IITRI

Report No. IITRI V6032-15

COMPOSITIONAL ANALYSIS OF LUNAR AND PLANETARY SURFACES USING NEUTRON CAPTURE GAMMA RAYS

to

Elmer Christensen, Code MAL
National Aeronautics and Space Administration
Washington, D. C. 20546

NASr-65(18)

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October 1, 1969 to December 31, 1969

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Washington, D. C. 20546

January 1970

FOREWORD

This is Report No. IITRI-V6032-15, under Contract No. NASr 65(18), entitled "Compositional Analysis of Lunar and Planetary Surfaces Using Neutron Capture Gamma Rays," covering the period from October 1, 1969 to December 31, 1969.

The following personnel have contributed to the work described in this report: J. H. Reed, principal investigator and J. W. Mandler, co-investigator.

Respectfully submitted,
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I. INTRODUCTION

The purpose of this research program is the continued development of the Combined Pulsed Neutron Experiment (CPNE) for lunar and planetary surface analysis. This experiment utilizes five different neutron analytical techniques (capture gamma-ray analysis, fast activation analysis, inelastic neutron scattering, thermal neutron die-away, and epithermal neutron die-away) which have been integrated into a single experimental package for the purpose of performing compositional analyses of planetary surfaces. Much of the earlier work was concerned with establishing the feasibility of using the different neutron techniques for the elemental analysis of bulk samples and with integrating the five techniques into a single package. Since the feasibility of the combined neutron experiment has been established, the major objectives now are to develop analytical techniques which will be used to derive from the data the maximum of information and to optimize the experimental parameters.

During this reporting period the major effort has been aimed at two specific tasks: (1) the development of computer techniques for the analysis of the data, and (2) studies which will aid in the determination of the final experimental parameters such as pulse rate and sampling times. A simulated capture gamma-ray spectrum of a moon rock returned from the Apollo 11 landing was generated (assuming laboratory conditions and a small sample) and analyzed using ALPHA-M. Investigations were initiated to simulate the capture gamma-ray plus activation spectra obtained from basalt, dunite, and granite using the combined neutron experiment. The TIME computer code was modified so that it could perform parametric studies to optimize the pulse rate. A meeting was held with R. L. Heath, R. G. Helmer, and J. E. Cline to discuss methods of data analysis and to obtain information concerning available computer programs for the analysis of gamma-ray spectra.

II. SIMULATION OF CAPTURE GAMMA-RAY SPECTRA

A. Capture Gamma-Ray Spectrum from a Moon Rock

Preliminary analyses of moon rocks returned from the Apollo 11 landing[1] indicate that the compositions are unlike those of any known terrestrial rock or meteorite. Although they were found to resemble earthly basalt, they exhibited an unusually high titanium, chromium, zirconium, and yttrium content and a very low sodium and potassium content. Since the capture gamma-ray technique is sensitive to many of these minor constituents, namely titanium, chromium, sodium, and potassium, it is of interest to see what type of a capture gamma-ray spectrum a moon rock would exhibit. A simulated capture gamma-ray spectrum from moon rock No. 61[1] was generated from spectra of individual elements obtained from Greenwood and Reed's atlas[2] of capture gamma-ray spectra. The simulated spectrum shown in Figure 1 was obtained after normalizing (using the 7.64 MeV iron peak) to an intensity obtainable with the combined neutron experiment. This spectrum is very similar in appearance to the capture gamma-ray spectrum from an earthly basalt except that the titanium contribution is much greater.

This simulated capture gamma-ray spectrum from moon rock No. 61 represents the spectrum which would be obtained under laboratory conditions using a small sample. Therefore, it represents the best capture gamma-ray spectrum which can be obtained using a 3 inch x 3 inch NaI(Tl) detector. The spectrum which would be obtained by the combined neutron experiment would exhibit degradation due to the attenuation of gamma rays in the bulk sample and a background due to neutron interactions in the detector and gamma rays from Compton scattering in the sample.

