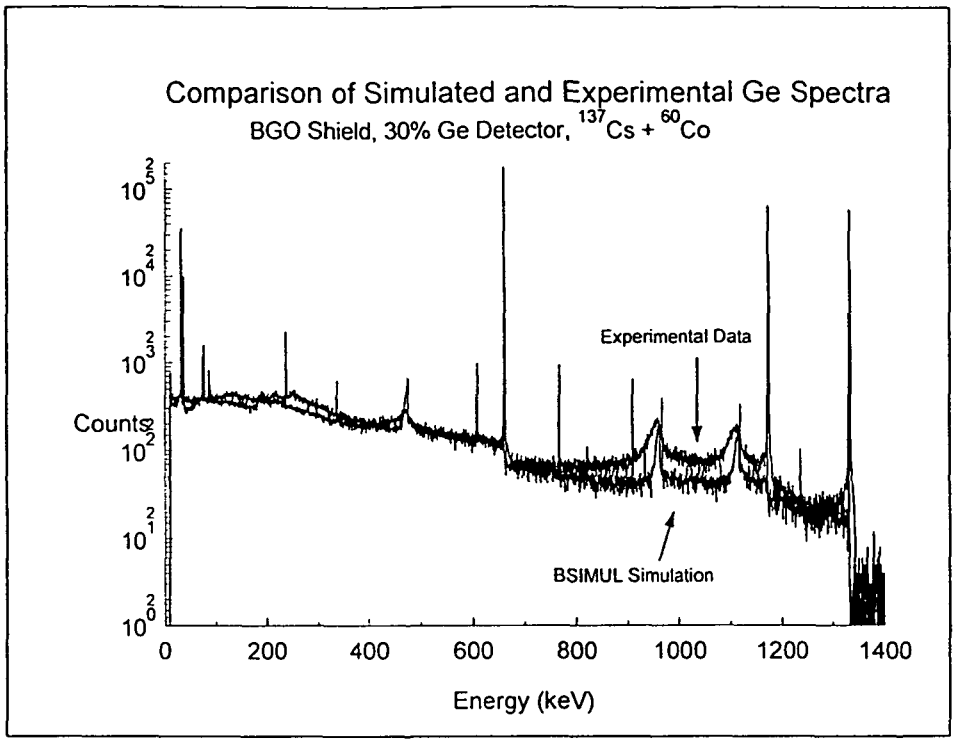

Figure 11. Comparison of BSIMUL data and experimental

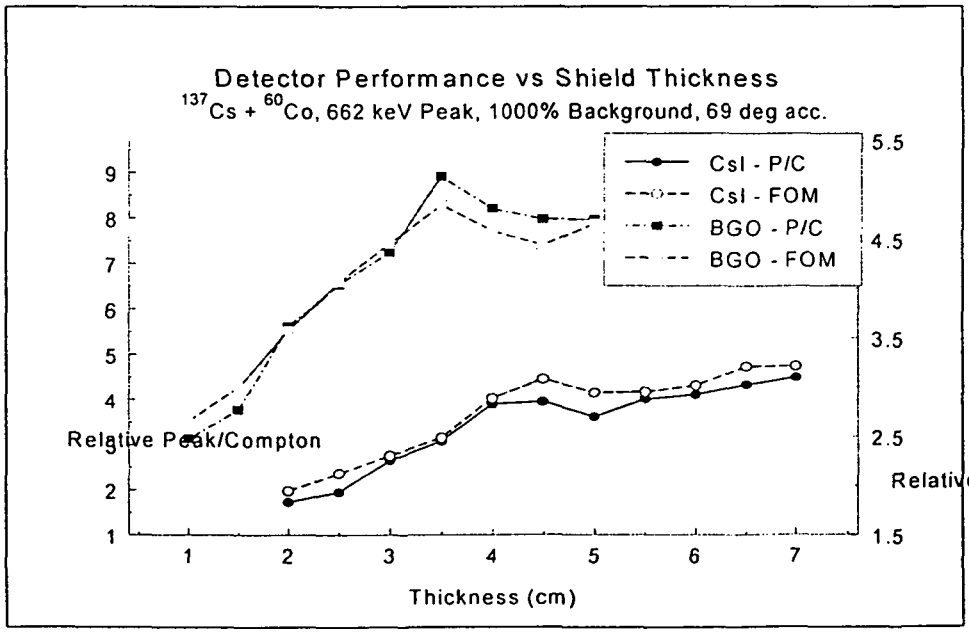

Figure 12. Performance vs. shield thickness, 1000% background, 69 deg acceptance angle

