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SUBROUTINES FOR THE MINUIT PROGRAM FOR THE DECONVOLUTION OF ANNIHILATION LINE

by

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Abstract: *The subroutines of the MINUIT program for the deconvolution of the Doppler broadened annihilation line and the results of the deconvolution in some metals and ionic crystals are presented. The effects of some parameters of the deconvolution are discussed.*

1. INTRODUCTION

In the annihilation process of a zero energy electron-positron pair the resulted two photons are emitted to opposite directions with energy of each photon equal to 511 keV. Due to the fact that the energy of electrons is different from zero the angle between these two photons is not exactly 180^0 and the energy is not exactly 511 keV (Doppler broadening of the annihilation line). The broadening of the line is measured using high resolution solid state detectors as Ge(Li) or intrinsic Ge.

In the measurement of the Doppler broadening of annihilation radiation using a solid state detector the FWHM of the resolution function is substantial compared to the FWHM of the Doppler broadened line.

In order to compensate the poor resolution of solid state detectors, computer programs designed to deconvolute Doppler broadened spectra have been developed by Hotz et al (H68), Rama Reddy and Carrigan (R70), Dauwe et al (D72), Jackman et al (J74) and Dannefaer and Kerr (D75).

This paper describes a deconvolution technique similar in some respects with (J74) and (D75) and the appropriate routines for the UNIVAC 1106 and PDP 11/34A.

The deconvolution program uses the MINUIT program (J77), modified for the UNIVAC 1106 and for the PDP 11/34A (D82), as the fitting program. The program computes the Fermi momentum of electrons and the contribution of core electrons in metals, the intensity of various components of annihilation in ionic crystals and the narrow component of para-positronium in ionic and molecular materials.

2. REVIEW OF THE METHOD*

The experimentally observed Doppler broadened spectrum F can be written as:

$$F_i = \sum_{j=1}^{n} R_{i-j} U_j \qquad (1)$$

where F_i is the value of F in channel i, R is the detector resolution function defined over 2n-1 channels, U is the unknown function for which we are searching, and n is the number of channels over which F and U are defined. The function R is determined experimentally using the 514 keV line of ^{85}Sr or ^{85}Kr. The spectra F and R are used in the program directly as recorded, except for the substraction of a constant background which is determined from the high energy side of each spectrum. The solution, U, to eq. (1) is determined in an iterative way, by assuming an initial test function U^1 which is folded according to eq. (1) to produce a function F^1. Then F^1 is compared, channel by channel, with F, and U^1 is modified to produce an improved test function U^2 according to:

$$U_i^2 = U_i^1 \left\{ \frac{\sum_{j=i-a}^{j=i+a} F_j}{\sum_{j=i-a}^{j=i+a} F_j^1} \right\}^n \qquad (2)$$

The correction to U^1_i is based on 2a+1 channel region centered on the ith channel (the value of a is determined from the width of the resolution function) for two reasons: First, it is desirable to use more than one channel in the correction ratio to reduce the effect of sharp statisti-

* The analysis is based mainly on (D75)

cal fluctuations in the experimental data which tend to produce oscillations in the modified test functions. Second, due to the smearing effect of the resolution function, a difference between F and F^1 over a region covering many channels centered on clannel i is, in part, a reflection of the difference between U and U^1 in channel i alone. The improved test function U^2 is then folded according eq. (1) producing a new F^2 function which is used to produce U^3 etc.
After each iteration the x^2:

$$x^2 = N^{-1} \sum_{i=1}^{N} (F_i - F_i^K)^2 / F_i \qquad (3)$$

is calculated. The iteration procedure is stopped if the rate of change of x^2 is fallen below a value specified by the user.
The exponent n in eq (2) has values either 1 or 2. This is required to reduce the number of iterations needed for the convergence of the deconvolution.

To obtain quantitative information a model is introduced and fitted to the solution obtained by iterations. The curve thus determined from the fitting is used as a new test function, and is folded with the resolution function and compared with the experimental spectrum by calculating the x^2 for the purpose of determining the goodness of the fit. At this point one iteration cycle is completed.

The number of iterations of the deconcolution process is usually 7-15 and depends on the shape of F. Greater number of iterations have from one side small effects into U and from the other introduces systematical deviations at the spectrum ends. These deviations are removed by the fitting. The iteration cycle is stopped usually after 2-6 cycles.