In order to determine the sensitivities for elemental detection which can be expected when analyzing the lunar surface using the capture gamma-ray technique, the simulated capture gamma-ray spectrum from moon rock No. 61 was analyzed using the ALPHA-M computer program. The results of this analysis, given in Table 1, indicate that the capture gamma-ray technique can yield accurate determinations for all the major elements (oxygen is determined using the activation spectrum which is obtained as part of the capture gamma-ray experiment) and many of the minor elements. Table 2 contains the sensitivities which can be expected using the capture gamma-ray technique. These sensitivities represent the best obtainable (for the given statistics) using the capture gamma-ray technique under laboratory conditions. The sensitivities attainable using the capture gamma-ray technique in the combined neutron experiment are expected to be slightly poorer than those in Table 2.

B. Capture Gamma-Ray Spectra from Basalt, Dunite, and Granite

Since the simulated capture gamma-ray spectrum from moon rock No. 61 shown in Figure 1 was obtained directly from a linear combination of elemental spectra from Greenwood and Reed's atlas, it represents the capture gamma-ray spectrum expected from the laboratory analysis of a small sample The sensitivities predicted using this spectrum will differ from those obtainable using the combined neutron epxeriment. Simulated spectra which more closely approximate experimental spectra are necessary in order to predict accurately the sensitivities expected from the combined neutron experiment.

As a first step in generating accurate simulated spectra from the combined neutron experiment, the elemental spectra from the atlas were attenuated. It was assumed that on the average all the gamma rays pass through 10 gm/cm^2 of sample before striking the crystal (earlier calculations indicated that about 50 percent of the gamma rays originate in the top 10 gm/cm^2 of the sample)

Table 1

ANALYSIS OF SIMULATED CAPTURE GAMMA-RAY SPECTRUM FROM MOON ROCK NO. 61

Element	Chemical Analysis	Analysis of Capture Gamma-Ray Spectrum
	Concentration (wt. %)	
Si	18.7	18.7 ± 0.6
Fe	12.4	12.6 ± 0.1
Al	5.8	5.9 ± 0.4
Ca	7.9	8.3 ± 0.3
Mg	5.4	7.6 ± 1.4
Na	0.37	*
K	0.15	0.14 ± 0.15
Ti	5.4	5.43 ± 0.02
Ni	0.0235	**
Cr	0.30	0.31 ± 0.08
Mn	0.24	0.18 ± 0.04

* Detection threshold for Na is 0.4 wt. percent.

** Detection threshold for Ni is 0.05 wt. percent.

Table 2

EXPECTED DETECTION THRESHOLDS FOR THE CAPTURE GAMMA-RAY TECHNIQUE

Element	Detection Threshold (wt. %)
Si	0.6
Fe	0.1
Al	0.4
Ca	0.3
Mg	1.4
Na	0.4
K	0.15
Ti	0.02
Ni	0.05
Cr	0.08
Mn	0.04
H	0.01
Cl	0.02

and that for the purpose of attenuation the sample matrix has the composition of concrete. This library of attenuated elemental spectra was then used to construct simulated capture gamma-ray spectra from basalt, dunite, and granite. The simulated spectra were normalized to experimental spectra using an energy region centered at 7.64 MeV and then an activation component was added to each yielding simulated capture plus activation spectra. The activation components were obtained from experimental delayed spectra (using the TIME code to determine the intensities to be used).

These simulated capture plus activation spectra were still not completely acceptable because they did not include background components due to neutron interactions in the crystal and Compton scattered gamma rays. As a first attempt at constructing the necessary backgrounds a preliminary background was formed for each of the three spectra by dividing the spectra into 10 channel groups, summing these groups, and then subtracting the groups of simulated data from the corresponding groups of experimental data. Each background curve thus obtained was smoothed to remove any possible structure and then added to its corresponding simulated spectrum yielding the solid curves shown in Figures 2, 3, and 4. The experimental spectra which we are attempting to simulate are indicated by point plots in Figures 2, 3, and 4.

A cursory examination of Figures 2, 3, and 4 yields the following conclusions. In general, the simulated capture plus activation spectra give a good approximation of the experimental spectra. Discrepancies occur in the titanium content of the basalt (the simulated spectrum overestimates the titanium contribution), the hydrogen content of all three samples (the simulated spectra all underestimate the hydrogen contribution although the discrepancy is small in the case of the basalt), and the activation contribution to the granite spectrum (the results from the TIME code seem to slightly underestimate the activation contribution). Despite these discrepancies (which may be due merely to erroneous normalizations of atlas spectra), the simulated spectra adequately approximate the experimental data.

