(JZS) Journal of Zankoy Sulaimani, December 2008, 11(1) Part A(9-19)
گۆڤاری زانكۆی سلێمانی ،كانونی یەكەمی 2008، بەرگ11(1) بەشی A لاپەڕە (9-19)

The Effect of Peak Area Estimation on the Gamma-Ray Spectrum Analysis.

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Abstract

This paper deals with a measured gamma-ray spectrum and designing a MATLAB program to perform peak finding procedure by using the differences of the experimental data as well as performing fitting process by using Newton-Gauss least square technique. Then, five different methods of peak area determination are proposed to analyze the symmetry lines of Po^{212} in the spectrum, and the comparison was done using the percentage variance reduction test.

Keywords: Nuclear physics, Gamma ray spectrum, Peak area determination.

Introduction

At the present, scintillation spectrometers are not considered as high-resolution devices anymore. Although they are still widely used for applications that need simplicity of using rather than high energy resolution, Germanium-Lithum, Ge(Li) , and High-purity germanium, HPGe, detectors have outdated them for using in gamma-ray spectroscopy[1].Especially High-purity Germanium (HPGe) detectors are frequently used to detect gamma rays for energy spectroscopy because of their unparalleled resolving power and high photon detection efficiency[2].

In this work the spectrum measured on HPGe-detector [3] and from the energy, efficiency and full width at half maximum, the calibration processes have been done. Fig. (1) shows the energy calibration curve which represents a polynomial of second degree but the coefficient of (x^2) is very small so it approaches to a straight line.

As is usual in gamma-ray spectrum analysis the smoothing process of the spectrum must be performed, then the main operation in analyzing gamma spectra begins, that is, peak finding process, which is the important ingredient of every gamma ray spectrum analysis. From references [4-8], a great variety of programs can be found in the literature for those purposes.

The peak finding algorithm is applied by a coded matlab program that determines the required parameters quantities for the peak analysis like, the boundary, the centroid, and the amplitude for each peak.

Then a matlab (m-file) code is focused on precisely evaluating spectral data in order to maximize the accuracy of two key components of spectral analysis, the net counts in all photopeak regions and nuclide identification [9].

The data analysis has been started by determining the energy and the area above the continuum for each peak. The energy identifies the element responsible for the gamma ray emission, and the area (number of counts) is proportional to the amount of that element [10].

A matlab program is constructed that uses the calibration constant as the inputs, then the recorded spectrum data (counts and channels) are read from an input text file.

Various applied forms have been proposed for representing a full-energy peak functions, most of them have been designated for a relatively narrow energy range, typically for radioactivity

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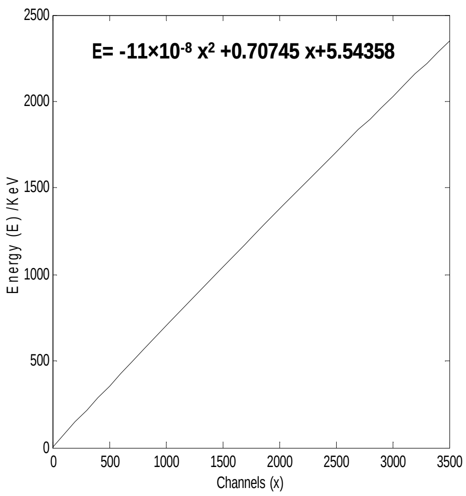

Fig.(1):The energy calibration curve

measurements. In the present work, it is a common practice to approximate the full-energy peaks by a Gaussian function with a polynomial function representing the background, as followed by the refs. [2, 11-14] and the estimation of the area of peaks superimposed on a continuum background is a very common practice in spectrometry.

Next, by using the starting values of the parameters, the basic feature of fitting is needed which represents a (Newton-Gauss) method for multi nonlinear systems of equations [15].

Finally the strong and symmetry gamma-ray lines are selected to find the photo peak areas by different methods in order to get the interesting results.

