Isotope Identification in the GammaTracker Handheld Radioisotope Identifier

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Abstract–**GammaTracker is a portable handheld radioisotope identifier using position sensitive CdZnTe crystals. The device uses a peak-based method for isotope identification implemented on an embedded computing platform within the device. This paper presents the run-time optimized algorithms used in this peak-based method of analysis. Performance of the algorithms is presented using measured data from gamma-ray sources.**

I. INTRODUCTION

THE Pacific Northwest National Laboratory (PNNL) is currently developing a rugged handheld radioisotope identifier with directional capabilities designed for search, survey, and characterization applications. The device, known as GammaTracker, uses an array of 18 2.25 cm^3 CdZnTe position sensitive crystals. This enables it to achieve a higher energy resolution as compared with other room-temperature devices and a higher relative efficiency than other CZT-based commercial systems. It performs in real-time automated calibration corrections, Compton imaging for directionality, and isotope identification. An internal representation of GammaTracker and its external packaging are shown in Fig. 1. Additional information about GammaTracker can be found in [1], [2], and [3].

Isotope identification within GammaTracker is implemented using a peak-based method of analysis, wherein the peak locations and intensities are determined from the spectra and then compared to a library of suspected radionuclide gamma-ray energies. Unlike template-based approaches, which require a comprehensive library of measured spectral templates, a peak-based method of analysis can identify a radionuclide not previously measured, as long as the corresponding gamma-ray energies and intensities are properly tabulated. In this work we present the run-time optimized algorithms used in the isotope identification process on GammaTracker and illustrate their performance on measured data from known gamma-ray sources.
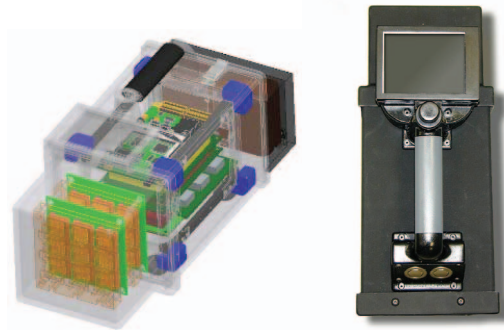
Fig. 1. Left: CAD drawing of the GammaTracker radioisotope identifier showing the device's internal electronics and array of CdZnTe crystals. Right: GammaTracker external packaging.

II. PEAK IDENTIFICATION

Fig. 2 shows the process involved in identifying the peaks in the spectrum and calculating the net area (counts) under each of the observed peaks. First an initialization file is read in and processed to provide information relevant to both peak identification and isotope identification. One important piece of information from this file is the detector's intrinsic resolution as a function of energy, given as quadratic polynomial coefficients. Then, for every measured gamma-ray spectrum that is acquired,

1. the spectrum is smoothed;
2. a filter is applied to extract the tentative peak locations and their widths;
3. regions of overlapping peaks (known as multiplets) are identified;
4. an underlying "background" continuum is estimated over all peak regions, including the multiplets;
5. the multiplet regions are resolved into their constituent peaks;
6. the count rate of each peak is calculated.

