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Processing of Gamma-Ray Spectra

THE DIVERGENCE FROM GAUSSIAN OF PEAK SHAPES IN GAMMA-RAY SPECTRA OBSERVED WITH GERMANIUM DETECTORS

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A formula for the fitting of gamma-ray peaks produced from solid state detectors is suggested, which takes account of possible distortion from a pure Gaussian shape. Comparative analyses of peaks using the formula, and an assumed Gaussian shape are presented showing the improvement in the fitting. When accurate peak energies are required in order to identify unknown nuclides, it is recommended that the expression provided is used, since the calculated peak positions are influenced by the extent of the distortion present.

Introduction

A multipurpose computer program called GASP has been developed and regularly updated at AERE Harwell over many years. It is used for the examination, modification and analysis of multi-channel pulse height spectra, originally from sodium iodide scintillation detectors, and subsequently from high resolution germanium detectors.

Part of the program is concerned with the analysis of peaks in observed spectra in order to estimate the intensities and energies of the peaks, since much of the work is concerned with identifying and quantifying nuclides during neutron activation analysis, and for unknown radioactive samples.

Peak analyses performed in GASP are made on the assumption that each peak can be represented by a Gaussian shape superimposed on a linear continuum. This assumption has been found to be closely obeyed with most spectra observed in this laboratory, but it was recognised that at high counting rates (>1000 cps) some distortion of peaks was likely. The distortion produces a skewed Gaussian shape

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peak with an approximately exponential tail on the low energy side of the peak. For accurate identification and quantitative analysis it is obviously important that the peak shape assumed should fit accurately the observed peaks.

Theoretical

Peak shapes

A large variety of empirical peak shape functions has been proposed, many of which have been summarised by McNELLES and CAMPBELL.[1] Generally these functions can be divided into two types.

(a) Those which use two or more ranges of channels over each peak, with a separate function describing the shape over each range. The functions are made continuous in magnitude and slope at the junction(s) of the ranges.

(b) Those which are the sum of several functions, each of which is continuous over the range of channels covering the peak.

In this laboratory several different combinations of functions of the type (a) have been applied. However none has provided a solution which behaved reasonably when attempts were made to fit them to observed peaks by an iterative minimisation of the sums of the squares of the differences between observed channel counts and the model.

Various functions of type (b) which when summed can produce a shape similar to the distorted peaks have been summarised by PHILLIPS and MARLOW.[2]

(i) *A simple Gaussian* shape, which is produced from an ideal detector response to single size pulses combined with Gaussian noise.

$$A \cdot \exp\left[-(X - X_0)^2/2 \cdot \sigma^2\right]$$

where A – the peak amplitude;
X_0 – the peak position;
σ – the peak resolution.

(ii) *Effects of pile up and incomplete charge collection* can remove pulses from the sharp single size pulses, producing an exponentially decaying distribution on the low energy side of the peak. It is also possible that the same effect may be produced by overswing in the amplifier/analyser system. When the exponential is combined with a Gaussian noise, a skew shaped peak is produced. The peak centre is moved slightly to lower position and an approximately exponential tail is prod-

uced on the low energy side of the peak.

$$N_1 B_1 \cdot \exp\left[\lambda_1 (X - X_0 + \lambda_1 \sigma^2/2)\right] \cdot \text{erf c}\left[(X - X_0 + \lambda_1 \sigma^2)/\sigma\right]$$

where N_1 – a normalisation factor ($= \sqrt{2\pi}\,\lambda_1 \sigma$);
B_1 – peak amplitude;
λ_1 – exponential constant for the tail;

$$\text{erf c}(z) = \frac{1}{\sqrt{2\pi}} \int_z^\infty e^{-x^2/2}\, dx.$$

(iii) *With high intensity peaks,* a much longer exponential tail is observed on the low energy side of the peaks, with an amplitude several orders of magnitude smaller than the main peak amplitude. This may be due to surface effect in the detector. The formula describing this tail is identical with that in (ii) with B_2 (the amplitude) and λ_2 (the exponential constant) being much smaller then B_1 and λ_1, respectively.

(iv) *A step in the underlying continuum* is sometimes observed between the high and low energy sides of the peak. When an intensity step is combined with Gaussian noise a smoothed step is produced over the position of the peak.

$$N_3 S \text{ erf c } [(X - X_0)/\sigma)$$

where N_3 – a normalisation factor ($= \sqrt{2\pi}\,\sigma$);
S – step amplitude;
X_0 – peak position;
σ – peak resolution.

If the step is regarded as a manifestation of the long exponential tail with $\lambda_2 \to 0$, the formula for the tail becomes identical with the step expression.

Other observers have found an exponential tail on the high energy side of the peak. PHILLIPS and MARLOW[2] do not find this form of distortion. It has not been found on peaks analysed in this laboratory.