The smoothing technique and fast Fourier transformation (FFT) process

In the measured spectra, because of having the noise peaks due to the statistical fluctuations in counts, smoothing technique can be applied to remove them and it divides the spectrum into many regions to aid in locating the peaks, in such a way that the smoothed values follow more closely the correct average spectrum shape and all smoothing techniques for gamma-ray spectra are based on the linear transformation of the measured data [16]. The methods of smoothing are divided into three categories - Fourier transform, least-squares adjustment of a polynomial, and digital filtering [17].The Fourier transform method is used in the present work by introducing the Fast Fourier Transform (FFT) to low-pass filter the data.

Here is an m-file for smoothing an array of ordinates (y's) that are in order of increasing abscissa (x's), but without using the abscissas themselves.

If we have (N) consecutive sampled values (h_k), for a smoothing interval (Δ).Now for an even number (N) the Fourier Transform (H) at all values of (f) in the range (-fc to fc) and for a variable of(t), as shown in Fig. (2), is given by [18]:

$$H(f_n) = \int_{-\infty}^{+\infty} h(t)\; e^{2\pi i f_n t}\, dt$$

$$\approx \sum_{k=0}^{N-1} h_k e^{2\pi i f_n t_k}$$

$$\approx \sum_{k=0}^{N-1} \mathbf{h_k e}^{2\pi i k n / N} \qquad \ldots\ldots\ldots (1)$$

Such that

$$\begin{cases} \mathbf{f_n = \dfrac{n}{N\Delta}} \\ \mathbf{f_c = \dfrac{1}{2\Delta}} \end{cases} \qquad \ldots\ldots\ldots\ldots\ldots (2)$$

Where $\mathbf{n = \dfrac{-N}{2}, \ldots, \dfrac{N}{2}}$

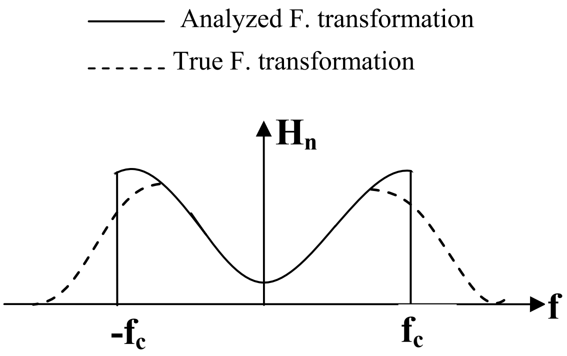

Fig.(2): Fourier transform (H_n) at all values of (f) from ($-f_c$ to f_c)[19]

The above equation is called the Fast Fourier Transform of the N-points (h_k) that are denoted by:

$$H_n = \sum_{k=0}^{N-1} h_k \, e^{2\pi i k n / N}$$

$$\therefore \quad H(f_n) = \Delta \, H f_n \quad \ldots\ldots\ldots\ldots (3)$$

Therefore its inverse form is given by

$$h_k = \frac{1}{N} \sum_{k=0}^{N-1} H_n \, e^{-2\pi i k n / N} \ldots\ldots\ldots (4)$$

Supposing that

$$W = e^{2\pi i / N}$$

Then (H_n) can be written as:

$$H_n = N \sum_{k=0}^{N-1} W^{nk} \, h_k \ldots\ldots\ldots\ldots (5)$$

Where W is an (n×k) matrix.

Danielson and Lanczoz showed that the discrete Fourier Transform of length (N) may be written as the sum of two discrete Fourier transforms, each of length (N/2) [19].