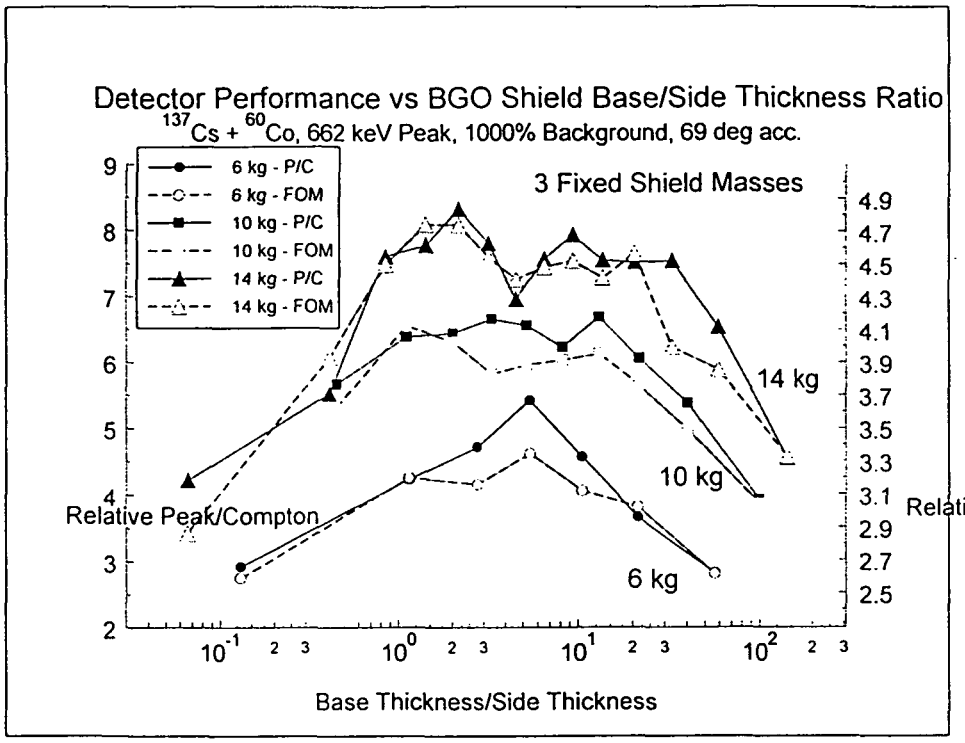

Figure 13. Ge detector performance vs. shield base thickness/side thickness

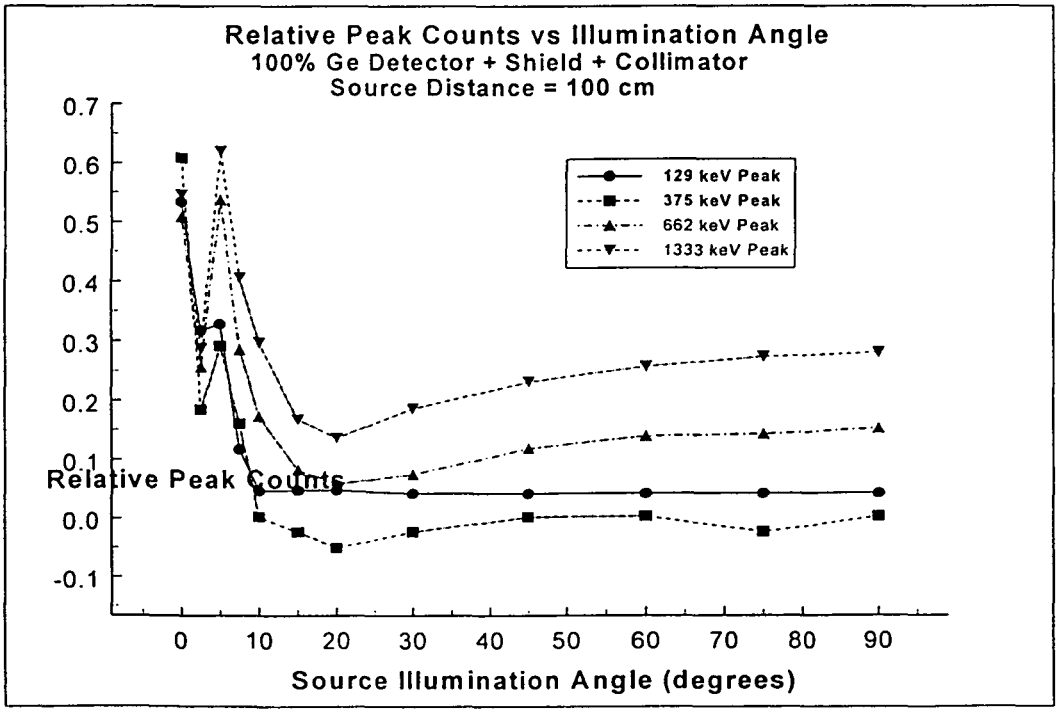

Figure 14. Plot of peak counts vs source illumination angle for various sources

Includes Constellation Technology Competition Sensitive Propriety Data

Progress on Related Work

ROBFIT

The work on the spectral analysis package ROBFIT was required through contract F08650-94-C-0006, for the Advanced Research Projects Agency and the U.S. Air Force. A new program, UNKFIT, has been added to ROBFIT. Its purpose is to fit spectra taken with Germanium detectors and produce a list of the isotopes present and their relative concentrations. UNKFIT is now in the integration and debugging phase. During the course of writing UNKFIT, we were able to realize an enormous simplicification in the automation of ROBFIT. This simplification was accomplished by including the functions previously done with a sequence of modules used to fit the background, fit the peaks, and then identify the isotopes. In a further simplication, UNKFIT now uses detector-specific characteristics. Only one menu file is now required.

These changes are expected to result in greater reliability and have been shown to reduce the total analysis time of a spectrum taken for 15 minutes to less than 5 minutes. In its present state, UNKFIT detects only the naturally-occuring background isotopes. Initially, these were identified at about the 5-sigma level in all but one of ten Monte-Carlo-generated test spectra. Current work includes debugging the UNKFIT module and adding isotopes of possible interest to the library.