Fitting procedure

Combination of the above expressions produces an unwieldly function with a multitude of parameters. Various methods have been suggested for fixing the values of some of the parameters, in order to reduce the computing time for the optimisa-

tion program. The four expressions below, together with the terms describing the linear background continuum relate the channel count with the channel position.

$$Y = A \cdot \exp[-(X - X_0)^2/2 \cdot \sigma^2] +$$

$$+ N_1 B_1 \cdot \exp[\lambda_1(X - X_0 + \lambda_1\sigma^2/2)] \cdot \text{erf c}[(X - X_0 + \lambda_1\sigma^2)/\sigma] +$$

$$+ N_2 B_2 \cdot \exp[\lambda_2(X - X_0 + \lambda_2\sigma^2/2)] \cdot \text{erf c}[(X - X_0 + \lambda_2\sigma^2)/\sigma] +$$

$$+ N_3 S \cdot \text{erf c}[(X - X_0)/\sigma] + CX + D$$

VARNELL and TRISCHUK[3] find empirical relationships between each of λ_1, λ_2, B_2 and σ (and also the high energy exponential tail constant) and the energy of the peak; they do not include A, the pure Gaussian function, or the step function S. Thus for any one peak only B_1 and X_0 are regarded as unknown, together with the constants describing the background continuum. However their observations are limited to peaks counted with a 20% dead time correction, this does not seem applicable to a general program for peak analysis.

PHILLIPS and MARLOW[2] use a computer program called HYPERMET, and analyse for all parameters. Before applying their minimisation procedure they set all initial values of parameters as accurately as possible; during the optimisation they constrain the values of the parameters to a range close to the initial values. Since in most cases they find that λ_2, B_2 and S are negligible this leaves five parameters to describe the peak shape, together with two parameters to describe the continuum shape. With high intensity peaks the number increases to eleven (including an extra parameter describing the continuum). This is a challenging task for any optimisation method, as they acknowledge.

In the present work, in common with VARNELL and TRISCHUK,[3] it is found that A (the pure Gaussian shape), and S (the step function) are unnecessary. As indicated earlier, when the value of λ_2 becomes very small the long tail function approximates to the step function. Fitting experimental data to the composite function has been performed using an optimisation procedure written by POWELL.[4] (The method uses a "quasi-Newton" method for minimisation of the sums of the squares which is balanced with a steepest descent correction. No provision of partial derivatives is required, since they are calculated during the minimisation procedure. However in order to obtain satisfactory minimisation, the parameters must be scaled. The routine also provides a method of calculating the variance/covariance matrix from the derivatives calculated during the minimisation). Initial values of

the eight parameters (B_1, λ_1, B_2, λ_2, σ, X_0, C and D) are estimated from the counting data before entering the program. If, during the optimisation the values of either λ_2 or B_2 become very small, it is found that the procedure is unable to reach a minimum for the sums of the squares of the differences. In this case the values of B_2 and λ_2 are fixed and the procedure re-entered. In almost all cases analysed this produces a fit to experimental peaks with a ratio of external to internal variances lying between 0.8 and 1.5, indicating a satisfactory fit of the formula to the observed peaks.

In the course of routine analyses, it often occurs that the spectrometer is calibrated against sources of known energy gamma-rays. During the calibration values of resolution are calculated and subsequently the resolution related to the energy by an empirical formula. When experimentally observed peaks are analysed, the value of the resolution is fixed from the calibration observations. Thus for a single peak there are seven parameters to estimate; for double peaks the values of B_2/B_1, λ_1, λ_2 and σ are assumed to be the same for both peaks giving nine parameters to estimate (multiple peaks are analysed only when the resolution is provided by the empirical formula).

Position of peaks

When performing activation analyses of samples of unknown composition the energies of observed gamma-ray peaks must be assessed accurately, since these energies are the main means of identifying the nuclide producing the activity. The relative intensities of the peaks may provide a confirmation of identification, if more than one gamma-ray is emitted by any nuclide observed.

It will be noted that the value of X_0, which is calculated from the fitting formula given, is not at the maximum count rate of the peak, but at a point higher in energy. The difference is dependent on the values of λ_1 and σ which appear in the exponential factor and in the erf c function. A difference is to be expected since all pulses produced by the detector have been assumed to have a probability of being reduced in size (governed by the exponential factor) be it by incomplete charge collection or overswing. It would be expected that the change in position X_0 from the peak maximum would be greater for larger counting rates whichever of the above explanations causes the effect. The value of λ_1 changes with counting rate and with energy, while σ varies with energy. Thus there is no simple relationship between the peak maxima and energy, although the values of X_0 can be related directly with energy.