One of the two, is formed from the even-numbered points of the original (N), the other forms the odd-numbered points, or

$$F_k = \sum_{j=0}^{N-1} e^{2\pi i j k n / N} \, f_j$$

$$F_k = \sum_{j=0}^{N-1} e^{2\pi i k (2j)/(N/2)} \, f_{2j} + \sum_{j=0}^{(N/2)-1} e^{2\pi i k (2j+1)/(N/2)} \, f_{2j+1}$$

$$\therefore \; F_k = \sum_{j=0}^{(N/2)-1} e^{2\pi i k (2j)/(N/2)} \, f_{2j} + W^k \sum_{j=0}^{(N/2)-1} e^{2\pi i k j/(N/2)} \, f_{2j+1}$$

$$\therefore \quad F_k = F_k^e + W^k \, F_k^o \quad \ldots\ldots\ldots\ldots (6)$$

That is called fast Fourier transform (FFT), where F denotes the k^{th} components of the Fourier transform of length (N/2) formed from the even components of the original f_j's .While F is the corresponding transform of length (N/2) forming the odd components.

Data evaluation and peak calculation

The data was processed with the gamma-ray analysis code of the matlab program to describe a gamma peak with its background in a spectrum consists of the following three steps [7]:

A) - Determination of the boundaries of a peak or grouping of peaks.

B) - Approximation and subtraction of the background

C) - Peak fitting of the net counts using a complex fitting process.

The program attempts to define the ranges of channels in the spectrum that lie significantly above the background, so it can be done by testing for the peak-to total curve ratio.

In order to develop a general approach to a nonlinear curve fitting, a Gaussian function is used to describe the principal component of the peak shape by taking into consideration the definition of the peak as total peak area after background subtraction. Let's consider that the set of discrete (yi) data is to be fitted by the general nonlinear function f(x,a) that represents a Gaussian function[14]:

$$y = f(x,\hat{a}) = a_1 \exp\left(\frac{-(x-a_2)^2}{2\ a_3^2}\right) + a_4 x^2 + a_5 x + a_6 \quad \ldots. (7)$$

Whwre a_1, a_2, a_3, a_4, a_5, and a_6 are the fitting parameters.

After performing the smoothing of the spectrum the (m-file) uses the smoothed regions to identify the peaks and their boundaries that the peaks can be localized by experimental data comparison [20].

It can be observed that the content of successive channels (N_{i-1}) and (N_i) will be such that only in the region where a peak begins to rise , i.e., the initial channel (j_i) ,centroid channel (J_c) and final channel(J_f) , see Fig.(3).

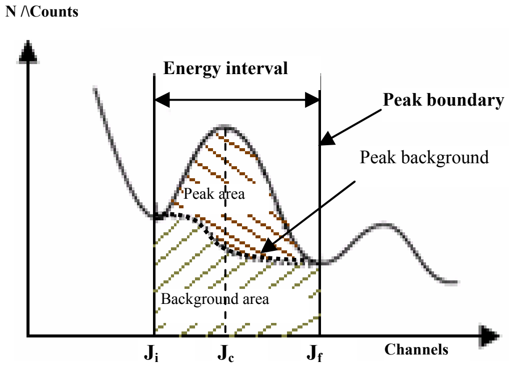

Fig.(3): Schematic portion of a natural gamma-ray spectrum illustrating the peak definition procedure [21].

Curve fitting

Knowing that ($\hat{x}$) and ($\hat{y}$) are the matrices of the respective channels and counts which are given by:

$$\left.\begin{array}{l} \hat{x} = [x_1, x_2, x_3, \ldots\ldots x_m] \\ \hat{y} = [y_1, y_2, y_3, \ldots\ldots y_m] \end{array}\right\} \quad \ldots\ldots\ldots (8)$$

for (m) counts on the peak.

While the matrix of the peak parameters ($\hat{a}$) is given by:

$$\hat{a} = [a_1, a_2, a_3, a_4, a_5, a_6] \quad \ldots\ldots\ldots. (9)$$

An estimate for the parameters can be applied by the programs itself, in such a way that the first three parameters (a_1, a_2 and a_3) represent the height, centroid, and the width of the peak respectively. The starting value (before the fitting technique) for (a_1) is determined from the values of the maximum count on the peak and those of (a_2 and a_3) are evaluated from the first and second momentum method from [10]:

$$\left.\begin{aligned} a_2 &= \frac{\sum x_i y_i}{y_i} \\ a_3 &= \sqrt{\frac{\sum (x_i - a_2)^2 y_i}{y_i}} \end{aligned}\right\} \quad \ldots..(10)$$

While for the background (a_4) is chosen to be zero, and (a_5 and a_6) are determined from the straight line joining the initial and final point on the peak.

