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Quality assurance features of "HYPERMET-PC"

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The γ-ray spectrum analysis code HYPERMET-PC has been significantly upgraded since its introduction in the first k_0-Users Workshop (1992). Some aspects of the implemented procedures in the new version 5.0, such as the novel approach to handle tandem LFC spectra and the benefit of using ortho-normal polynomials for fitting efficiency curves will be outlined. Having realized the importance of quality assurance in applied γ-ray spectrometry, additional utilities have been incorporated for checking system parameters: nonlinearity, energy resolution, etc. The new Nuclide Identification routine makes the program suitable for qualitative analysis both of NAA and PGAA type.

Introduction+

Instrumental, multielement NAA makes stringent demands on applied γ-ray spectrometry. Following the irradiation, the measured γ-ray spectra are often very complex, containing hundreds of peaks with many multiplets and the underlying background also has an irregular shape. When short-lived isotopes are also present, the peak shapes in the spectrum are not uniform and change from measurement to measurement as a function of system characteristics and counting rate.

Consequently, the importance of selecting a dedicated evaluation software package cannot be overemphasized. We have years of favourable experience with the spectrum analysis code HYPERMET[1] which allows the dynamic variation of the peak and background shape parameters utilizing an effective non-linear fitting algorithm. This motivated our decision to develop an interactive version with user-friendly graphics and internal database to meet the ever growing demand for fast, semi automatic spectrum analysis.

While maintaining the main features of the original code, the body of the program was rewritten in C++ and adapted to the IBM PC operating system. The menu structure and the ease in spectrum processing together with a number of Windows-like features make this program an attractive choice for every γ-ray spectroscopist. Here the basic principles of some new modules in version 5.0 will be outlined.

The Quality Assurance package

This new menu consists of three modules for the determination of full-energy peak efficiency-, system nonlinearity- and full width at half maximum (FWHM) curves versus γ-energy. Although these functions are essential for system calibration in the first place, they represent the most important performance parameters of the applied γ-spectrometer, thus being most appropriate for QA purposes as well. In the course of programming, one governing principle was to require the minimum input from the user in order to save manpower and minimize human errors.

Full-energy peak efficiency

This is one of the most fundamental parameters in k_0-based NAA which should be absolute to allow corrections for true coincidence losses. Following the proven approach of MOENS,[2] $\varepsilon_{p,geo}$ can be determined for an actual geometric counting configuration using calculated solid angles and a "reference" efficiency curve[3] $\varepsilon_{p,ref}$. The latter is generally constructed by measuring a number of absolutely calibrated point sources (^{137}Cs, ^{241}Am, etc.) together with some "home-made" secondary sources (^{110m}Ag, ^{182}Ta, etc.) at a large distance from the detector. Input data such as decay periods, peak areas and associated errors etc. are usually entered into spreadsheet to calculate individual points of the efficiency vs. energy curve. Then a set of efficiency values are read-in to an other program for curve fitting. Obviously, this procedure is rather time consuming and is subject to a number of errors.

By contrast, HYPERMET-PC takes all input spectral data from peak table files. Furthermore, a special, editable ASCII file serves for peak identification containing certification data for the applied sources together with decay data for isotopes selected for calibration (^{152}Eu, ^{133}Ba, etc). Note that, during the fit, all kinds of errors are considered, including errors in half-lives, source strength, absolute intensity, etc. A typical efficiency curve fitting a 6th order polynomial to about 60 points is shown in Fig. 1. In the 60–3200 keV energy range, 0.5–1% overall uncertainty has been attained.

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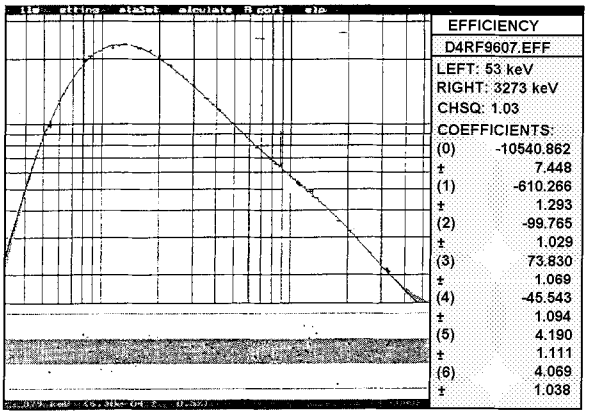

Fig. 1. Efficiency curve of a 36% HPGe detector fitted with 6th order polynomial (etalon sources: ^{241}Am, ^{109}Cd, ^{133}Ba, ^{152}Eu; home-made sources: ^{56}Co, ^{182}Ta, ^{110m}Ag)

