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ANALYSIS OF GAMMA-RAY SPECTRUM OBTAINED WITH CDZNTE-DETECTORS USING THE ROOT CERN SOFTWARE FRAMEWORK

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ABSTRACT

Semiconductor CdZnTe gamma spectrometers allow the implementation of new radiation monitoring technologies. However, the energy resolution from 5 to 10 keV and the small size of the detector may result in the detector being unable to resolve photopeaks with very close energies. Algorithms deduce the source identity from the spectrum and must rely on a well-established peak separation in cases where multiple sources are involved. Some techniques exist, but they are computationally expensive, both in memory and processor speed. Typically they can lead to critical performance problems when run on single board computers. To solve this problem, spectral deconvolution methods such as Gold or Richardson-Lucy algorithms have been proposed, that somewhat resolve the complex spectrum. The realized functions of spectra processing implemented in the ROOT CERN allow solving the indicated contradictions. The article presents the results of using ROOT CERN on a single-board computer for analyzing the spectra measured with a CdZnTe spectrometer. The results show that the spectral deconvolution methods used have high accuracy and efficiency in the deconvolution of complex spectra.

Keywords: Gamma-ray spectroscopy; spectra analyzes software; ROOT CERN; CdZnTe-detector; peak searching algorithm

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1. INTRODUCTION

A new approach to ensuring safety when using radiation sources and nuclear facilities is currently being developed [1]. It aims to minimize the risks of unplanned or accidental exposure from any additional sources [2].

It is important to note that the energy resolution of spectrometers based on CdZnTe detectors is in the range from 5 to 12 keV, which is worse than for HP(Ge) to much better than NaI(Tl) [3]. Book [4] contains great examples of spectra for different measurement conditions. In [5] the dependences of the measurement quality on the metrological characteristics of the detectors and the parameters of the total absorption peaks calculated during the analysis of the measured gamma spectra are given. Thus, the software plays an important role in assessing the quality of the measuring system as a whole [6].

Of course, there are many known gamma spectrum analysis programs that are available both free of charge and commercially [7]. There are free versions of commercial programs with limited functionality. But the main problem is that the well-known software is designed to work with traditional detectors. The exception is the software provided by the developers of CdZnTe spectrometers. It should also be noted that this is mainly closed software, which limits the range of tasks to be solved for determining the characteristics of radiation sources. At the same time, the development of software for the analysis of gamma spectra with the use of new information technologies is now actively developing [8].

In principle, two areas can be distinguished here:

– improvement of the algorithms for calculating the parameters of the total absorption peaks, i.e. expanding the capabilities of traditional software [9];

– the use of artificial intelligence methods, first of all, for the analysis of the all spectrum [10, 11].

Both directions have strengths and weaknesses. The use of modern data processing algorithms makes it possible to increase the sensitivity, i.e. to

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reduce the minimum detectable activity, and the accuracy of the spatial localization of radiation sources [12]. But the analysis results are highly dependent on the measurement conditions. Artificial intelligence technologies can improve the quality of isotope identification, but there are limitations in quantifying radiation sources. Obviously, in the future, research will be carried out aimed at combining these two areas [13].

But the analysis of gamma-ray spectra is widely used in high-energy physics. One of the key and generally recognized tools for data analysis in the HEP is the ROOT CERN software framework [14].

In our work, we consider the application of the ROOT CERN software framework for the analysis of gamma spectra of the obtained CdZnTe spectrometers. For the time being, we will restrict ourselves to algorithms for searching for peaks of total absorption. But in the future, ROOT CERN can be used to solve problems using artificial intelligence methods [14].

2. MODEL OF GAMMA-RAY SPECTROSCOPY

The spectrum $\Phi(x^{(1)}, x^{(2)}, \dots, x^{(n)})$ is understood as the distribution of the number of particles or events over the measured values (parameters) $x^{(1)}, x^{(2)}, \dots, x^{(n)}$ reduced to some standard conditions. The parameters $x^{(i)}$ can be the investigated physical (energy) or space-time characteristics of the particles. In this case, talking about the radiation spectrum. In the case when the parameters $x^{(i)}$ are the observable physical (energy) or space-time characteristics speak about the instrumental spectrum [15].

When analyzing, two types of measured parameters should be distinguished – discrete (energy for gamma radiation, charge, particle mass, analyzer channel number) and continuous (time intervals between events, signal amplitude, spatial variables). One of the main characteristics of nuclear radiation is the energy spectrum. And nuclear physics research most often has to deal with energy spectra, so the term "spectrum" is often used for the concept of "energy spectrum". The spectral line is understood as the radiation spectrum related to one transition between discrete energy levels [16, 15]. Considered formally discrete, such radiation is characterized by some average energy $\bar{E}$ and distribution (spectrum) $\Phi(E)$, which is called the line shape [15]. The real line width is mainly determined by the Doppler effect, which depends on the nature of the motion of the decaying nuclei [17]. The spectral line shape characterizes the radiation associated with one energy transition. A distinction is also made between the emission spectrum of a nuclide – the total spectrum of radiation relating to all transitions of a given type, and the emission spectrum of a source – the total spectrum of radiation of a given type, relating to all nuclides contained in the source [5].