The conclusions which can be drawn from the comparison of the simulated and the experimental capture plus activation spectra are (1) the TIME code can adequately predict the capture and activation contributions to the spectrum, (2) the assumption that on the average the gamma rays pass through about 10 gm/cm^2 of sample before striking the detector is adequate, and (3) an experimental spectrum can successfully be simulated using the atlas spectra. However, before simulated spectra can be used to predict the sensitivities which the combined neutron experiment can attain, a closer look at the background due to neutron interactions in the detector and Compton scattered gamma rays will be made. In particular, an attempt will be made to obtain an analytic expression for this background so that it can be added to the individual elemental spectra. These elemental spectra are needed for the library used in ALPHA-M. Also, the effects of resolution smearing will be investigated in an attempt to take into account small angle scattering of gamma rays.

III. ANALYSIS OF EXPERIMENTAL PARAMETERS

Studies concerning the optimization of experimental parameters such as pulse rate, sampling times, neutron output, and analyzer dead time are continuing. The TIME code[3] which was written to aid in these studies was modified to require as input the ratio of the effective number of capture gamma rays to background (activation plus natural activity) gamma rays produced per neutron pulse instead of the ratio of capture gamma-ray intensity to background gamma-ray intensity at the end of the neutron burst. This change enables TIME to perform parametric studies to optimize the pulse rate.

Some results from parametric studies performed using the modified TIME code are given in Table 3. This table gives the number of capture gamma rays and background gamma rays expected to be detected during the given sampling intervals. In these calculations the average analyzer dead time was assumed to be 40 μsec (a value obtained from experimental spectra) and the thermal neutron half lives were obtained from Reference 4 (145 μsec for basalt, 190 μsec for granite, 296 μsec for dunite). The ratio of the effective number of capture gamma rays to background gamma rays produced per neutron pulse (for a given neutron output) were determined by performing a parametric study of this ratio using TIME and comparing the results with experimental data. The values used were 2.20 for basalt, 1.40 for dunite, and 1.05 for granite.

The results shown in Table 3 indicate that the intensity of the capture gamma-ray spectrum can be substantially increased by changing from the 100-330 μsec window (used in previous experimental studies) to a 20-480 μsec window. As expected, the ratio of capture gamma rays to background gamma rays detected exhibit a decrease of about a factor of two and the number of capture gamma rays detected per unit time doubles

Table 3 RESULTS OF PARAMETRIC STUDIES USING TIME CODE

Sample	Pulse Rate (pps)	Gate Opened (μsec)	Gate Closed (μsec)	Capture Gamma Rays Detected	Background Gamma Rays Detected	Number of Pulses
Basalt	494	100	330	3380	274	5000
Basalt	494	1570	1800	20	449	5000
Basalt	494	20	600	5081	348	5000
Basalt	494	20	480	4820	318	5000
Basalt	1000	20	480	4666	798	5000
Dunite	494	100	330	2441	545	5000
Dunite	494	1570	1800	163	673	5000
Dunite	494	20	600	4096	814	5000
Dunite	494	20	480	3821	690	5000
Dunite	1000	20	480	3783	1284	5000
Granite	494	100	330	2633	597	5000
Granite	494	1570	1800	20	839	5000
Granite	1000	20	480	3750	1478	5000

when the pulse rate is doubled. The effects on the sensitivities of these changes in window and pulse rate are as yet unknown. Investigations to determine the effects of intensity and the ratio of capture gamma rays to background gamma rays will be initiated when an acceptable library of simulated elemental capture gamma-ray spectra from bulk samples has been generated. We strongly suspect that changing the window to 20-480 μsec will result in an increase in sensitivity for a given sampling duration.

IV. MEETINGS

A Combined Pulsed Neutron Experiment Meeting was held at the Goddard Space Flight Center on November 19 and 20, 1969. The purpose of the meeting was to duscuss and to determine the direction and emphasis of future developmental work. For planning purposes it was assumed that the CPNE would be used on a lunar rover with extended surface exploration capabilities. Accepting that the feasibility of the CPNE has been established, two areas of development require considerable work.