All papers published up to now assume that in the deconvolution technique the line which is to be deconvoluted must be symetric, so a suitable background must be substracted to remove the asymetry of a line measured with a solid state detector. Two different background functions were used:

The first background function has the form:

$$B_i = B_L - (B_L - B_H)\, S_i / S \qquad (4)$$

where B_L and B_H are the background values at low and high energy of the spectrum, S_i is the area up to the ith channel and S the area of the whole spectrum.

The second background function is based on the error function. Its shape is:

$$B_i = \frac{H}{2}\left(1-\mathrm{erf}\left(\frac{i-i_0}{\sqrt{2}\sigma}\right)\right) \qquad (5)$$

where $H=B_L-B_H$, i_0 is the channel of the peak and erf (x) is the error function. The background substraction is performed before the starting of the first iteration cycle.

3. THE PROGRAM

The routine for the deconvolution of the 511 keV line was included in the MINUIT program with the name STAND. To call the subroutine STAND the command card STANDARD was used. The form of the command card is:

STANDARD WORD7(1) WORD7(2)..... WORD7(7)

WORD7(1) determines the selection way of U^1 for the kth iteration cycle. WORD7(1) equals to 1 at the first call of the STAND and determines that $U^1_i=F_i$. WORD7(1) equals to 3 at the other calls of the STAND and determines that the U^1 is determined from the fitting parameters. The value of WORD7(2) determines the number of the deconcolution iterations.

The logical diagram of the routine STAND is shown in fig. 1. The routine FCN is written involving the suitable model for the fitting. The logical diagram of the routine FCN is shown in fig. 2. The COMMAND CARDS were used with the following order.

```
STANDARD    1   N1   }
MINIMIZE             } first cycle
STANDARD    3   N2   }
CALL FCN    6        } second cycle
MINIMIZE             }
STANDARD    3   N3
   .
   .
   .
   .
END
```

Subroutine FCN is called with IFLAG=6 after the second, third.... STANDARD. Calling FCN with IFLAG=6 MINUIT resets all flags related with the previous minimum and the covariance matrix (J75). This is needed because after STANDARD there is a new set of U_1.

4. EXPERIENCE WITH THE PROGRAM AND DISCUSSION

The routines STAND and FCN are written to use with the program MINUIT working on the UNIVAC 1106 or on the PDP 11/34A.

The deconvolution program is tested in our laboratory since 1975 using Doppler broadened lines from annihilation in metals and ionic crystals. Typical results are shown on table 1 and fig. 3. The solid state detector used was an intrinsic Ge 200×5 mm^3 with resolution 1.08 keV at the 514 keV of ^{85}Kr. The fitted model was a parabola plus a gaussian for metalic samples and a sum of two or three gaussians for the ionic crystals.

The substraction of suitable background, like (D75), (J74) and others to make symetric the annihilation line before the deconvolution process should be reexamined. The following must be considered:

The asymetry of the annihilation line is mainly due to incomplete charge collection at the ends of the detector. There is also the same asymetry, for the same reasons, into the experimentally obtained resolution function. The asymetry of the resolution function may be written as a sum of three main terms.

$$R=R_1+R_2+R_3 \tag{6}$$

From the superposition theorem, as applied to the convolution, we have:

$$F=R*U=(R_1+R_2+R_3)*U=R_1*U+R_2*U+R_3*U \tag{7}$$

where * represents the convolution process.

The right way to substract a background will only be «for example» substraction of the R_1 from R and correspondingly the R_1*U from F which is unknown before the end of the deconvolution. Any substraction of «a suitable background» from F leads to the distortion of U.

The experience of the authors shows that, when «suitable background» substracted from F, the results were: (i) distortion of U at the low energy side, (ii) large value of x^2 from the fitting and (iii) large fluctuations of the fitting parameters. In contrast if background did not substracted then: (i) U was symetric, (ii) small value of x^2 was obtained

from the fitting, (iii) the stability of the fitting parameters was excellent and (iv) F was very satisfactory reproduced from the convolution of the U, from the fitting parameters with R, as it is clearly shown in fig. 4.

All the above shows that the background substraction is not needed because all reasons for making non symetric the annihilation line are included in the resolution function.