The immediate goal of a spectrometric experiment is to measure the spectrum, i.e. definition of the function $\Phi(x^{(1)}, x^{(2)}, \dots, x^{(n)})$. In such an experiment, a spectrometer is used to register particles and analyze their characteristics. The essence of the analysis is to transform the studied characteristics of particles *V* (energy, mass) into the observed physical characteristics *x* (amplitude of the electric pulse). The result of such an experiment is a set of values $x_i^{(1)}, x_i^{(2)}$ ... (*i*=1, …, *n* –is the measurement number). As the spectrum $\Phi(x)$, we will consider the spectrum of particles detected by the spectrometer. Then $\Phi(x)dx$ is interpreted as the average number of particles recorded per unit time, for which the parameter *x* lies in the interval (*x*, *x*+*dx*).

Due to the specificity of nuclear-physical processes, the transformation of the physical characteristics of a particle into a measured value is not unambiguous. Therefore, the measured emission spectrum will not coincide with the true emission spectrum. Let $\mathrm{G}(x, V)$ be the conditional probability density of recording the value of the output signal equal to *x*, provided that the particle had the value of the physical parameter *V*. This function is called the response function of the spectrometer. Then the measured spectrum $\mathrm{U}(x)$ is related to the emission spectrum by the relation

$$\mathrm{U}(x) = \int \mathrm{G}(x, V)\Phi(V)\mathrm{d}V. \qquad (1)$$

The functions $\mathrm{U}(x)$ and $\Phi(V)$ are close to each other only if $\mathrm{G}(x, V)$ is close to the δ-function. The task is to reconstruct the radiation spectrum $\Phi(V)$ from the known $\mathrm{U}(x)$ and $\mathrm{G}(x, V)$. Equation (1) is the 1st kind integral Fredholm equation.

Let us consider this in more detail in relation to gamma radiation.

The instrumental spectrum is complex due to the peculiarities of the registration of gamma radiation with proportional detectors. In addition, there are both natural and technological limitations on how accurately the detection system can register the energy of a Gamma-ray detection event. The natural limitation of the accuracy of determining the energy arises mainly due to statistical fluctuations associated with the processes of charge formation in the detector. Total absorption peak positions can also be distorted by electronic effects such as noise, pulse aliasing, incorrect pole-to-zero setup, and the

like. In addition, the real spectrum of gamma radiation of the sample may differ significantly from the spectra obtained in laboratory conditions [18].

The instrumental spectrum of monoenergetic gamma radiation in the "narrow beam" geometry consists of three main components – the peak of total absorption, the peak of emission, and a continuous distribution on the left side due to Compton scattering (Fig. 1.).

The peculiarity of the used detector is that the total absorption peak is not a simple Gaussian due to the peculiarities of the physics of transport of charge carriers (electrons and holes) in the process of collecting the charge arising from the interaction of a gamma quantum with the detector material. There are several approaches to the representation of instrumental spectra when registering gamma radiation with detectors based on CdZnTe and CdTe [19]. The method describedin [20] was adopted as the basis for the model of the peak shape of the total absorption. The difference lies in taking into account the departure peak, and this is not provided for by any of the methods mentioned.

An example of the spectrum of an calibration source is shown in Fig. 2.

Common to all modes of the total absorption peak in detectors based on CdZnTe is taking into account the "pulling" of the left half of the total absorption peak due to the contribution of the slower "hole" component. Another common feature of the models of instrumental spectra of CdZnTe detectors is the use of parameters obtained experimentally [21, 22].

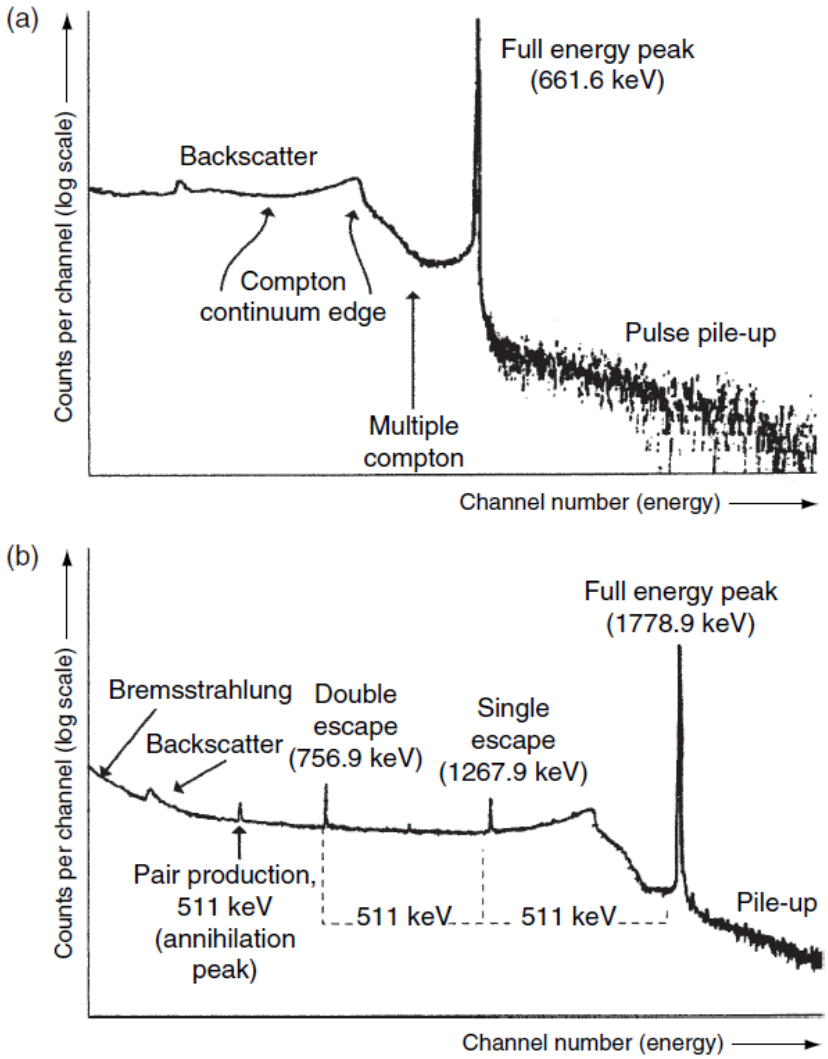


Fig. 1. **Typical data acquisition scheme used with modern radiation detectors [18] Example spectra illustrating the various spectral features expected: (a) ^{137}Cs; (b) ^{28}Al**