1. Study configuration parameters, having as a goal the reduction of the experimental weight to a reasonable value.
2. Study various aspects of electronics and environment pertinent to the integration of the CPNE to the rover.

Listed below are sixteen questions that were generated at the meeting. When these questions are answered the CPNE should be defined, permitting breadborading and field testing.

1. What is the maximum sensitivity for each technique (capture, inelastic, epithermal die-away, and thermal die-away) based on independent measurements using a geometry that is optimum for each technique?
2. How is the CPNE effected by replacing the molybdenum attenuator with a beryllium attenuator?
3. To what degree is the capture sensitivity dependent on reflector thickness? How does the reflector influence the inelastic scattering, epithermal die-away and thermal die-away?
4. What is the capability of the experiment, with and without reflector, to measure the minor elements?

5. Is the weight of the reflector and/or the shadow shield worth the redundancy it provides in the measurement of hydrogen?
6. To what degree is performance and sensitivity sacrificed if the 3 in. x 3 in. NaI(Tl) detector is replaced by a 2 in. x 3 in. NaI(Tl) detector?
7. What weight savings is realized if the 3 in. x 3 in. NaI(Tl) detector is replaced by a 2 in. x 3 in. NaI(Tl) detector? (This would include the smaller attenuator.)
8. What radiation level and energy spectrum is produced by the RTG that is to be used on the dual mode roving vehicle?
9. What would be the effect of the RTG radiation on the CPNE performance capability?
10. What requirements should be included in a "radiation quality specification."
11. What requirements would the CPNE impose on the space craft and what environment is required by the experiment (storage and operational)?
12. Is it desirable and practical to incorporate the He^3 cadmium detector on the probe center line?
13. What are the telemetry requirements and specifications?
14. Will the experiment be required to operate at night?
15. Are specifications available for space qualified linear signal processing components?
16. Will a data multiplexer be developed and available for this experiment?

Studies aimed at answering these sixteen questions will be the basis of the research to be undertaken during the coming year.

On December 5, 1969 IITRI personnel met with R. L. Heath, R. G. Helmer, and J. E. Cline at the Idaho Nuclear Corporation. The purpose of this meeting was to discuss methods of data analysis and to obtain information concerning available computer programs for the analysis of gamma-ray spectra. Various methods for the analysis of gamma-ray spectra, including the GAUST, "library," and Trombka approaches (see report No. IITRI V6032-14 for brief discussions of these approaches) were discussed. The consensus was that the "library" approach seemed to be the most appropriate for the capture gamma-ray portion of the CPNE.

We obtained listings of the computer programs GAUSS 3 and SYSPHUS at this meeting and discussed GAUSS 5 (a more recent version of GAUSS 3). SYSPHUS uses the "library" approach to analyze gamma-ray spectra obtained using NaI(Tl) detectors and it contains several desirable features not available in ALPHA-M. GAUSS 3 and GAUSS 5 are programs used to analyze gamma-ray spectra obtained using Ge(Li) detectors. GAUSS 5 has the added feature of being able to search a spectrum and locate peaks. We plan to make these codes operational at the IITRI computer facility and investigate their usefulness in the analysis of our data.

V. FUTURE WORK

The investigations concerning the simulation of spectra from the CPNE will continue. In particular, the background due to neutron interactions in the detector and Compton scattered gamma rays will be closely studied. A crystal activation spectrum will be obtained and incorporated in the library of capture gamma-ray spectra. The goal of these investigations will be the acquisition of a library of simulated elemental capture gamma-ray spectra from bulk samples. This library will be used in the analysis of simulated basalt, dunite, and granite spectra for the determination of the sensitivities attainable using the CPNE.

The studies concerning the optimization of the pulse rate, gate times, and neutron output will continue. The TIME code will be used to predict the optimum parameters on the basis of the detected number of capture and background gamma rays. Simulated spectra obtained using these parameters will then be analyzed in order to determine their effects on sensitivity.