In order eq. (7) to be satisfied and yielded the best representation for (n) utilized peak data points(x,y),it must be determined a nonlinear set of the square differences such that [6]:

$$S = \frac{[y_k - f(x_k, a)]^2}{y_k} \quad \ldots\ldots (11)$$

and it must be optimized by taking its derivative to find the best values of the parameters. i.e.,

$$\Phi_i = \frac{\partial S}{\partial a_i} = -\frac{2[y_k - f(x_k, a)]^2}{y_k} \times \frac{\partial f(x_k, \hat{a})}{\partial a_i} = 0 \quad \ldots (12)$$

Eq.(12) is a set of nonlinear equation like

$$\hat{\Phi}(\hat{x}, \hat{a}) = \begin{cases} \hat{\Phi}_1(\hat{x}, \hat{a}) = 0 \\ \hat{\Phi}_2(\hat{x}, \hat{a}) = 0 \\ . \\ . \\ \hat{\Phi}_m(\hat{x}, \hat{a}) = 0 \end{cases} \quad \ldots\ldots.. (13)$$

which can be solved numerically by using Newton's method to find the parameters [16].

In each step n-multidimensional system of equations can be solved and continued with the provided iteration condition until stopping the iteration and reaching the best values of the parameters from equation:

$$a^{[i+1]} = a^{[i]} - J^{-1} . \Phi(x, a^{[i]}) . \Delta^{[i]} \quad \ldots. (14)$$

The scalar $\Delta^{[i]}$ limits the value of the step length in an admissible region around the current solution. While index (i) is for the iteration and (J) is the Jaccobian matrix, its elements may be calculated from the differences with providing the initial parameters firstly and it can be written as the following [22]:

$$J = \Phi(x, a^{[i]}) = \begin{pmatrix} \frac{\partial \Phi_1}{\partial a_1} & \frac{\partial \Phi_1}{\partial a_2} & \cdot & \cdot & \cdot & \frac{\partial \Phi_1}{\partial a_n} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \frac{\partial \Phi_n}{\partial a_1} & \cdot & \cdot & \cdot & \cdot & \frac{\partial \Phi_n}{\partial a_n} \end{pmatrix} \quad \ldots.(15)$$

The programming algorithm of the fitting (Newton m-file) have the following input parameters:

1) - Initial parameters that are determined from the boundary (m-file) code for each peak.

2) - Tolerance (tol=1e-6), in order to be continued the iteration until the norm (norm<=tol) such that [23]:

$$norm = \frac{\sqrt{\Delta_1^2 + \Delta_2^2 + \ldots + \Delta_n^2}}{n} \quad \ldots\ldots (16)$$

3) - Maximum number of iterations

4) - Counts and channels of the peak so they are determined from the peak searching (m-file). But, the output of the (Newton m-file) are the final values of the parameters ($\quad, i = 1,....6$) and the number of the iterations. Fig.(4) shows the schematic representation of the matlab program.

Methods of peak area determination

According to the previous works in these fields, one of the methods of peak area evaluation may be the analytical method. In this method the fitting process finds a best Gaussian shape and the area under the curve is represented by the integration of the Gaussian function (GF). Then the integration can be replaced by its numerical method by using trapezoidal method [24,25]:

$$A_j \approx h[\frac{GF_i + GF_f}{2}] + h \; GF_j \quad .... (17)$$

For $j = 1, ... , n-1$, and by noting that the indices (i and f) specify the initial and final values of the Gaussian function such that in general for index (k) and channel (x_k):

$$GF_k = GF(x_k) \quad .... (18)$$

While (n) and (h) are the number of points and the step size, given by [26]:

$$\left. \begin{array}{l} h = \dfrac{x_f - x_i}{n} \\ x_k = x_i + k\; h \end{array} \right\} \quad .... (19)$$

The second method is the digital data, for well-resolved peaks, the simple summation of counts above the estimated background continuum is probably as good as any method of finding the peak area.For the digital data method the region of interest ROI-summation is quite tolerant of small variations in peak shape and provides an accurate and straightforward estimate of the precision of the net peak area [10].