The spectrum is initially smoothed so that it can be used by any of the algorithms that follow. A smoothed spectrum is required for deconvolution of the multiplet regions and estimation of the peak region continuum, but it is optional in all other routines. A nine knot least squares "Savitzky-Golay" filter [4] was chosen in a compromise of speed and accuracy. The filter works by performing a local polynomial regression over the data neighboring a given point in order to determine its smoothed value. A set of pre-computed knots makes this process efficient. The method preserves peak features much better than other filters, such as moving average filters, and can be coded to be just as fast.
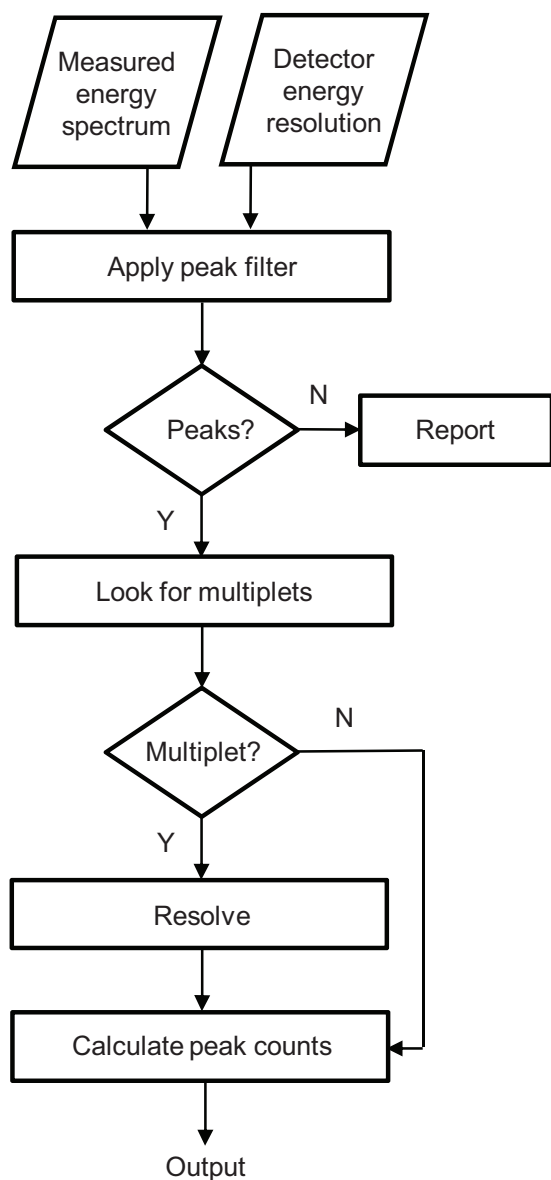
Fig. 2. Flow chart of the peak finding algorithm.

After smoothing, a tentative list of peak locations is determined by cross-correlating a zero-area square pulse of varying width against the raw gamma spectra, resulting in a curve that reflects the degree of correlation between the two inputs. The width of the square pulse is varied based on the energy resolution of the spectrum, where the square of the full width at half maximum is proportional to energy. Maximums in the filter's output that lie above a user-defined sensitivity threshold are considered peaks. The width of each peak is estimated using the width of the hump associated with this maximum. A visual of the process can be seen in Fig. 3 on a measured spectrum containing ^{133}Ba and ^{60}Co. Given a sensitivity of three, seven tentative peaks are identified in the figure, one of which is a false peak at 1102 keV. The sensitivity is one of the variable parameters in the algorithm that may need to be fine-tuned based on the performance of a

given detector. A square pulse was used in the filter instead of a Gaussian in order to avoid the calculation of an exponent $n \times m$ number of times, where n is the number of spectra channels and m is the width of the pulse in channels. The isotope identification process is currently being run using the on-board integer based microprocessor, so avoiding complex floating point calculations like this is essential to optimize speed. Further, the peak identification capabilities of the Gaussian and square pulse digital filters were nearly identical in a series of tests that were conducted using CZT spectra.
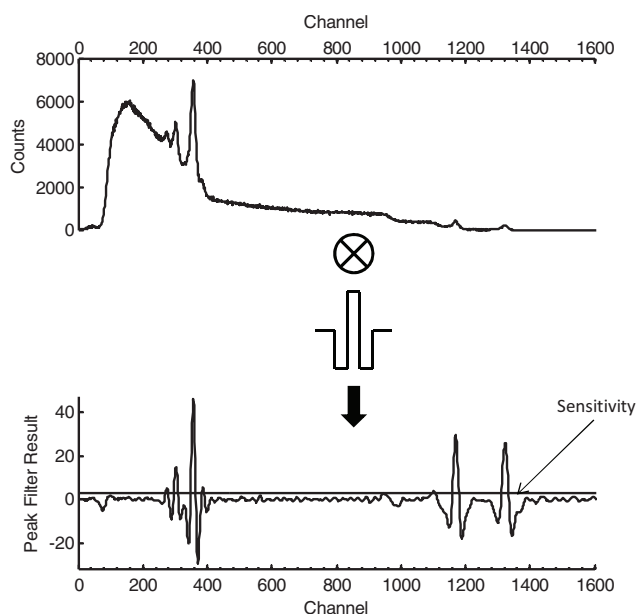

Fig. 3. Illustration of the peak finding matched filter algorithm using a zero-area square pulse of varying width as the matched filter kernel. The maximums of the resulting curve that lie above the "sensitivity" represent found peaks.