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4. W. R. Mills and W. W. Givens, "Neutron Die-Away Experiment for Lunar and Planetary Surface Analysis - Phase II," Final Report July 3, 1967 to June 28, 1969, Mobil Research and Development Corporation.

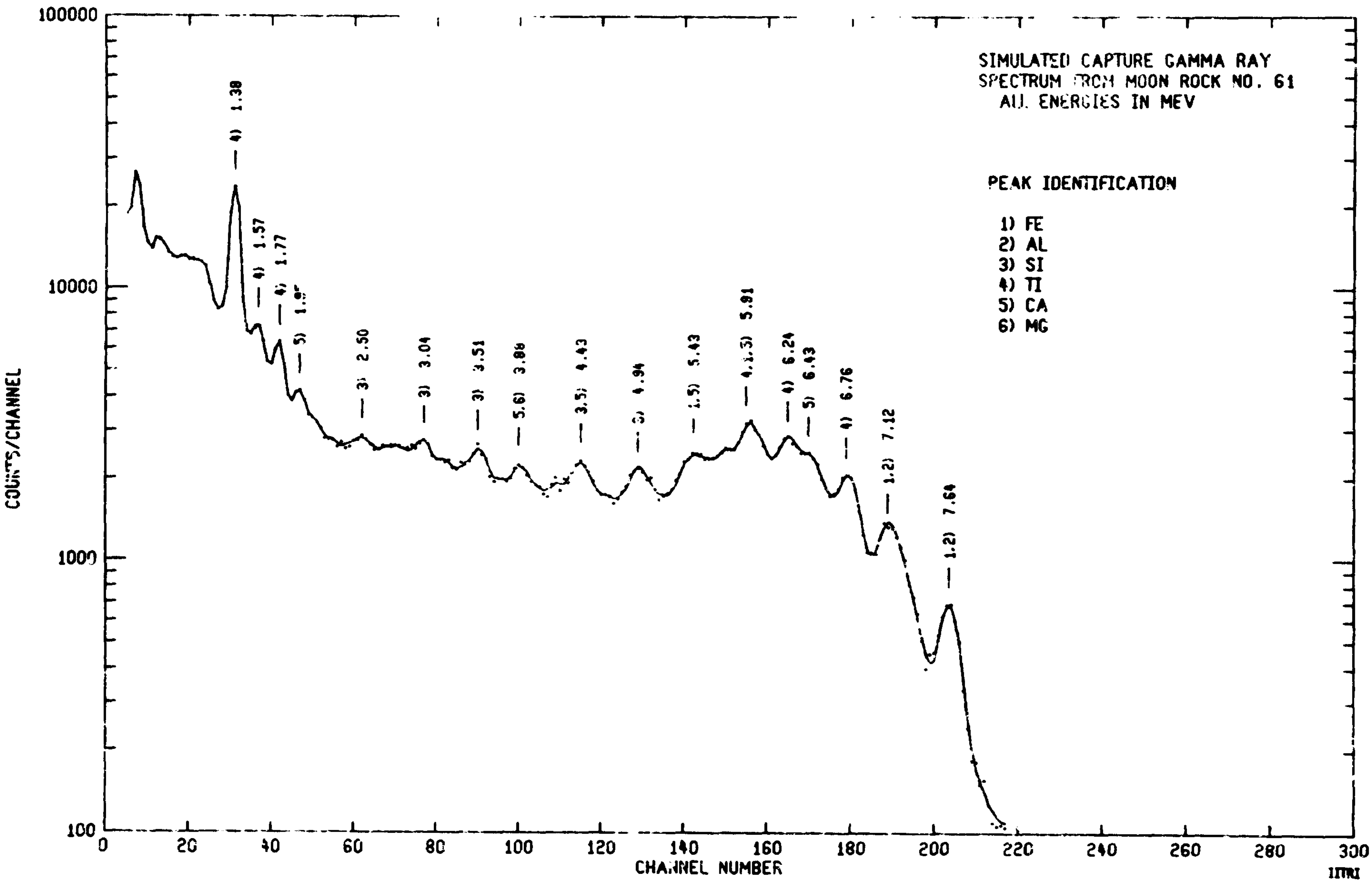

Figure 1 SIMULATED CAPTURE GAMMA-RAY SPECTRUM FROM MOON ROCK NO. 61

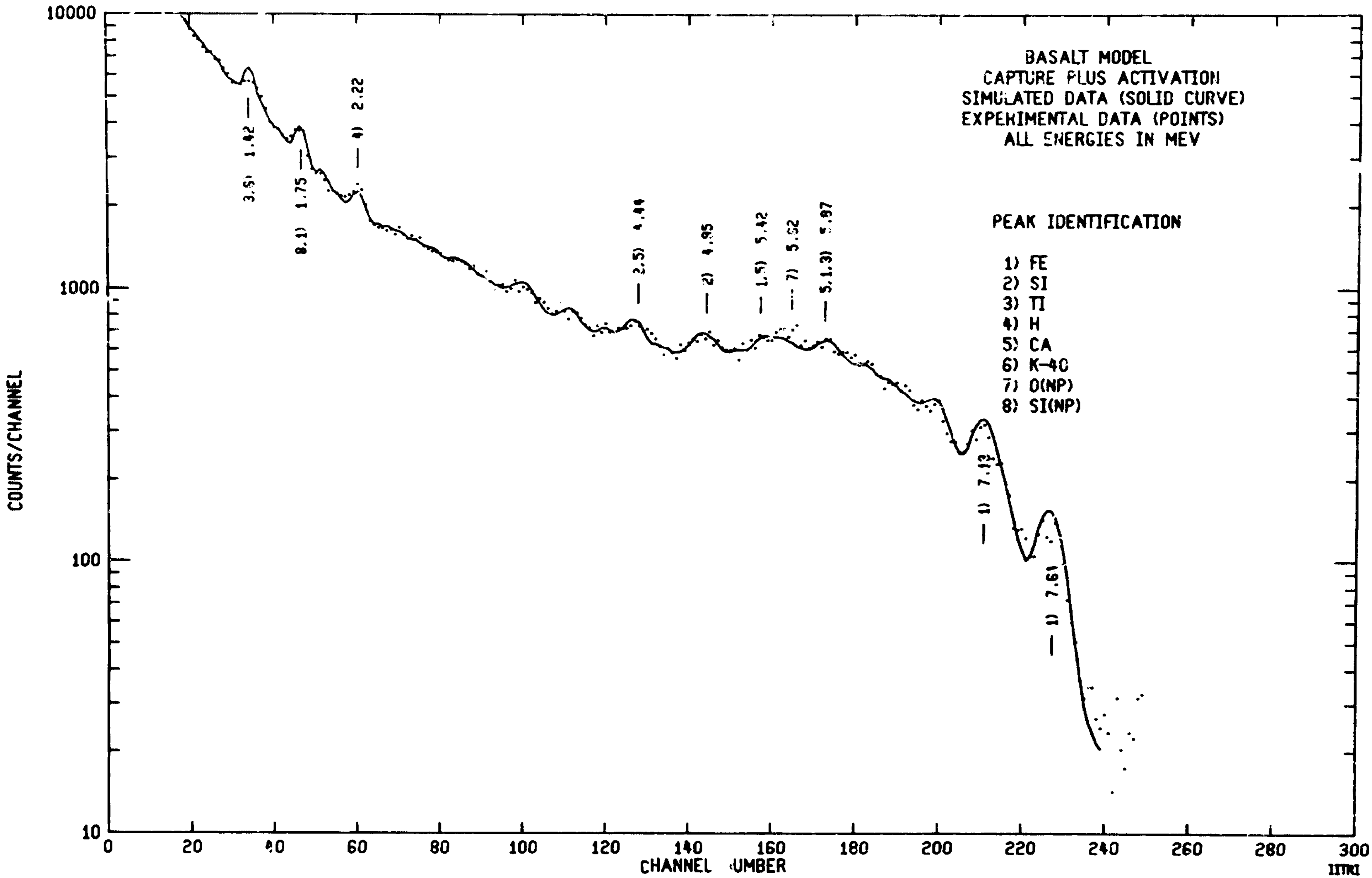