Due to which the reviews proposed many ways that can be abbreviated as following:

a)- Total peak area [27]

$$A_j = F_j - (F_\ell + F_r)\,(r - \ell + 1) * 0.5 \quad .... (20)$$

Where (ℓ and r) are the channel numbers at left side and right side of the peak respectively, and F_j is the count for channel (j).

b)-Wasson modified (TPA) method [10]

$$A_j = F_j - (n + 0.5)\,(B_n + B_{-n}) \; ...... (21)$$

Where (n) is the number of the counts on each side of the peak, and B_n is count of the background corresponding to channel (n).

c) - Covell's method [27]

$$A_j = F_j - (n + 0.5)\,(F_n + F_{-n}) \quad ...... (22)$$

d)-Quittner's method [21]

$$A_j = F_j - B_j \quad .... (23)$$

To calculate the total area (A) for each method, the partial areas (A_j) in the eqs.(17 , 20-23) should be added , i.e.,

$$A = \sum_j A_j \quad .... (24)$$

Taking into consideration that for the methods of eqs.(21-23) , the peaks must be symmetry due to the counts distribution .Therefore, the index of the sum for those methods ($j = -n, ..., n$); but for the method of total peak area method , eq.(20), it has the range ($j = l, ..., r$).

Results and discussion

From the peak positions (centroids) and the calculated areas, the peak energies and peak intensities can be determined. After that, the relative intensity is evaluated by dividing the individual peak intensity by the standard line intensity[28] ,that is, the line of energy (609.62 KeV) in our measured spectrum .

In general to compare a column of calculated values of a variable (R) with a column of a measured (experimental) quantity (R\`) the percentage Variance Reduction test (VR) is used, that is, computed from equation [23]:

$$VR = 100 \times \left\{ 1 - \frac{\sigma(R)}{\sigma(R')} \right\} \quad \ldots\ldots \; (25)$$

Knowing that σ(R) and σ(R\`) are the respective variances according to theoretical(R) and experimental values (R\`) such that for (n-values), they are given by:

$$\left.\begin{aligned} \sigma(R) &= \sum_{j=1}^{n} (R_j - R'_j)^2 \\ \sigma(R') &= \sum_{j=1}^{n} (R'_j - R'_{av})^2 \end{aligned}\right\} \quad \ldots\ldots.. \; (26)$$

Since the peak areas are not measured experimentally, then the average value of the five used methods for each peak has been found and listed in a column of average areas (Aav) for comparing the methods. Table (1) represents the five mentioned methods for peak area estimation and the average areas for about (27) symmetry photopeaks of (Po^{212}-element).

It is clear that in gamma ray spectroscopy one of the important measurable quantities is the peak energy and the relative intensity which depends on the area under the peak, and therefore methods of peak area estimation [8]. Table (2) tabulates the calculated energies (E) and the relative intensities (R) to be compared to those of the measured values (those were taken from the nuclear data sheets [26]).

Table (1): The calculated peak areas using five different methods.