Thus when an unknown spectrum is being analysed for peak energies it is important that those spectra which show distorted peaks should be analysed using

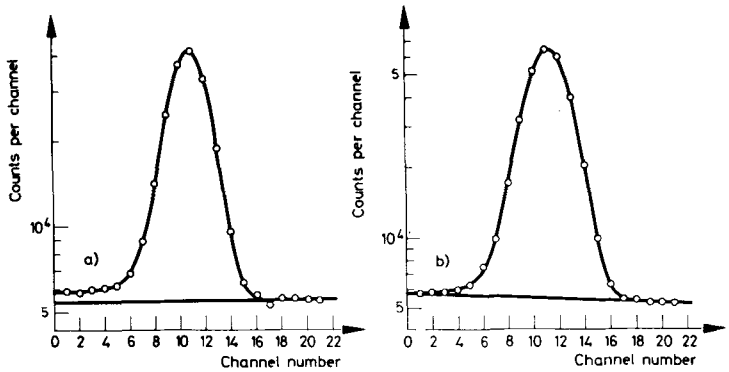

Fig. 1. Graphs of the recommended formula fitted to single peaks

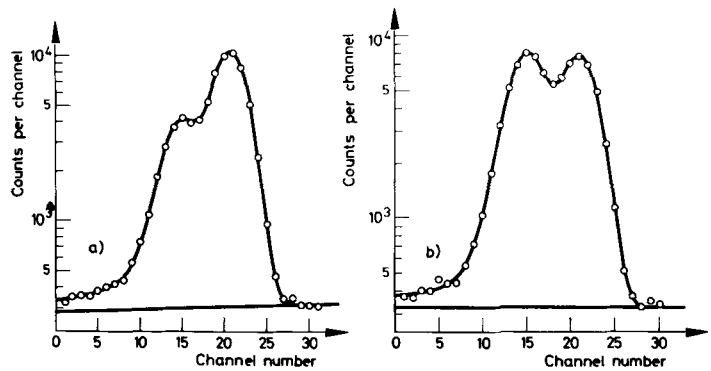

Fig. 2. Graphs of the recommended formula fitted to double peaks

the formula given above, since X_0 is the position at which the analysed peak would have been were there no distortion. (It should be noted in passing that the formula given by PHILLIPS and MARLOW[2] differs from the one given above, such that although the peak shape described is identical with the above formula, the value of X_0 given is $\lambda_1 \sigma^2/2$ lower than that given here. The formulae given by VARNELL and TRISCHUK[3] and by McNELLES and CAMPBELL[1] are similar to the present formula).

Experimental

Observations

Fig. 1 a and b show graphs of the recommended formula fitted to single peaks and Fig. 2 a and b illustrate fitting to double peaks. The values of the parameters found by the fitting routine are given in Tables 1 and 2, and for comparison the

Table 1
Parameters for fitting pure Gaussian peaks to single peaks

	Fig. 1a		Fig. 1b	
	Present formula	Pure Gaussian	Present formula	Pure Gaussian
Position	11.52	10.75	11.91	11.17
Area	14 200	14 190	24 390	25 440
σ	1.593	1.572	1.730	–
λ_1	1.243	–	1.362	–
λ_2	0.033	–	0.383	–
Variance ratio	1.51	16.25	1.08	25.09

Table 2
Parameters for fitting pure Gaussian peaks to double peaks

	Fig. 2a		Fig. 2b	
	Present formula	Pure Gaussian	Present formula	Pure Gaussian
Position 1	15.56	14.62	16.02	14.90
Area 1	16 290	18 010	38 110	39 100
Position 2	21.56	20.58	22.01	20.90
Area 2	49 530	49 600	38 000	37 050
σ	1.733	1.947	1.763	2.052
λ_1	0.995	–	0.802	–
λ_2	0.107	–	0.075	–
Variance ratio	0.71	7.88	1.78	13.91

values of parameters found for fitting pure Gaussian peaks to the same data. (The zero offset in all figures is greater than 1000 channels). Points to be noted from the tables are:

(1) The ratio of the external to internal variance is very much smaller with recommended formula, indicating that the calculated curve is much closer to the observed points when the present formula is used rather than a pure Gaussian.

(2) Most areas quoted are similar in the two methods of fitting. However the lower energy peak of the double peak fit shows a discrepancy when the pure Gaussian peak shape is assumed. Since the observed peaks have a tail on the low energy side, some of the counts which should appear in the higher energy peak have been credited to the lower energy peak when the pure Gaussian shape is assumed.

(3) The position of the peaks from the two methods are different by over 1 channel in some cases. The actual differences are fractionally larger than would be expected when the maxima of the present formula are calculated. Since the peaks are distorted the centre of the pure Gaussian fit is low because the fitting routine attempts to compensate for the low energy tail by moving the centre of the fit to a lower energy.

(4) The values of the σ from the two different expressions are different. The pure Gaussian fit attempts to compensate for the low energy tail by increasing the width of the Gaussian.

Conclusions

It has been shown that high intensity gamma-ray spectra obscured with a solid state detector show shapes of peaks which differ from a pure Gaussian shape. A suggested formula provides a close representation of the peak shapes. The values of the peak areas found differ very little from those found from use of a Gaussian shape, but significant differences are found in values of the peak position and peak resolution.

A point of interest is that application of the present formula to fitting single peaks may take a factor of three times more computer time than when a Gaussian shape is used for fitting. For double peaks the tail penalty in using the formula may be only a 50% increase.

References

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