Once the tentative peak locations and widths are determined, sets of overlapping peaks are found and a continuum "background" is calculated over all peak regions, including both multiplets and singlets. Finding the multiplet regions is necessary because their constituent peaks need to be resolved before any reasonable peak area calculation can be made. The estimated widths for these peaks from the peak filter are usually far from accurate because of the overlap. Given a smoothed spectrum as input, the background continuum under each peak region is modeled using a smoothed series of step functions drawn from the left side of the region to the right. One step is used for each individual peak and its height is proportional to the height of the peak above it, relative to the other peaks. An example stepped background for a multiplet region can be seen in Fig. 4. Here the ^{133}Ba 384 keV and 356 keV multiplet from the Fig. 3 spectra is highlighted. Step functions have proven more accurate as a peak background because they help to account for the pulse pileup of degraded full-energy events between the peak and its Compton edge [5], [6]. Smoothing of the

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steps is required to account for the line broadening process inherent in gamma-ray spectra.

Singlet peaks at this point only need to be integrated by summing the counts that lie between the raw spectral data and the estimated background. Multiplets, however, must be resolved into their constituent component peaks. The technique of simply drawing a line between each peak overlap point, subtracting off the background, and integrating can only give a crude estimation of the counts in each of the peaks. Instead, a non-linear least squares fitting procedure must be used that perhaps defaults to this gross sum method if the fit diverges. The fitting procedure first subtracts off the continuum "background" from the raw spectral data over the span of the multiplet. Initial guesses for the peak model parameters must then be made based on the existing peak data that has been acquired thus far. For GammaTracker a standard Gaussian has been chosen as the model even though a more technically correct model for CZT spectral peaks is a Gaussian with an exponential tail. Experiments with the code have shown that a Gaussian peak model is adequate. A non-linear fitting procedure using the Levenberg-Marquardt algorithm [7] is then undertaken to fit a sum of Gaussians to the continuum subtracted raw data in the multiplet, given the initial parameter estimations for each Gaussian and the uncertainty in the raw data due to Poisson counting statistics. If the fit is divergent or grossly inaccurate, a singular value decomposition linear least squares method is used as backup. It will never diverge from a solution, but it assumes a very accurate initial estimation of the peak locations and full width at half maximums for good results. Only the height of the constituent Gaussians is considered in the fit. If the linear method itself is grossly inaccurate then the simple integration method mentioned earlier is used. Fig. 4 shows a successful fit for the ^{133}Ba 384 keV and 356 keV multiplet. After fitting, the area of each Gaussian is calculated in addition with its uncertainty using the propagation of errors. This information is instrumental in the identification of the isotopes.

III. ISOTOPE IDENTIFICATION

The isotope identification code within GammaTracker is a descendent of the GRPANL Germanium spectra analysis code suite [6]. Its strategy is to use gamma-ray information from a library of sought-after nuclides to compose a list of candidate nuclides that pass a series of tests, and then resolve the relative disintegration rates of the nuclides from among the spectra peaks. A flow chart outlining the isotope identification process is shown in Fig. 5.
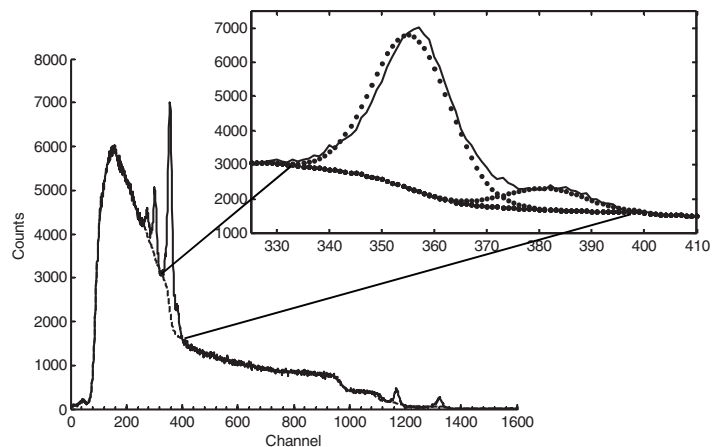