***Source*: [18]**

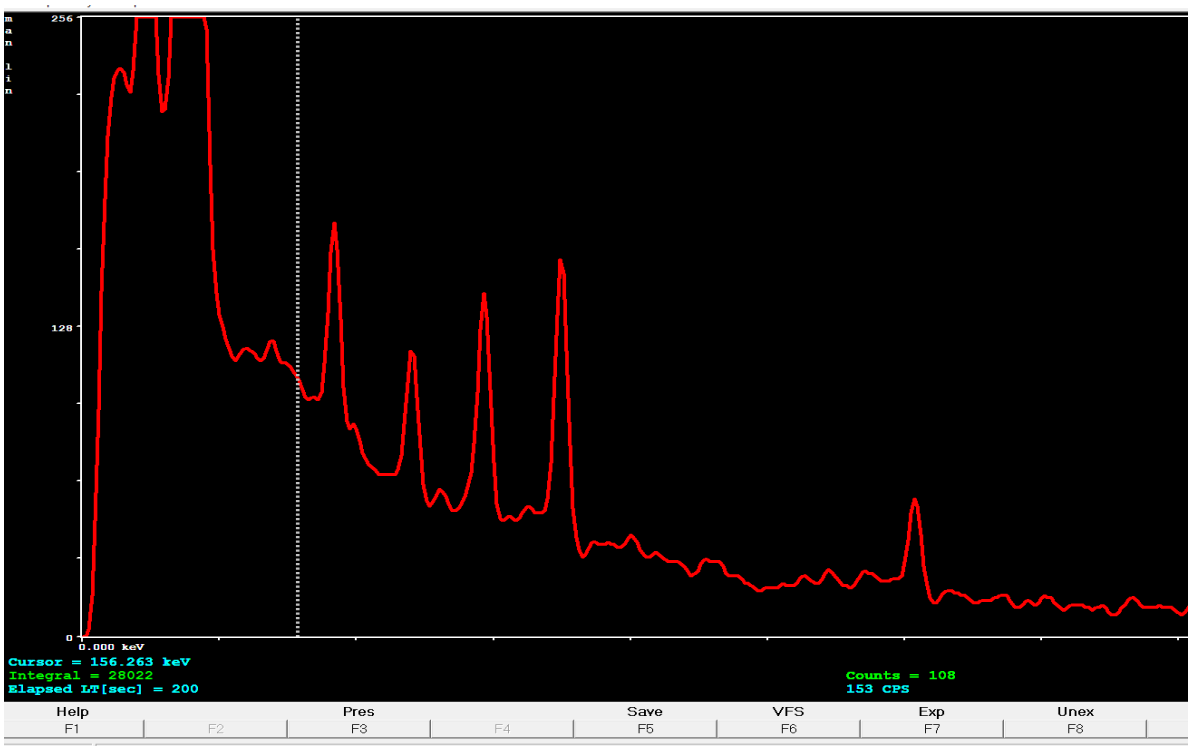


Fig. 2. **Gamma-ray spectra ^{133}Ba**
***Source*: compiled by the author**

Taking into account the above features of the detector, the following analytical representation of the total absorption peak was used to describe the response function of the CdZnTe spectrometer [22]:

$$n(E_i) = n_0 \exp\left[-\frac{(E_i - E_0)^2}{2\sigma^2}\right] + n_0 F_t(E_i), \qquad (2)$$

where

$$F_t(E_i) = \{A \cdot \exp[B(E_i - E_0)]\}\left\{1 - \exp\left[\frac{C(E_i - E_0)^2}{2\sigma^2}\right]\right\}\delta$$

– is the function describing the left "tail" of the peak of total absorption due to the later collection of charge by holes (F_t – symbol t from "tail" is the remainder), $n(E_i)$ – is the number of counts in the channel corresponding to the energy of-quanta, E_i, n_0;
– is the peak amplitude, E_0 – is the centroid of the peak, σ^2– dispersion of the Gaussian distribution, $FWHM = 2\sigma\sqrt{ln2}$ – is the full width of the photopeak at half its height, A – is the parameter that determines the amplitude of the function F_t, B – is the parameter that determines the decay of the function F_t, C – is the parameter that determines the "cutoff" of the function F_t, $\delta = 1$ at $E_i < E_0$ and $\delta = 0$ at $E_i > E_0$.

In this case, the emission peak will be described by a Gaussian distribution similar to the first term of equation 3, shifted by the value of the experimentally determined parameter [23]. The dependences of the values of parameters A and B on the recorded radiation energy obtained in laboratory studies with exemplary sources are given in [24].