The test spectrum ztcase9.sp, shown in Figure 15, was a background spectrum taken for 72 hours in a room containing a depleted fuel rod that was fully shielded by lead bricks. The spectrum has been fully analyzed and the isotopes and their relative activities are listed in Table VI. The program is now able to report the uncertainty with which an isotope is known to be missing from the spectrum as well as to be present. For instance, in the case of ^{239}U the results can be interpreted as evidence that this isotope is missing.

Table VI. Isotopes Found in the Background Spectrum ztcase9.sp.

Isotope	Activity relative to Bi 214	Error in relative activity
Bi 214	1.	.00324
Ac 228	.4998	.0112
Cf 252	.3119	1.17
Am 244	.00258	.0004
Am 243	.001224	.00116
Am 241	.04849	.0103

U 239	.002484	.0230
Np 239	.01564	.00256
U 235	.0499	.00537
Th 234	2.133	.173
Pa 233	.002646	.000964
Pa 231	.02171	.00717
Th 228	2.335	.305
Th 227	.008366	.00640
Ra 226	1.573	.173
Rn 219	.05646	.00654
Pb 214	.9114	.0261
Pb 212	.5227	.0277
Bi 212	.5849	.0113
Pb 211	.06563	.00839
Pb 210	1.042	.197
Ti 208	.1919	.00484
Sm 151	269	95.1
La 146	.009242	.00102
Ba 142	.02338	.00215
Cs 137	.008366	.000386
Pa 134	1.329	.0578
Te 133	.007349	.00165
Te 133m	.002175	.000306
Xe 133	.04282	.00720
Sn 130	.0004989	.000538
Sn 132	.002874	.000482
I 132	.01477	.00293

I 129	.1457	.0328
In 127	.003770	.000780
Sn 127	.005990	.00112
Sn 126	.06098	.00894
Cd 119	.007802	.000701
In 119	.07988	.0183
Tc 108	.01746	.00160
Ru 106	.5493	.514
Tc 105	.04410	.00817
Zr 95	.003118	.000988
Nb 95	.03256	.00391
Nb 94	.0009307	.000210
Rb 89	.004132	.00144
Y 88	.0001841	.000166
Se 85	.01185	.00127
Sr 85	.001052	.000394
Co 60	.001630	.000124
K 40	4.748	.0361