In the original form of (D75) the exponent n of eq. (2) has a value equal to 2. This exponent was needed for fast convergence of the deconvolution. For our system for the measurement of the broadening of the annihilation line (1.08 keV at the 511 keV, 60eV/ch) the value of n equals to 1. If n equals to 2 the convergence of the deconvolution was very slowlly and required too many iterations to have the same x^2 value as if n equals to 1. Additionally, in this case, there is distortion of the U^K.

The execution of the program takes 5-10 min CPU time on UNIVAC 1106 and 30-45 min on PDP 11/34A.

Because the complication of the whole process and the complex calculations during the deconvolution process, it is very difficult, but not imposible, the accurate computation of the fitting parameter errors. These errors are estimated to be 1-2% for the Fermi momentum or the standard deviation of the Gaussians and 4-6% for the intensities of the different components.

TABLE 1

Results of deconvolution of annihilation line in metals and ionic crystals. (Second and third columns for metals are Fermi momentum and contribution of core electrons. Γ_1, Γ_2, Γ_3 in miliradians, I_1, I_2, I_3 %).

Material and Conditions	RESULTS					
	Γ_1	I_1	Γ_2	I_2	Γ_3	I_3
NaCl 293°K	8.64	88.1	16.0	9.1	3.13	2.8
NaCl 11°K	8.62	94.5	20.9	5.5	—	—
NaCl 150 kRad	8.56	89.6	20.9	7.2	4.16	3.4
NaCl 2.5 MRad	8.64	87.8	18.9	8.9	3.37	3.3
Al 293°K	6.6	19.				
Cu 293°K	5.5	65.				
Zn 293°K	6.3	50.				
Ag 293°K	4.7	70.				
Cd 293°K	5.5	52.				
Sn 293°K	6.4	41.				
Au 293°K	4.8	79.				
Pb 293°K	6.1	38.				
In 82°K	5.79	46.6				
In 288°K	5.78	46.2				
In 420°K	5.82	42.2				

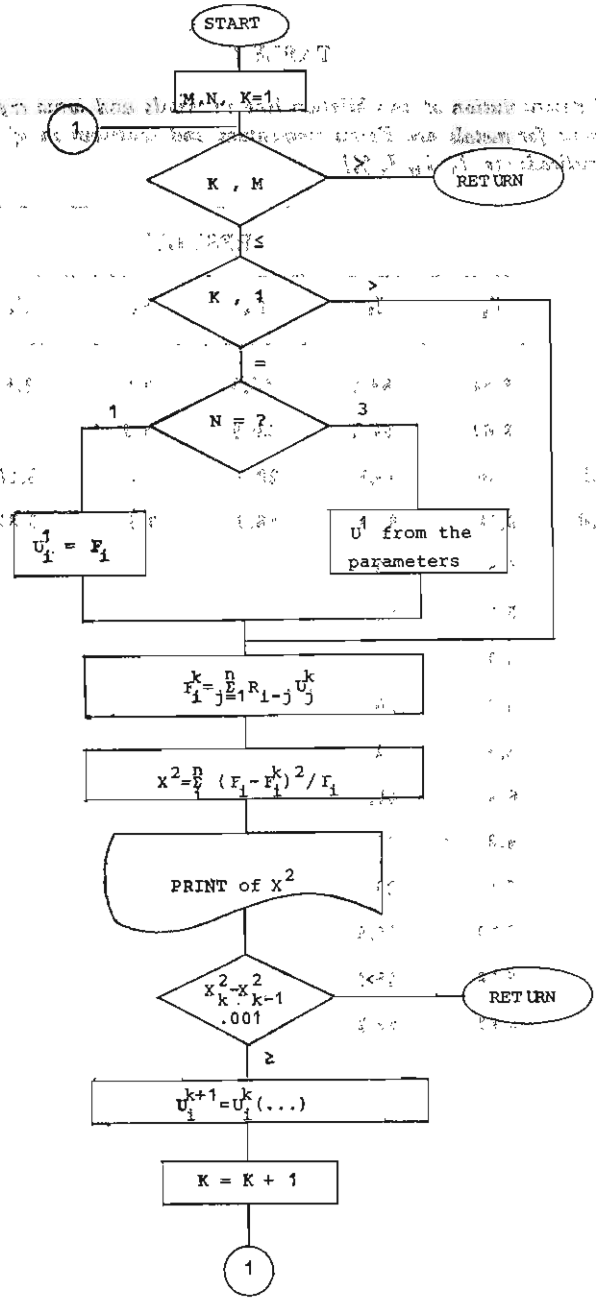

Figure 1. The logical diagram of the subroutine STAND for the deconvolution of annihilatation line.