To represent the Compton distribution $\mu(E, E_i)$, the method of statistical tests (Monte Carlo method) was used, which is the most effective when considering the transfer of radiation in matter due to the statistical nature of this process [25]. This is explained by the fact that elementary scattering events take place on a free electron and therefore the properties of the crystal are not essential. In addition, scattering has a continuous spectrum of secondary particles and large statistics are needed for its correct representation; therefore, it is optimal to use the Monte Carlo method. In the Monte Carlo method, the random motion of a particle is considered as a certain trajectory, and the state of the particle at each nodal point is played out using random numbers from the corresponding distributions. It is shown that modern algorithms for the implementation of this method make it possible to achieve modeling accuracy up to 1-2 % [22]. The implementation of the Monte Carlo method used was described in more detail earlier [22].

The distribution $\mu(E, E_i)$ is the probability of scattering of a secondary electron in the energy interval (α_1, $\alpha_1+d\alpha_1$) and is determined by the Klein-Nishina formula [17]:

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$$W(\alpha_1)d\alpha_1 = A(\alpha)f(\alpha,\alpha_1)d\alpha_1, \frac{\alpha}{1+2\alpha} \le \alpha_1 \le \alpha$$

$$f(\alpha,\alpha_1) = \frac{\alpha_1}{\alpha} + \frac{\alpha}{\alpha_1}\left(\frac{1}{\alpha} - \frac{1}{\alpha_1}\right)\left(2 + \frac{1}{\alpha} - \frac{1}{\alpha_1}\right), \quad (3)$$

where: α, α_1 – is the energy before and after scattering in units of electron mass; $A(\alpha)$ – is the normalization constant. In this case, the maximum energy of a Compton electron is determined by the formula [18]

$$E_{kmax} = \frac{E}{1+\frac{mc^2}{E}}. \quad (4)$$

For monoenergetic gamma radiation, the maximum energy E of a Compton electron is calculated using formula (4), and then a model of the Compton distribution is constructed using the Monte Carlo method. When simulating the required section of the instrumental spectrum, the obtained distribution is multiplied by a correction factor, which is a constant of the detector and determines its characteristic as the "Compton / peak" ratio.

Then the differential energy spectrum $d\varphi(E)/dE$ for a large number of gamma quanta in the decay scheme has the form

$$d\varphi(E)/dE = \sum_{i=1}^{M}\left[n_i(E) + n_{esc}(E) + \mu(E,E_i)\right], \quad (5)$$

where M – is the number of gamma lines in the decay scheme of the isotope under study.

Since the experimental spectrum $U(E)$ is discrete, the theoretical spectrum is also transformed into a discrete form with a given energy window ΔE

$$\varphi(E) = (d\varphi(E)/dE)\,\Delta E. \quad (6)$$

The presented relations (5) and (6) describe the functions U (x) and G (x, V) from expression (1) in relation to the gamma radiation spectra measured by the CdZnTe spectrometer.

3. ROOT CERN OBJECT-ORIENTED FRAMEWORK

3.1. General Description ROOT

ROOT is an object-oriented framework aimed at solving the data analysis challenges of high-energy physics developed and supported by CERN [14]. It was originally designed for particle physics data analysis and contains several features specific to this field, but it is also used in other applications such as astronomy and data mining [26]. With ROOT you can [26]:

Save data You can save your data (and any C++ object) in a compressed binary form in a ROOT file. The object format is also saved in the same file: the ROOT files are self-descriptive. Even in the case the source files describing the data model are not available, the information contained in a ROOT file is be always readable. ROOT provides a data structure, the tree, that is extremely powerful for fast access of huge amounts of data – orders of magnitude faster than accessing a normal file.

Access data Data saved into one or several ROOT files can be accessed from your PC, from the web and from large-scale file delivery systems used e.g. in the GRID. ROOT trees spread over several files can be chained and accessed as a unique object, allowing for loops over huge amounts of data.

Mine data Powerful mathematical and statistical tools are provided to operate on your data. The full power of a C++ application and of parallel processing is available for any kind of data manipulation. Data can also be generated following any statistical distribution and modeled, making it possible to simulate complex systems.

Publish results Results can be displayed with histograms, scatter plots, fitting functions. ROOT graphics may be adjusted real-time by few mouse clicks. Publication-quality figures can be saved in PDF or other formats.

Run interactively or build your own application You can use the Cling C++ interpreter for your interactive sessions and to write macros, or you can compile your program to run at full speed. In both cases, you can also create a graphical user interface.

Use ROOT within other languages ROOT provides a set of bindings in order to seamlessly integrate with existing languages such as Python and R.

The inclusion of a C++ interpreter (CINT until version 5.34, Cling from version 6.00) makes this package very versatile as it can be used in interactive, scripted and compiled modes in a manner similar to commercial products like MATLAB.

With PyROOT, ROOT's Python-C++ bindings, you can use ROOT from Python. PyROOT is HEP's entrance to all C++ from Python, for example, for frameworks and their steering code. The PyROOT bindings are automatic and dynamic: no pre-generation of Python wrappers is necessary.

With PyROOT you can access the full ROOT functionality from Python while benefiting from the performance of the ROOT C++ libraries.

Analysis Once you get data, either real or simulated events, you can start browsing them with the ROOT browser, that allows you to quickly plot the distribution of your quantities (simply double click on variables). A productive way of working is to write a C++ macro, testing each command step by

step with the Cling interpreter – writing a Python program using PyROOT bindings is a very good option too. When you are satisfied with your macro, you may consider converting it into a compiled library or stand-alone application, to achieve the maximum speed.