Fig. 4. Resolution of a ^{133}Ba multiplet region into its constituent Gaussian peaks from a GammaTracker spectra containing both ^{133}Ba and ^{60}Co. The stepped continuum "background" is evident under the peaks.

The algorithm initializes by accepting the peak data from the peak identification code and reading in the library of nuclides and a table describing the detector's relative efficiency as a function of energy. A minimalist approach to the nuclide library is best. It should contain nuclides that the analyst is most interested in finding in order to minimize false positive identifications. Linked to each nuclide in the library is a list of gamma-ray energies that will help to identify the nuclide, the branching ratios of the gamma-rays, and up to two other gamma-rays associated with each given gamma-ray line. Redundancy between the primary lines and the associated gammas is allowed in order to maximize results. Also allowed in the library is a designation for lines that should be missing for a specific nuclide. This gives the code the ability to properly identify a nuclide that shares many of the same lines as another nuclide in the library.

Determining the nuclides in the library that are consistent with a given set of observed peaks in the spectrum involves looping through each observed peak and energy line in the library and executing two tests for each (peak, energy line) combination. The tests are mathematical in nature and return a probability between 0 and 1 that the given energy line is a match for the peak. The most obvious test determines the degree at which the energy of a gamma-ray line in the library and the energy of the observed peak match. A Gaussian curve of the form

$$ f(x) = \exp\left(-\left(\frac{E_{line} - E_{peak}}{FWHM_{peak}\kappa} \right)^2 \right) $$

gives sensible results. Here E_{line} is the energy of the gamma-ray line in the library, E_{peak} is the energy of the observed peak, κ is a tuning factor, and $FWHM_{peak}$ is the full width at half maximum of the observed peak. The full width at half

maximum allows more leeway for wider peaks. An example of the energy test is given in the top portion of Fig. 6.
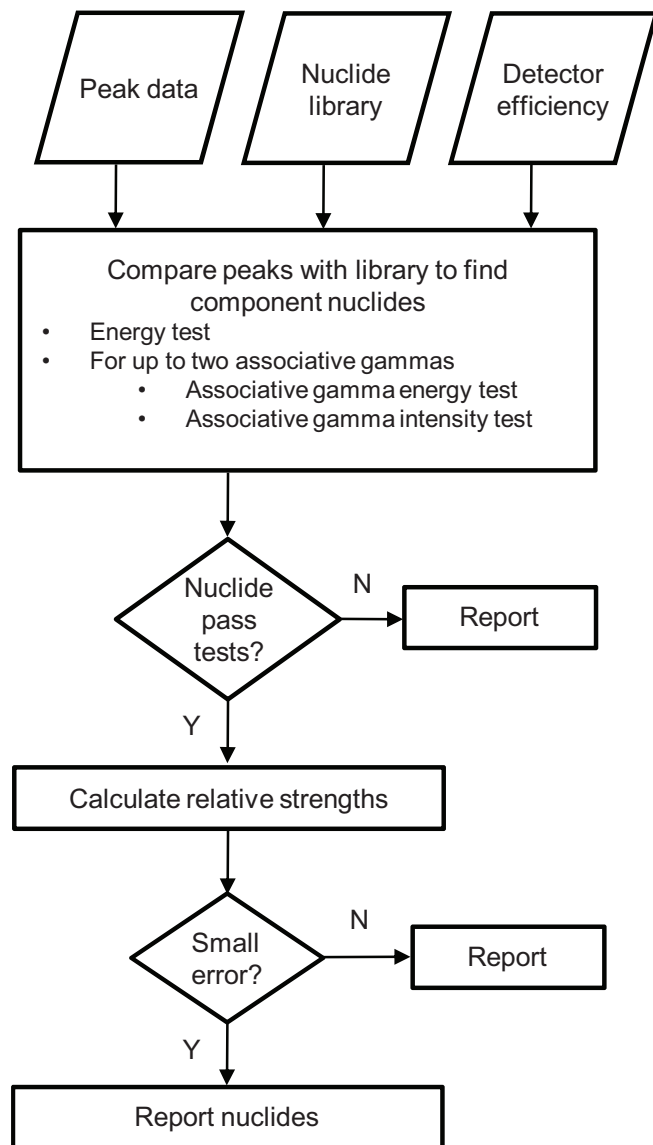