N	A1	A2	A3	A4	A5	Aav
1	825.96	825.05	827.11	826.2	826.05	826.074
2	533.93	536.77	535.37	533.45	533.69	534.642
3	26959.81	26952.4	26957.14	26957.14	26960.28	26957.36
4	1024.88	1022.31	1026.5	1019.24	1023.27	1023.24
5	464.19	463.02	465.02	463.89	462.58	463.74
6	363.11	359.23	366.23	362.77	365.47	363.362
7	2291.17	2291.79	2293.35	2290.35	2290.53	2291.438
8	742.94	741.78	743.46	740.46	742.2	742.168
9	265.06	263.99	267.48	264.13	265.28	265.188
10	4824.91	4822.92	4822.31	4824.31	4823.12	4823.514
11	657.81	658.61	657.88	657.67	656.01	657.596
12	317.33	315.49	318.66	316.5	318.53	317.302
13	1962.67	1960.68	1962.71	1962.71	1962.7	1962.294
14	510.36	509.83	508.96	511.36	508.52	509.806
15	1233.41	1232.42	1233.46	1233.96	1233.51	1233.352
16	498.64	498.91	497.33	497.93	498.74	498.31
17	772.69	772.52	772.49	771.19	771.59	772.096
18	591.98	590.55	590.01	591.64	592.09	591.254
19	191.29	191.29	190.35	192.15	192.38	191.492
20	306.87	307.03	305.47	306.46	306.52	306.47
21	687.32	687.5	688.89	687.39	686.93	687.606
22	3437.21	3439.69	3438.16	3438.16	3437.69	3438.182
23	63.94	62.89	64.3	63.29	63.98	63.68
24	468.17	467.82	468.87	468.67	468.21	468.348
25	876.13	876.93	876.13	876.18	877.15	876.504
26	94.76	94.25	94.77	95.05	94.79	94.724
27	294.15	294.36	294.15	294.15	294.16	294.194

Table (2): The peak energies (E) and the relative intensities calculated in the present work compared with those of the nuclear data sheets [26].

Present work							Nuclear data sheets	
N	E / KeV	RI1	RI2	RI3	RI4	RI5	E /KeV	RI
1	389.12	1.091	1.131	1.196	1.159	1.235	388.88	0.803
2	454.81	0.717	1.198	0.925	0.822	0.751	454.77	0.651
3	609.62	100	100	100	100	100	609.312	100
4	665.61	3.144	3.578	3.322	3.093	3.116	665.453	3.167
5	703.18	0.989	0.952	0.969	0.968	0.97	703.11	1.024
6	720.01	0.877	1.148	0.981	1.163	1.079	719.86	0.822
7	768.77	10.95	11.165	11.286	11.047	11.045	768.356	10.72
8	806.35	2.701	2.433	2.945	2.900	2.543	806.174	2.646
9	1071.16	0.5100	0.402	0.614	0.415	0.600	1069.96	0.599
10	1120.18	32.78	32.438	32.43	32.69	32.89	1120.287	32.75
11	1155.51	3.532	3.587	3.53	3.47	3.331	1155.19	3.536
12	1207.61	1.016	0.95	1.177	0.963	1.161	1207.68	0.978
13	1238.16	12.73	12.73	12.74	12.74	12.74	1238.1	12.56
14	1281.21	3.671	3.662	3.652	3.672	3.622	1280.96	3.102
15	1377.92	8.69	8.506	8.512	8.612	8.731	1377.669	8.677
16	1401.75	2.798	2.993	2.645	2.776	2.899	1401.5	2.755
17	1408.22	4.657	4.653	4.559	4.359	4.458	1407.9	4.664
18	1508.57	4.953	4.843	4.755	4.912	4.954	1508.22	4.577
19	1543.53	0.433	0.617	0.534	0.624	0.634	1543.32	0.434
20	1661.67	2.475	2.510	2.386	2.4763	2.486	1661.28	2.495
21	1729.14	6.494	6.493	6.496	6.4864	6.475	1729.595	6.334
22	1764.17	33.097	33.108	33.106	33.106	33.1	1764.494	33.41
23	1838.69	0.627	0.487	0.6409	0.4913	0.628	1838.86	0.781
24	1847.25	4.696	4.692	4.6979	4.6978	4.697	1847.42	4.599
25	2204.26	11.296	11.293	11.299	11.299	11.3	2204.21	11.02
26	2293.64	0.554	0.483	0.645	0.7512	0.654	2293.4	0.662
27	2447.36	3.398	3.798	3.799	3.7991	3.798	2447.86	3.406

values (those were taken from the nuclear data sheets .