Incidentally, note that, because the C++ specifications do not fix the size of integer and floating point variables (they only provide limits), ROOT provides also machine-independent definitions of different integer and floating point variables with fixed representation. Sometimes, such definitions are necessary to deal with your data, for example when they are the binary output of some device, in which case your variables must have the same representation as the output words of such device.

Most often, the result of your data analysis is best displayed as histograms. ROOT provides a very rich set of functionalities for histogram creation, manipulation and drawing, and can save high-quality plots in a number of different formats.

3.2. Advanced Spectra Processing in ROOT

Now ROOT includes advanced spectral pro-cesssing implemented in TSpectrum Class [27]. This class contains advanced spectra processing functions for:

– One-dimensional background estimation.
– One-dimensional smoothing.
– One-dimensional deconvolution.
– One-dimensional peak search.

The basic function of the 1-dimensional peak searching is in detail described in [28]. It allows to identify automatically the peaks in a spectrum with the presence of the continuous background and statistical fluctuations – noise [29]. The algorithm is based on smoothed second differences that are compared to its standard deviations. Therefore it is necessary to pass a parameter of sigma to the peak searching function. The algorithm is selective to the peaks with the given sigma. This function searches for peaks in source spectrum the number of found peaks and their positions are written into structure pointed by one_dim_peak structure pointer.

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However, when we have noisy data the number of peaks can be enormous. One such an example is given in Fig. 5. Therefore it can be useful to have the possibility to set a threshold value and to consider only the peaks higher than this threshold. The value in the center of the peak value[i] minus the average value in two symmetrically positioned channels (channels i-3*sigma, i+3*sigma) must be greater than the threshold. Otherwise, the peak is ignored.

The algorithms of background estimation are based on Sensitive Non-linear Iterative Peak (SNIP) clipping algorithm. The smoothing algorithms are based on the convolution of the original data with several types of filters and algorithms based on discrete Markov chains. The peak searching algorithms use the smoothed second differences and they can search for peaks of general form. The deconvolution (decomposition – unfolding) functions use the Gold iterative algorithm, its improved high resolution version and Richardson–Lucy algorithm. In the algorithms of peak fitting we have implemented two approaches. The first one is based on the algorithm without matrix inversion – AWMI algorithm. It allows it to fit large blocks of data and large number of parameters. The other one is based on the calculation of the system of linear equations using Stiefel-Hestens method. It converges faster than the AWMI, however it is not suitable for fitting large number of parameters [27].

SpectrumDeconvolution function implemented in ***TSpectrum*** is used for spectrum analysis. This function is used to strip-off known instrumental function from source spectrum. It is achieved by deconvolution of source spectrum according to response spectrum using Gold or Richardson-Lucy algorithms [31]. Value – numeric vector of the same length as y with deconvoluted spectrum (Fig. 3).

Both methods search iteratively for solution of deconvolution problem [32]

$$y(i) = \sum_{j=1}^{n} h(i-j)x(j) + e(i), \qquad (7)$$

in the form

$$x^k(i) = M^k(i)x^{(k-i)}(i). \qquad (8)$$

For Gold method:

$$M^k(i) = \frac{x^{(k-i)}(i)}{\sum_{j=1}^{n} h(i-j)x(j)}. \qquad (9)$$

For Richardson-Lucy:

$$M^k(i) = \sum_{l=0}^{n} h(i-l)\frac{x^{(k-1)}(l)}{\sum_{j=1}^{n} h(l-j)x^{(k-1)}(j)}. \qquad (10)$$

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Here $h(i-j)$ in (7) is calculated based on $d\varphi(E)/dE$ in (5).

4. RESULT AND DISCUSSION

Often in publications ROOT criticized for the complexity and unnecessary functionality. Therefore, the main task of this work was to test the possibility of using basic algorithms of the TSpectrum ROOT class for analyzing the gamma radiation spectra measured by CdZnTe on a single-board computer (Fig. 4). The requirement to use a single board computer is a key condition for creating a modern mobile spectrometer [32].

Therefore, the analysis of the spectra was carried out on a single-board computer running the Ubuntu 18.04 operating system. The amount of RAM is 4 GB, SD – 64 GB. Version ROOT 6.14.06. Python was used to work with the analyzer and spectra processing programs. PyROOT was used as a software interface for working with ROOT [33].

Some examples with the results of spectra processing are shown. Fig. 5, Fig. 6, Fig. 7 and Fig. 8 show the analysis of the gamma-ray spectrum of ^{235}U obtained by measuring a special reference source. Fig. 5 shows the instrumental radiation spectrum of an exemplary source of Uranium with an initial enrichment of 20 % in ^{235}U. Fig. 6 shows the peak search results for the entire spectrum at different scales. The spectrum presented very well illustrates the problem of large differences in the intensities of the detected radiation for energies below 300 keV and for energies of about 1000 keV. Therefore, Fig. 7 shows a portion of the spectrum with a gamma-ray line of ^{238}U. A quantitative analysis of this peak is very important for instrumental assay of the initial enrichment of nuclear fuel [37]. This spectrum clearly demonstrates the contribution of Compton scattering at low energies. Methods implemented by TSpectrum can also be used to reduce Compton scattering fusion, an example is shown in Fig. 9 for a point source of ^{137}Cs. Fig. 8 shows a photopeak with low statistical significance; it is quite well identified. A distinctive feature of the low intensity peaks is symmetry, in contrast to the peak in Fig. 7.