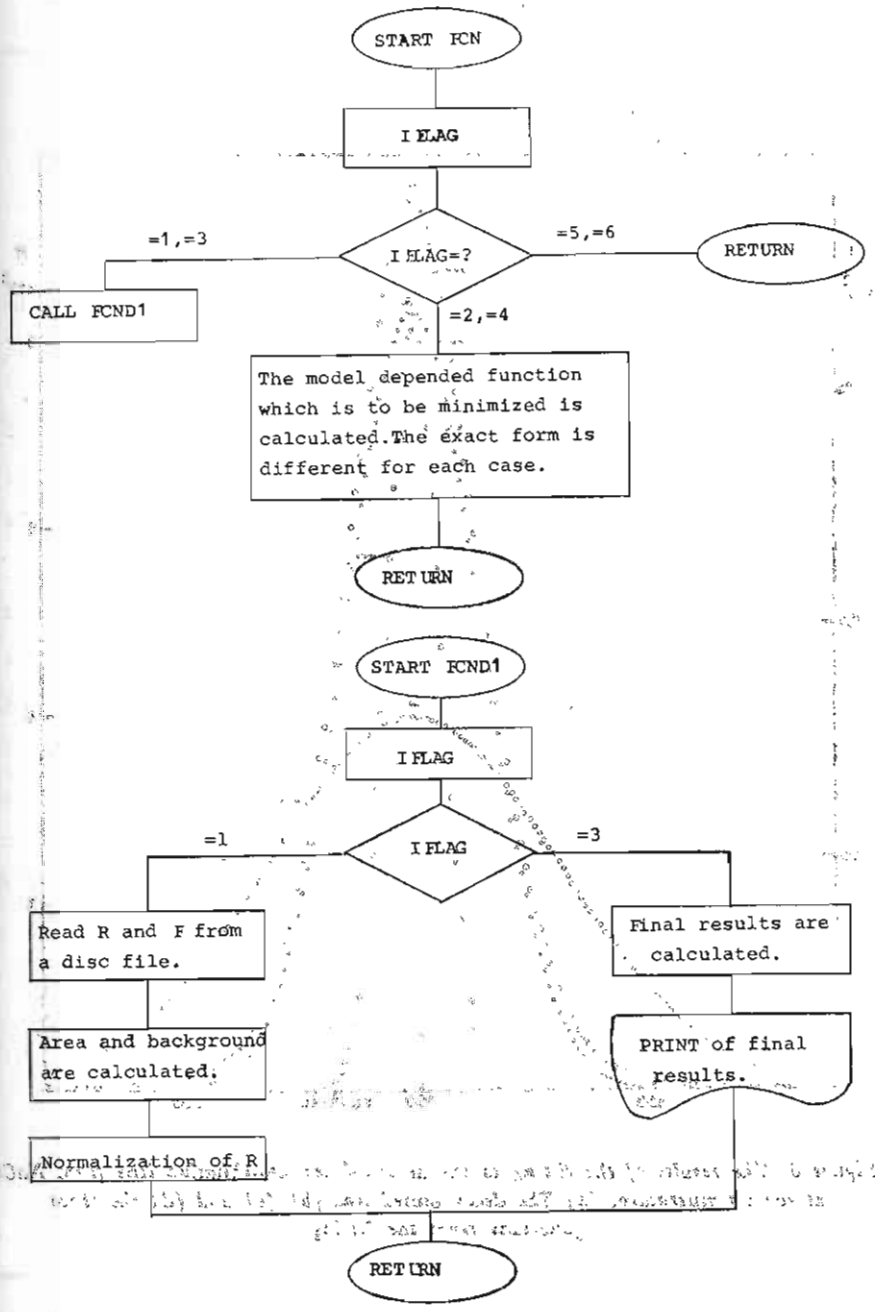

Figure 2. The logical diagram of the subroutine FCN for the fitting of the suitable model to the results of deconvolution.