Fig. 5. Flow chart of the isotope identification algorithm.

The second test focuses on the associated gammas of the emission line specified in the library. It performs an energy test against the observed peak energies in a similar manner as above. If this passes with a high enough confidence then a comparison is made between the expected intensity of the associated gamma versus the observed intensity of the corresponding peak. The probability returned by the test is a measure of how similar these values are. Of course, the observed associated gamma peak could be comprised of emissions from multiple nuclides, so that must be considered in the test. The opposite could occur too, but that is less likely since the primary library energy lines should be chosen so that interferences are minimal. A suitable probability curve given these requirements is shown at the bottom of Fig. 6. After both tests are finished, their probabilities are multiplied and

compared against a user-defined threshold. Only nuclides that pass are considered in the final step of the analysis. Nuclides are also cut if a required missing peak from the library is present in the list of observed peaks.
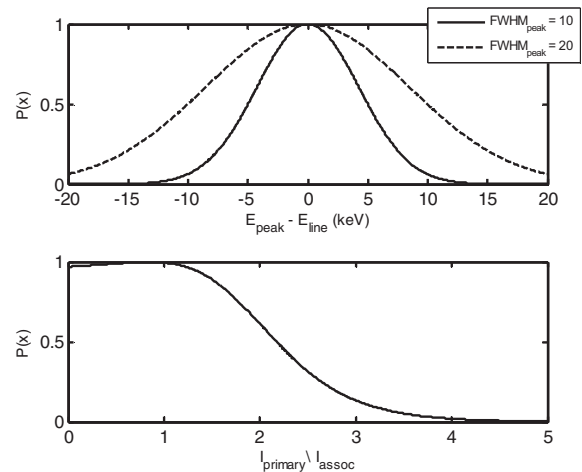

Fig. 6. Top: Function used in the isotope identification energy test. Bottom: Function used in the associated gammas intensity test.

The isotope identification process could be finished if the candidate nuclides did not share any peaks at the gamma-ray line energies given in the library. This is not always the case, however. The peak intensities are technically a linear combination of the nuclide disintegration rates with the branching ratios as coefficients. Assuming Y_i is the ith peak, A_j is the jth nuclide and X_{ij} is the branching ratio of the jth nuclide at the ith peak energy, we have

$$Y_i = \sum_{j=1}^{J} A_j X_{ij} ,$$

for a total of J nuclides. Given uncertainties in the peak intensities, a general least squares process solves this set of equations for the disintegration rates of the nuclides and their uncertainties, σ_j. Nuclides with relative uncertainties, $\sigma_j / A_j \times 100\%$, above an acceptable threshold are removed from the reported results. GammaTracker only reports the list of isotopes found and not their disintegration rates.