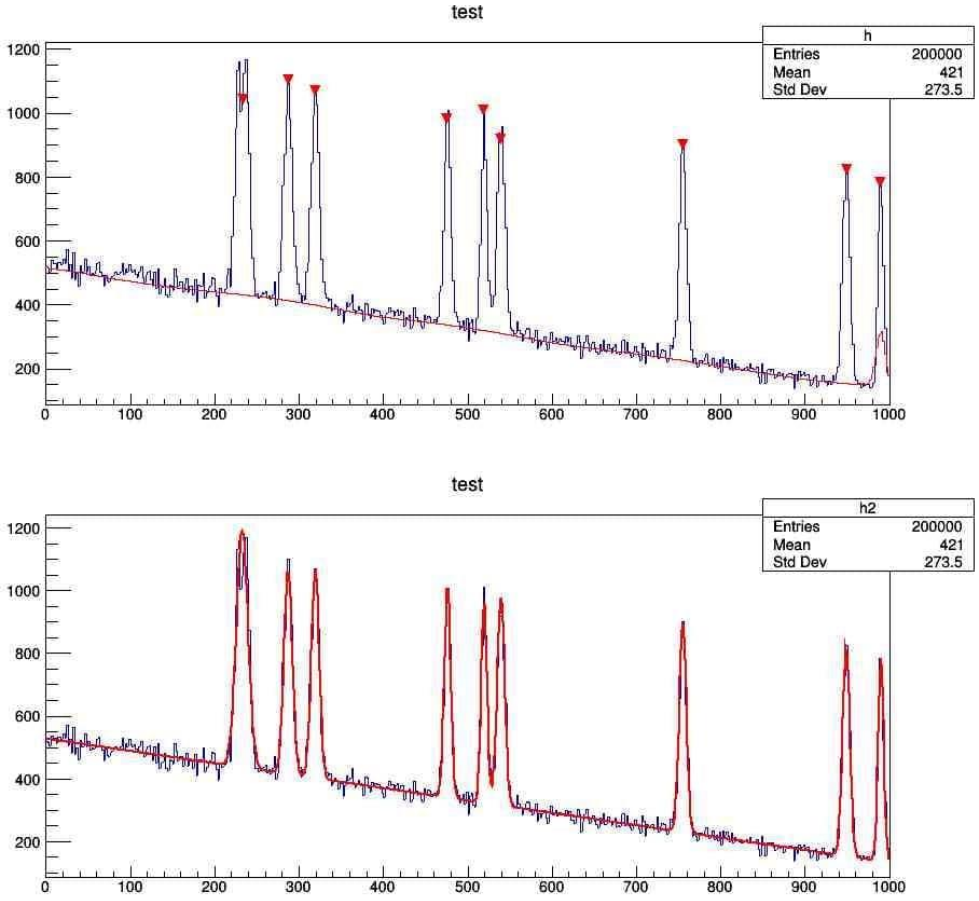


Fig. 3. **Gamma-ray spectra processing. Test deconvolution**
***Source*: [27]**

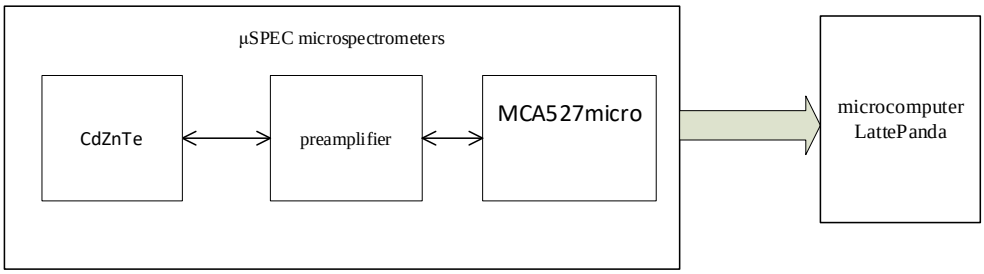


Fig. 4. **CZT-spectrometer operation**
***Source*: compiled by the author**

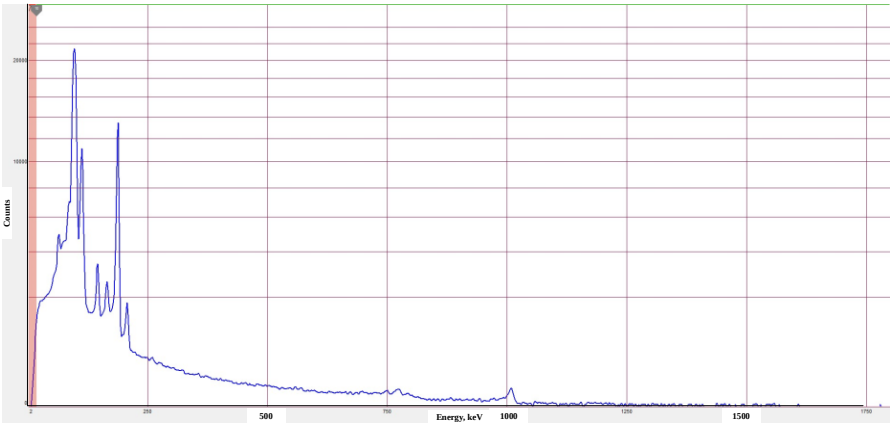
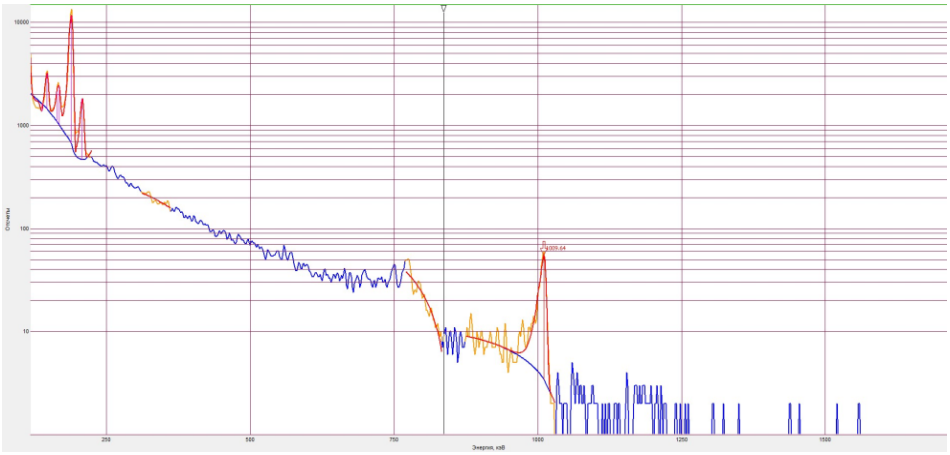