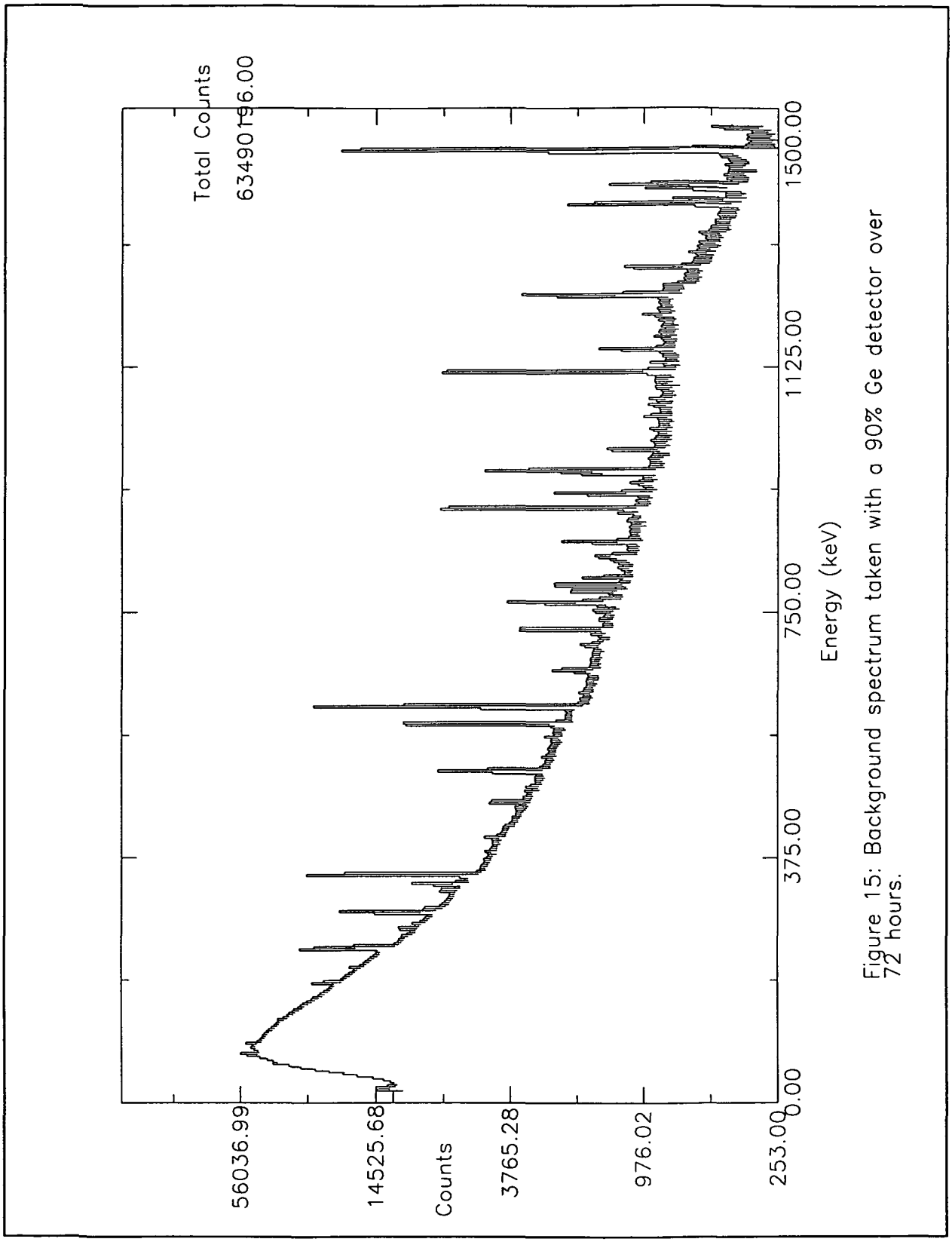

Figure 15: Background spectrum taken with a 90% Ge detector over 72 hours.

Plans

Gamma-ray Spectrometer Modeling Studies

During the coming year, the modifications to BSIMUL will be completed. 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. New subroutines will be written that will allow the operator to model a detector and shield of any configuration. Since removing the symmetry requirements will slow the calculation, the subroutines that currently take advantage of cylindrical or rectangular symmetry will be used where possible. The convolution program will be integrated into BSIMUL, so that a spectrum will be given an accurate peak shape automatically. The result of these changes will be a program that is much easier to use than the current version.

BSIMUL has been tested and works well at energies ranging from 50 keV to 1500 keV. Testing of the x-ray and high energy gamma-ray regions will be performed. The low energy range will be extended from 10 keV to 1 keV so that both x-ray florescence and gamma-ray systems can be simulated. The program can be used to model the behavior of any desired detector system.

The x-ray simulations will be verified with spectra obtained using a HgI_2 detector. The detector will be used in conjunction with active and passive shielding materials to provide a thorough test of the program at x-ray energies.

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16. Abstract

Progress made during 1995 on the Monte-Carlo gamma-ray spectrum simulation program BSIMUL is discussed. Several features have been added, including the ability to model shields that are tapered cylinders. Several simulations were made on the Near Earth Asteroid Rendevous detector.

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