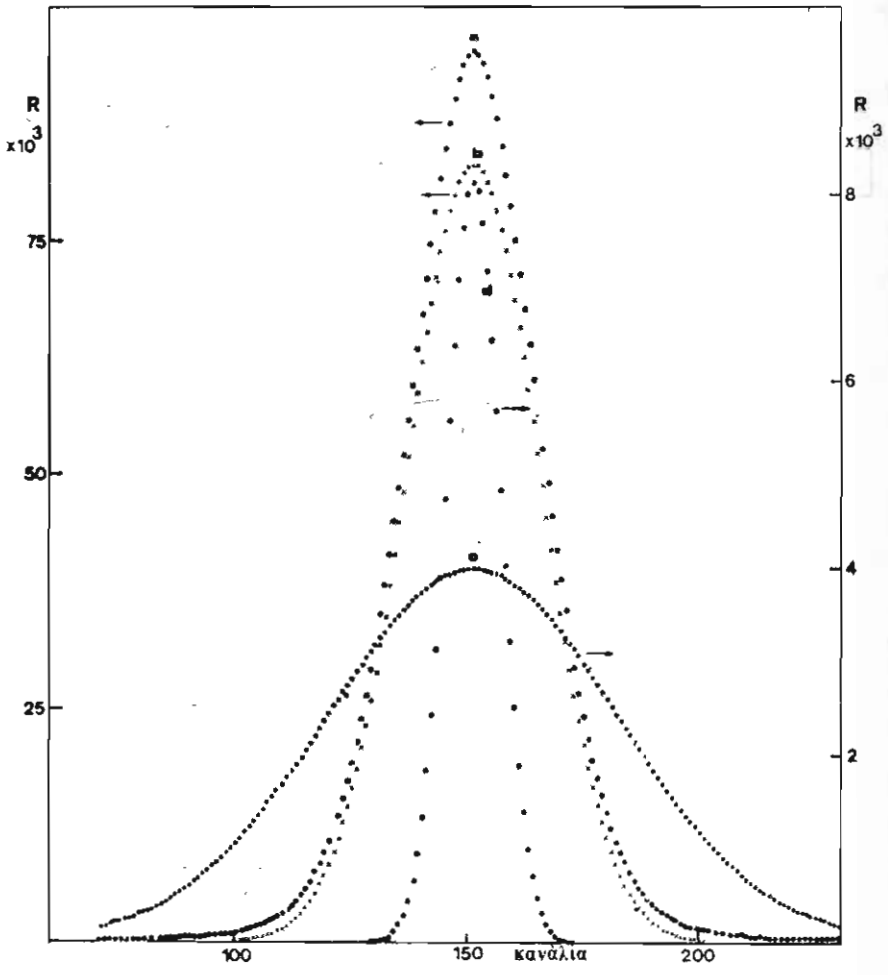

Figure 3. The results of the fitting to the deconvoluted annihilation line from NaCl at room temperature. (a) The deconvoluted line (b), (c) and (d) the three gaussians from the fitting.