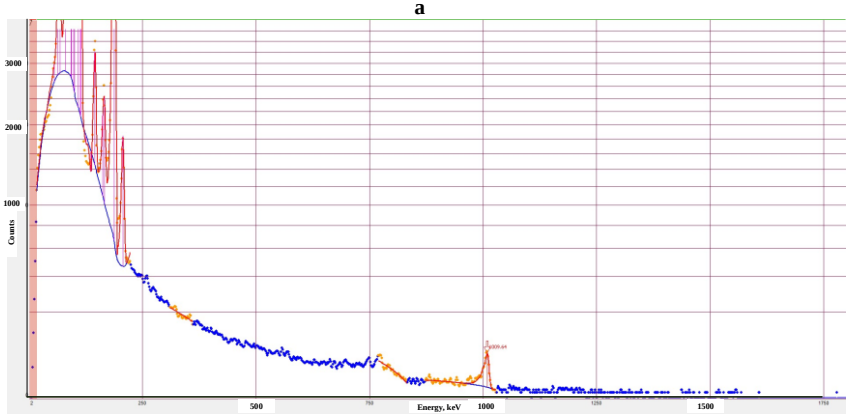


Fig. 5. **Gamma-ray spectra processing**
***Source*: compiled by the author**



a



b

Fig. 6. **Gamma-ray spectra processing:**
a) logarithmic scale; b) quadratic scale
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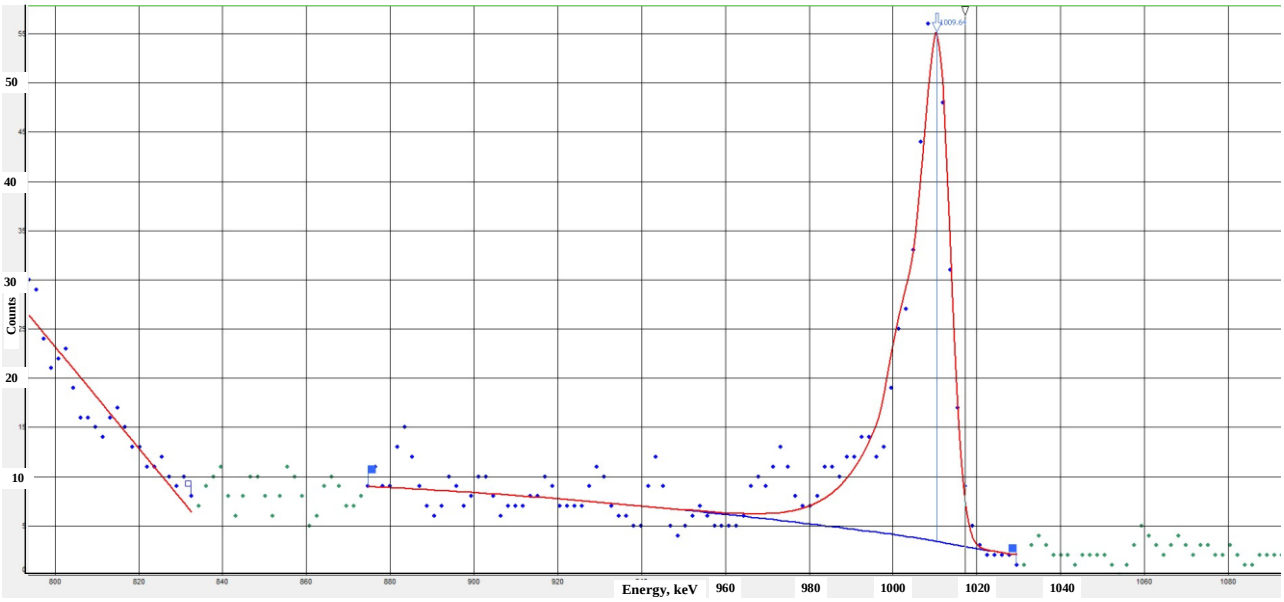