Figure 2 COMPARISON OF SIMULATED AND EXPERIMENTAL CAPTURE PLUS ACTIVATION SPECTRUM FROM BASALT

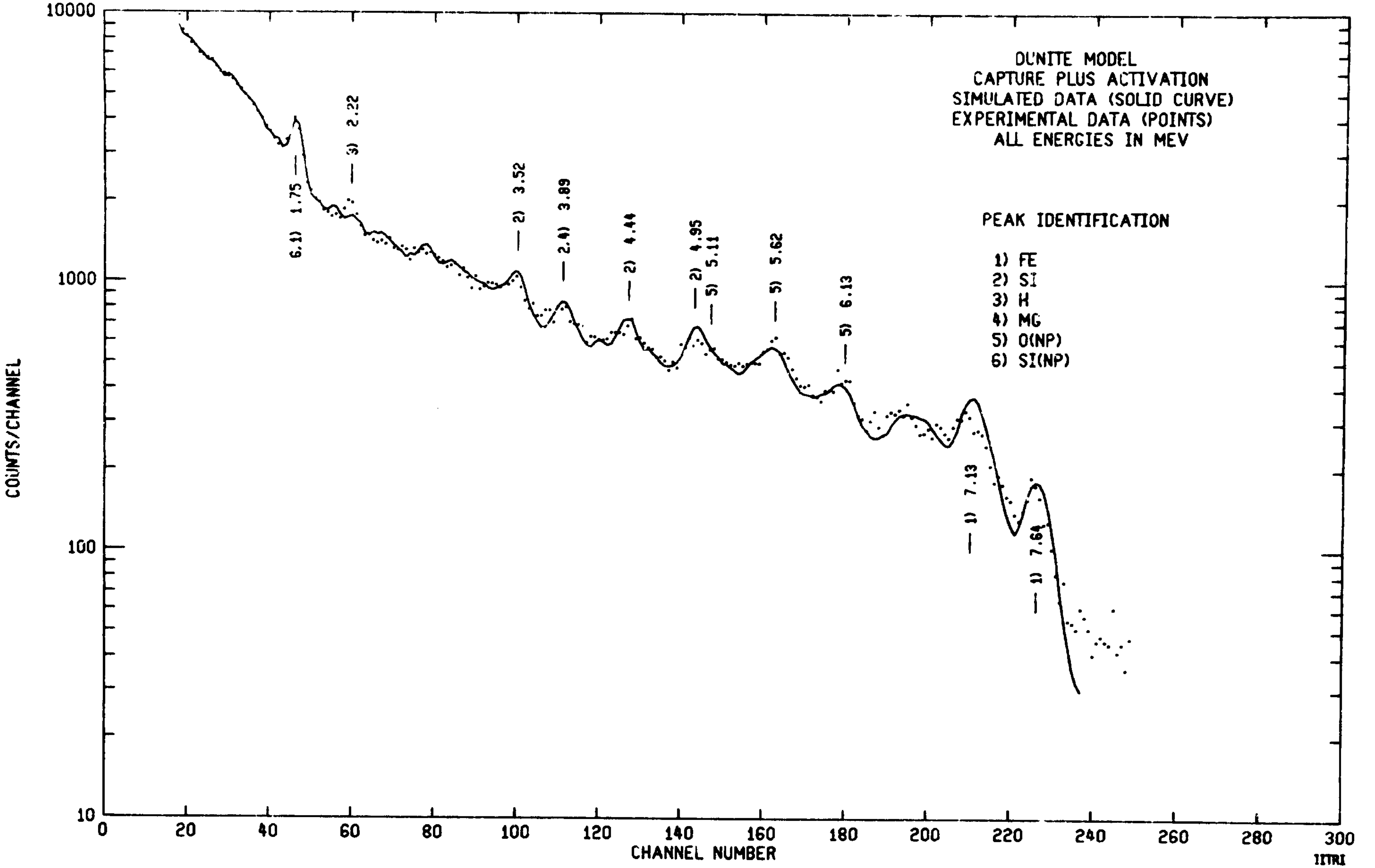

Figure 3 COMPARISON OF SIMULATED AND