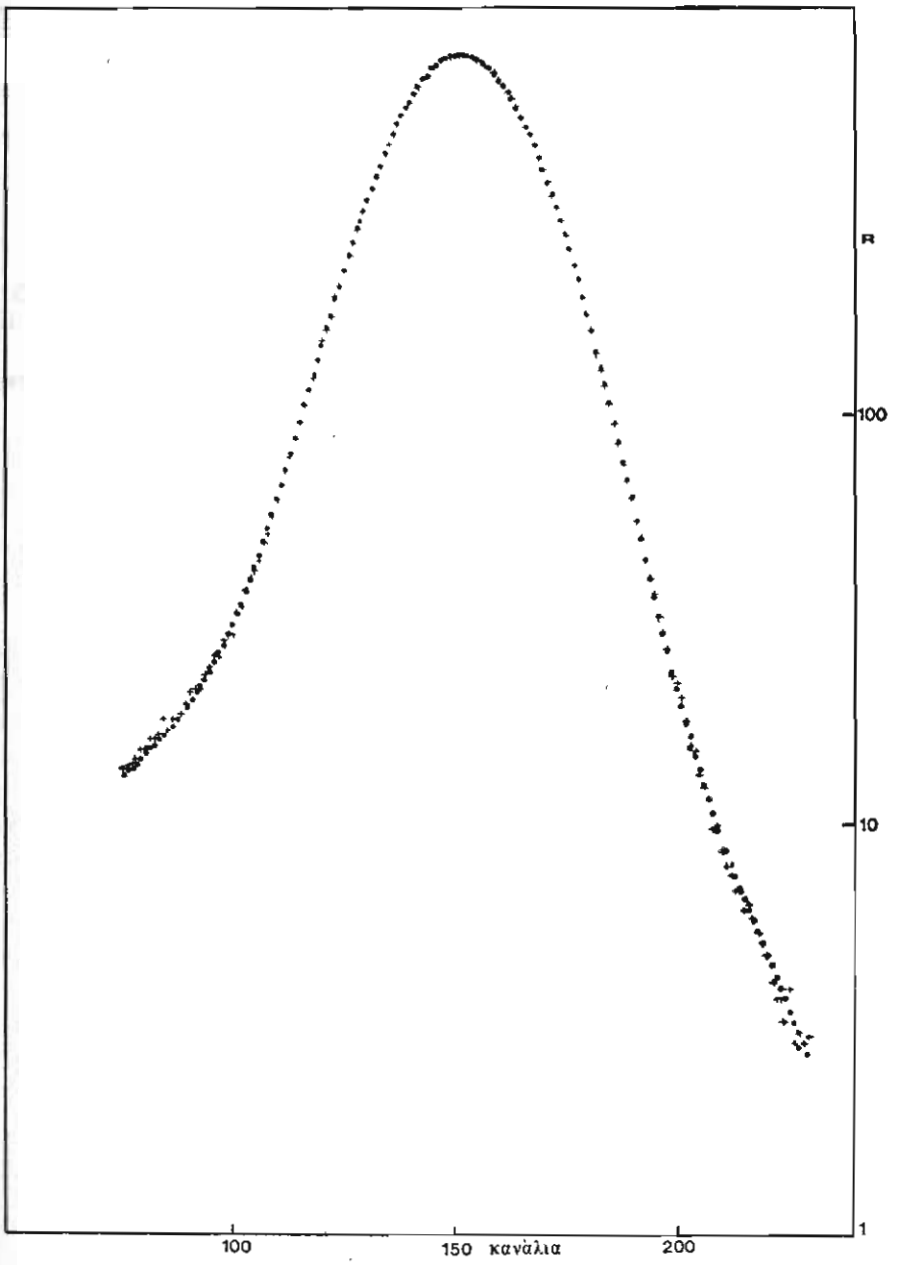

Figure 4. Experimental data (+) and the convolution of the model function with the resolution function (.) for NaCl at room temperature without background substraction.

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ΠΕΡΙΛΗΨΗ

ΥΠΟΓΡΑΜΜΑΤΑ ΓΙΑ ΤΟ ΠΡΟΓΡΑΜΜΑ MINUIT ΓΙΑ ΤΗΝ DECONVOLUTION ΤΗΣ ΔΙΑΠΛΑΤΥΣΜΕΝΗΣ ΛΟΓΩ ΦΑΙΝΟΜΕΝΟΥ DOPPLER ΓΡΑΜΜΗΣ ΤΗΣ ΕΞΑΫΛΩΣΗΣ.

ὑπὸ

ΧΑΡΔΑΛΑ Μ., ΔΕΔΟΥΣΗ ΣΠ. καὶ ΧΑΡΑΛΑΜΠΟΥΣ ΣΤΕΦ.

Ἐργαστήριο Ἀτομικῆς καὶ Πυρηνικῆς Φυσικῆς
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Παρουσιάζονται μιὰ μέθοδος deconvolution τῆς διαπλατυσμένης λόγω φαινομένου Doppler γραμμῆς τῆς ἀκτινοβολίας ποὺ ἐκπέμπεται ἀπὸ τὴν ἐξαΰλωση ζεύγους ἠλεκτρονίου-ποζοτρονίου, οἱ ὑπορουτίνες γιὰ τὸ deconvolution καὶ ὁ τρόπος χρήσης τοῦ προγράμματος MINUIT γιὰ αὐτὴν τὴν ἀνάλυση. Ἡ μέθοδος καὶ τὸ πρόγραμμα χρησιμοποιήθηκαν γιὰ τὴν ἀνάλυση φασμάτων ἀπὸ ἐξαΰλωση στὰ μέταλλα, στοὺς ἰοντικοὺς κρυστάλλους καὶ στὰ μοριακὰ ὑλικά. Οἱ ὑπορουτίνες γιὰ τὸ deconvolution μποροῦν νὰ δουλέψουν τόσο στὸν UNIVAC 1106 ὅσο καὶ στὸν PDP 11/34A τοῦ ἐργαστηρίου.