Fig. 7. **Gamma-ray spectra processing**
***Source*: compiled by the author**

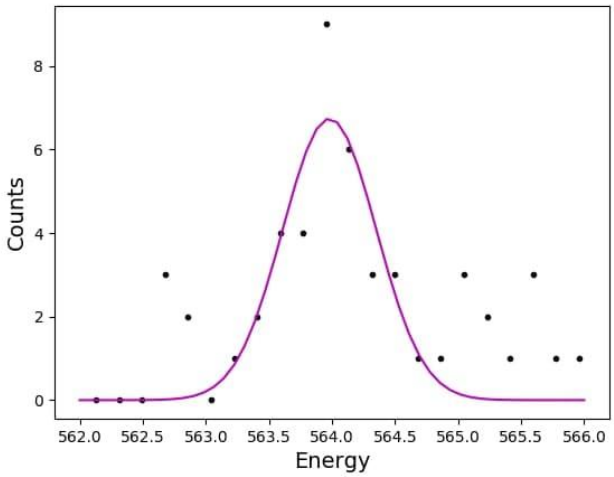


Fig. 8. **Gamma-ray spectra processing. Peaks fit**
***Source*: compiled by the author**

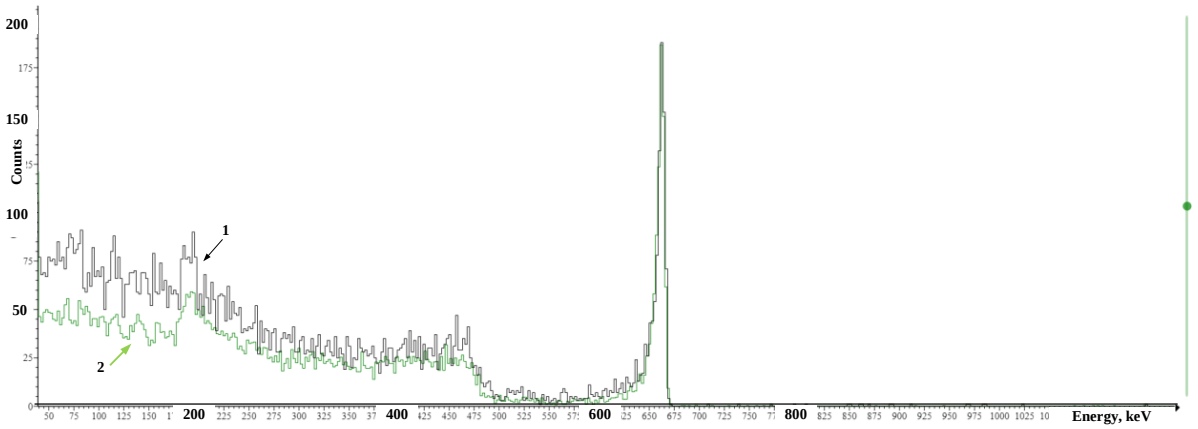


Fig. 9. **Gamma-ray spectra processing. Contribution of Compton scattering**
***Source*: compiled by the author**

CONCLUSION

As already noted, one of the problems of creating a mobile CdZnTe spectrometer is the contradiction between the requirements for high efficiency of the algorithms for processing the measured spectra and the computational capabilities of the spectrometer processor. The results obtained showed the possibility of processing one-dimensional gamma-radiation spectra using the methods implemented in the TSpectrum ROOT class on a universal single-board computer running the Ubuntu operating system. PyROOT was used as a software interface for working with ROOT, ROOT's Python-C ++ bindings, you can use ROOT from Python.

The result obtained made it possible to determine the direction of future research on the use of ROOT for

– processing of multidimensional spectra

– analysis of poorly identified photo peaks using neural networks.

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АНАЛІЗ СПЕКТРІВ ГАММА-ВИПРОМІНЮВАННЯ, ОТРИМАНИХ CDZNTE-ДЕТЕКТОРОМ, З ВИКОРИСТАННЯМ ПРОГРАМНОГО ПАКЕТА ROOT CERN

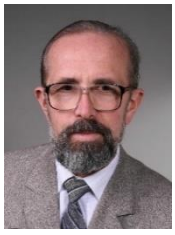
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АНОТАЦІЯ

Напівпровідникові гамма-спектрометри CdZnTe дозволяють впроваджувати нові технології радіаційного контролю. Однак енергетичний дозвіл від 5 до 10 кеВ і невеликий розмір детектора можуть привести до того, що детектор не зможе визначити фотопікі з дуже близькими енергіями. Алгоритми ідентифікації джерела по спектру і повинні покладатися на чітко встановлений поділ піків у випадках, коли використовується декілька джерел гамма-випромінювання. Існують ефективні методи аналізу спектрів, але вони вимагають великих обчислювальних ресурсів як з точки зору пам'яті, так і з точки зору швидкості процесора. Зазвичай вони можуть призвести до критичних проблем з продуктивністю при роботі на мікрокомп'ютерах. Для вирішення цієї проблеми, були запропоновані методи розкладання спектра, такі як алгоритми Голда або Річардсона-Люсі, які в деякій мірі дозволяють ідентифікувати піки в складному спектрі. Реалізовані в ROOT CERN функції обробки спектрів дозволяють вирішити зазначені суперечності. У статті представлені результати використання ROOT CERN на мікрокомп'ютері для аналізу спектрів, виміряних за допомогою спектрометра CdZnTe. Результати показують, що використовуються методи аналізу спектрів мають високу точність і ефективністю при розкладанні складних спектрів.

Ключові слова: гамма спектрометрія; програмне забезпечення аналізу спектрів; ROOT CERN; CdZnTe-детектор, алгоритм пошуку піків

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