EXPERIMENTAL CAPTURE PLUS ACTIVATION SPECTRUM FROM DUNITE

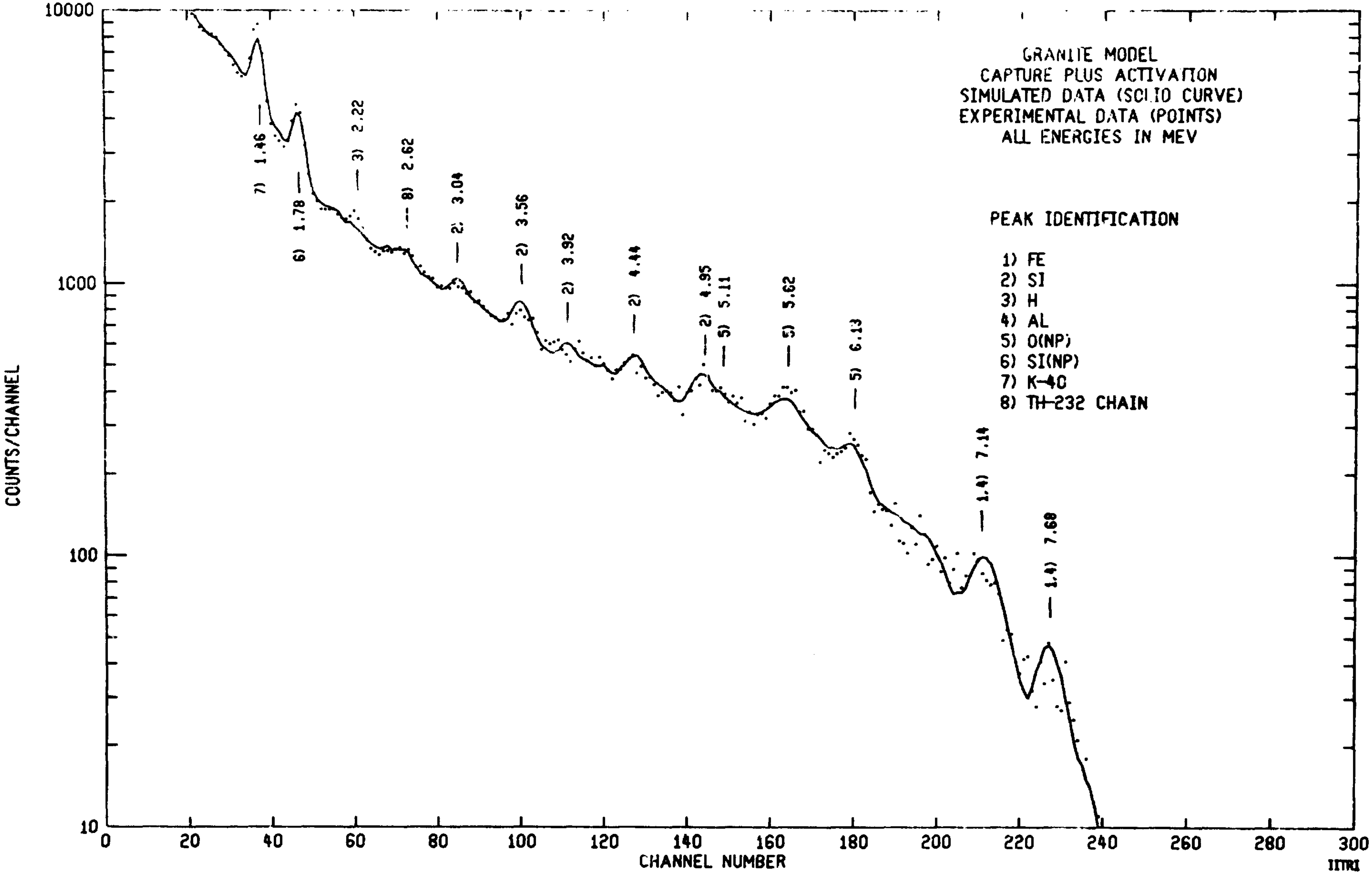

Figure 4 COMPARISON OF SIMULATED AND EXPERIMENTAL CAPTURE PLUS ACTIVATION SPECTRUM FROM GRANITE