Fig. 7 shows the results from running the spectra from Fig. 4 through the isotope identification process. Both ^{133}Ba and ^{60}Co were identified from a total of 19 nuclides in the library. The solid vertical lines represent gamma-ray lines from the library that were successfully matched to their respective peaks. The dashed lines are from other nuclides in the library. Notice in the figure that the second peak in ^{60}Co (at 1332 keV) was not matched because of energy calibration errors, yet identification was still possible because two lines were used in the library. The "sensitivity" of the identification process can be relaxed by adjusting a parameter if necessary. The results from the least squares fit yielded a disintegration rate of

3.34×10^9 pCi for ^{60}Co and 1.199×10^{10} pCi for ^{133}Ba, and relative uncertainties of 2.3% and 0.7%, respectively.
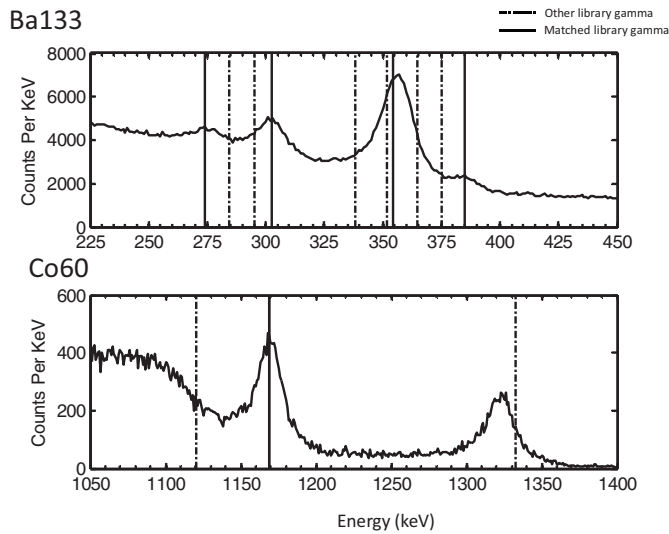

Fig. 7. Visual of gammas from an input nuclide library matched to the sample spectrum in Fig. 4 during the isotope identification process.

IV. CONCLUSION

The GammaTracker handheld radioisotope identifier uses a peak-based method of analysis in its isotope identification implementation. The first half of the process involves peak identification. In the algorithm, an initial list of candidate peaks is found using an optimized cross-correlation procedure against a square pulse of zero area. Multiplet regions are then identified and a stepped background is estimated for all peaks using a smoothed version of the spectra. The muliplet regions are resolved using non-linear least squares and the intensities of all observed peaks are calculated. Isotope identification takes place in the second half of the process. Here a library of sought-after peaks is compared against the set of observed peak information from the spectrum. A series of tests is conducted to determine the nuclides most likely responsible for producing the peaks present in the spectrum. A least squares approach is then undertaken to resolve the nuclide disintegration rates amongst the observed peaks and to calculate a relative error. The isotope identification process successfully identified ^{133}Ba and ^{60}Co from a GammaTracker spectra set using a library of 19 nuclides.

REFERENCES

[1] C. Seifert, et al., "First Light for the GammaTracker Handheld Radioisotope Identifier," submitted to the *IEEE Nuclear Science Symposium Conference Record*, N14-1, 2009.
[2] M. Myjak, "Real-Time Compton Imaging for the GammaTracker Handheld CdZnTe Detector," *IEEE Trans. Nucl. Sci.*, Vol. 55, No. 2, pp. 769-777, April 2008.
[3] M. Myjak, et al., "Electronics System for the GammaTracker Handheld CdZnTe Detector", *IEEE Nuclear Science Symposium Conference Record*, N15-139, 2007.
[4] A. Savitzky, M.J.E. Golay, "Smoothing and Differentiation of Data by Simplified Least Squares Procedures," *Analytical Chemistry*, Vol. 36, pp. 1627-1639, 1964.
[5] H. W. Stockman, "Microprocessor-based reduction of gamma spectra: A fast method for deconvolution of overlapped peaks," *Nucl. Instr. Methods*, Volume 274, Issue 1-2, pp. 314-318.
[6] R. Gunnink, W.D. Ruhter, J.B. Niday, "GRPANL: A Suite of Computer Programs for Analyzing Complex Ge and Alpha-Particle Detector Spectra," UCRL-53861, Vol. 1 (May 1988).
[7] W. Press, W. Vetterling, S. Teukolsky, B. Flannery, *Numerical Recipes in C++*, 2nd ed., Cambridge University Press, 2002, pp. 686-694.