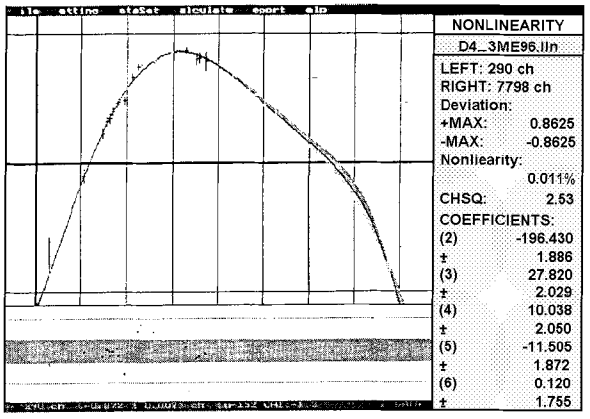

Fig. 2. Nonlinearity of a γ-ray spectrometer (36% HPGe, Amp: CI 2026, ADC: CI 8715, MCA: ACCUSPEC/B) *Y*-axis: 1 channel deviation/div.; *X*-axis: 1 K channel/div.

Beside several advantages (no need for spreadsheet, ease in fine tuning, etc.) two unique features should be stressed. First, the program uses orthogonal polynomials[4] which prevent curve oscillations and provide an unambiguous fit. This is a distinct advantage over methods splitting the energy range into 2–4 parts and fitting different polynomials for each segment with trial and error.[5] Second, efficiency values from uncalibrated sources are automatically normalized when at least one source is absolutely calibrated in the set. This greatly simplifies the use of "home-made" secondary standards, e.g., ^{56}Co, ^{182}Ta, etc. Moreover, it allows the user to make a calibrated source by fitting the data points of the new source together with those determining the absolute efficiency curve.

System nonlinearity

This parameter can be measured by injecting pulses of variable amplitudes at the preamplifier input from a highly stable pulse generator. A faster and more convenient way is to determine the nonlinearity curve[3] from the same set of spectra (^{152}Eu, ^{182}Ta, etc.) already used for efficiency calibration. Fitting a regression line to the apparent peak energies and plotting, after normalization, the deviation from literature energy values a nonlinearity curve can be obtained (Fig. 2).

As seen, the maximum deviation can be kept within ±1 channel (usually ±0.5 keV) if the spectrometer is calibrated at least in two channels near the range limits. By selecting a 0–3.2 MeV range (needed when measuring the short-lived ^{49}Ca, ^{37}S, etc.) the ^{56}Co is the only isotope emitting such high energy γ-rays with well known energies and intensities. A suitable source can be fabricated easily by irradiating a thin Fe foil in a cyclotron's proton beam utilizing the ^{56}Fe(p,n)^{56}Co reaction. Since ^{57}Co and ^{58}Co will also be produced from other relevant Fe isotopes, the 122 keV–3.3 MeV energy range can be covered with only one source. The code, therefore, will be extended to support the "Triple Cobalt Isotopes" method for QA studies.

FWHM versus γ-ray energy function

Similar to the procedures described above, the full width at half maximum (FWHM) values can also be derived and depicted as a function of γ-ray energy from the same set of calibrating spectra. Figure 3 shows the individual FWHM points together with the Sqrt(a+b*E) function describing the theoretically expected peak resolution. As seen, the agreement is excellent. The parameters of this curve can then be used as constraints for unfolding spectra recorded at low counting rates. As turned out, the above mentioned flexibility of the HYPERMET-PC program should sometimes be restricted in order to attain a better fit for heavily convoluted peaks.

Other options

New program modules have been implemented[6] for handling loss-free corrected spectra recorded in Dual Spectrum mode. In the case of peak distortion caused by the malfunction of electronics (improper P/Z settings, etc.), a new utility allows "manual" fit to sum up the areas of the main and side peaks similarly to the trapezoid method.

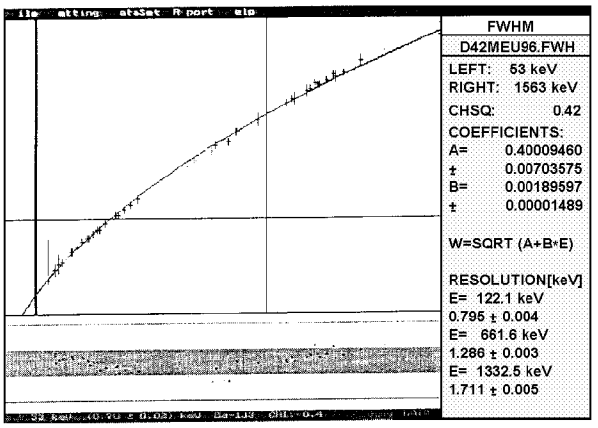

Fig. 3. FWHM versus γ-ray energy function measured with a 36% HPGe detector

Precise energies obtained with the help of a nonlinearity correction greatly facilitates nuclide identification, which can also be performed by the program using the new Nuclide Identification routine, developed for both INAA and PGAA as a new option to version 5.0.

Finally, the context-sensitive hypertext help, which is built in the new version and is also available as a separate Windows help file, is also noteworthy. Detailed explanation of these and other new features will be given elsewhere.

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