Now by applying eqs.(25 , 26) for Table (1) by supposing that (R_j) represents the elements of each column of the calculated areas(i.e., A1,A2,A3,A4, and A5) and (R'_j) symbolize to the average areas for the five methods (Aav) , the first columns of Table (3) has been obtained.For further comparison, eqs.(25, 26) can also be used for Table (2), but this time it is assumed that (R_j) represents the elements of each column of the calculated relative intensities (i.e., RI1,RI2,RI3,RI4, and RI5) and (R'_j) is for the experimental (or measured) relative intensities, the second of third columns of the results are listed in the Table (3). From Table (3), by taking into consideration the values of (VR) for both the areas and the relative intensities, one can observe that the analytic method for area estimation values greater than the others, indicating that the analytic method is a good one for the area calculation. In the other hand Table (3) reveals degree of goodness for the other four methods (digital data methods) that also it points out to the fifth one (Quittner's method) as a first one among the digital data methods for area determination.Also, from Table (3) it can be noticed that the corresponding errors for the calculation process (, i.e., 100-VR) [23] in the areas are less than those of the relative intensities, which can be ascribed to errors due to the instrumentations.

Table (3): The percentage variance reduction test (VR) for the results.

M	Area			Relative intensity		
	σ(R)	σ(R`)	VR	σ(R)	σ(R`)	VR
1	15.07	681775157.38	99.99999778990	0.90	10382.55	99.99133
2	63.50	681775157.38	99.99999068678	2.07	10382.55	99.98001
3	44.41	681775157.38	99.99999348560	1.65	10382.55	99.98407
4	29.38	681775157.38	99.99999569039	1.55	10382.55	99.98509
5	25.24	681775157.38	99.99999629769	1.41	10382.55	99.98640

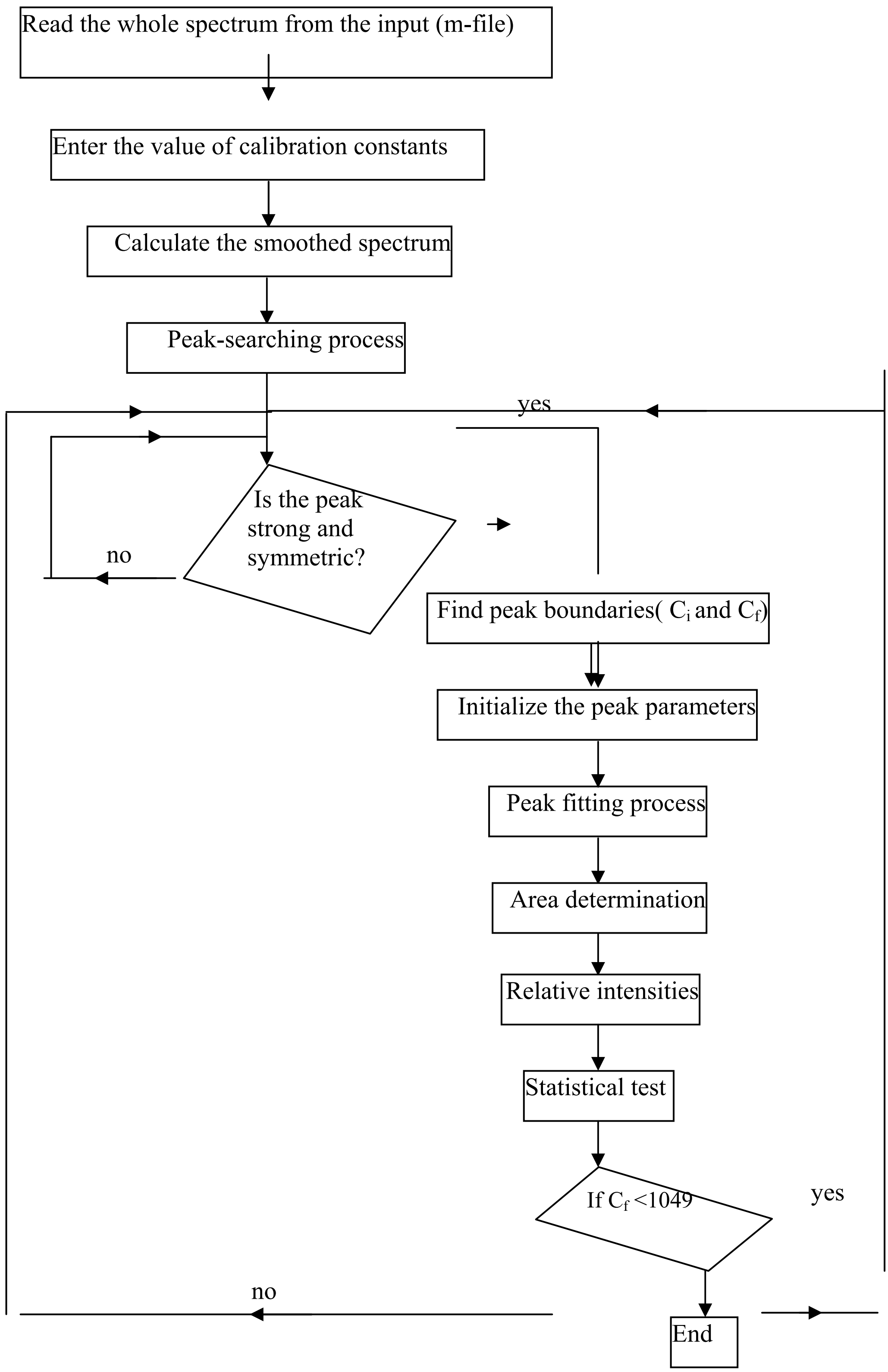

Fig.(4) :Schematic representation of the program.

Conclusion

On view of the obtained results, one can point out that for the peak area calculation the two methods of the digital data directly, and proper approximative function can be used for fitting the given shape inclusive background, where the second method gives the good results compared with the first.

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كاریگەری دۆزینەوەی روبەری لەتكەكان لەسەر شیكردنەوەی شەبەنگی تیشكی گاما.

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پوختە

ئەم توێژینەوەیە مامەڵە دەكات لەگەڵ شەبەنگێكی پێوراوی تیشكی گاما و بەرنامەیەكی (MATLAB) دانراوە بۆ ئەنجامدانی پرۆسەی دۆزینەوەی لوتكە بە بەكارهێنانی جیاوازیەكان لەكۆمەڵەخاڵە پراكتیكیەكاندا و هەروەها ئەنجامد انی پرۆسەی جووتبون ئەویش بەبەكارهێنانی رێگەی كەمترین چوارگۆشەی نیوتن –گاوس (Newton-Gauss) .

ئنجا پێنج رێگە ی جیاواز بۆ دۆزینەوەی رووبەری لوتكە بیشاندران بۆ شیكاركردنی هێڵە چوونیەكەكانی ناوكی تیشكاوەری Po^{212} ی ناو شەبەنگەكە و لە پاشاندا بەراورد كردنی بۆ ئەنجام درا بە بەكارهێنانی تا ڤیكردنەوەی رێژەی سەدی جیاوازی كەمكراوە.

تأثير ايجاد مساحة الذروات على تحليل طيف اشعة گاما.

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الخلاصة

تم في هذا البحث تحليل طيف كامي مقاس و صمم برنامج (MATLAB) لإنجاز عملية أيجاد الذروات بأستخدام الفروقات للبيانات العملية .أنجزت أيضا عملية التطابق بإستخدام طريقة المربعات الصغرى لنيوتن-كاوس (Newton-Gauss). ثم عرض خمس طرق مختلفة لأيجاد مساحة الذروة لتحليل الخطوط المتماثلة داخل الطيف لتحليل ذروات (Po^{212}) داخل الطيف، و كذالك أجريت المقارنة بواسطة النسبة المؤوية للتباين المختزل .

Received on 17/7/2007 Accepted 23/9/2007

وەرگیراوە لە 2007/7/17 پەسندكراوە لە2007/9/23