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A comparison of different peak shapes for deconvolution of alpha-particle spectra

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ABSTRACT

Alpha-particle spectrometry is a standard technique for assessing the sample content in terms of alpha-decaying isotopes. A comparison of spectral deconvolutions performed adopting different peak shape functions has been carried out and a sensitivity analysis has been performed to test for the robustness of the results.

As previously observed, there is evidence that the alpha peaks are well reproduced by a Gaussian modified by a function which takes into account the prominent tailing that an alpha-particle spectrum measured by means of a silicon detector exhibits. Among the different peak shape functions considered, that proposed by G. Bortels and P. Collaers, Int. J. Rad. Appl. Instrum. A 38, pp. 831–837 (1987) is the function which provides more accurate and more robust results when the spectral resolution is high enough to make such tailing significant. Otherwise, in the case of lower resolution alpha-particle spectra, simpler peak shape functions which are characterized by a lower number of fitting parameters provide adequate results.

The proposed comparison can be useful for selecting the most appropriate peak shape function when accurate spectral deconvolution of alpha-particle spectra is sought.

1. Introduction

Alpha-particle spectrometry is an effective technique for assessing the sample content in terms of alpha-decaying isotopes. Spectrometers make use of two distinct detector technologies, grid ionization chambers or ion-implanted silicon detectors. Grid ionization chambers are widely used with bulk samples, however their 2π geometry implies the detection of backscattered alpha particles which makes the interpretation of the spectra challenging [1,2]. The standard case is to deal with thin samples, usually realized by means of electrodeposition [3], and in such a case the standard equipment is a spectrometer mounting an ion-implanted silicon detector [4,1].

Alpha particles have discrete energies but when their energy is measured by means of a silicon detector it exhibits a peak representing a broad distribution proportional to their activity, with a well known asymmetry [5,6]. Steinbauer et al. [4] demonstrated that the measured energy distribution is mainly due to the detector response function. In particular, such a function is determined by the elastic collisions with bound electrons and nuclei. Therefore, the energy distribution for alpha particles entering the sensitive volume of the detector is determined by the Gaussian distribution of electronic and nuclear energy-loss straggling. However, alpha particles entering in the sensitive region of the detector also transfer their energy to electrons by inelastic collisions, causing excitation and ionization. Such a process is found to be responsible for a non-Guassian contribution to the measured energy distribution, which is the reason for the observed tail on the low-energy side of the peak.

Different alpha-decaying isotopes emit alpha particles at specific energies whose measured energy peak distributions may overlap due to the limited attainable energy resolution of the spectrometers based on silicon detectors. The problem of identifying the isotopes and determining their activities is therefore a matter of deconvolving the different contributions to the measured spectra e.g., [7]. Spectral deconvolution requires a mathematical function to describe the shape of the energy peak distribution for fitting the measured spectrum. Several authors have proposed different peak shapes e.g., [6,8–10,11–17], all of them being based on the convolution of a Gaussian function with one or more exponential functions. The main differences lie in the number and the slope of the exponential functions adopted.

In this work a comparison of spectral deconvolutions performed adopting different peak shape functions is carried out. A

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Table 1
Deconvolution fitting parameters (Appendix A) and their estimated uncertainties of the most significant ^{239}Pu and ^{240}Pu peaks of the alpha-particle spectrum 5535. Deconvolutions obtained adopting L'Hoir [6], Bortels and Collaers [11], Koskelo et al. [14], and García-Toraño [16] are compared to deconvolutions obtained adopting a simple Gaussian as peak shape. Nominal energies (μ in keV) and transition probabilities (A in %) from the libraries are reported for direct comparison. Inconsistent values are reported in bold.

5535						
		^{239}Pu			^{240}Pu	
		$\alpha_{0,4}$	$\alpha_{0,2}$	$\alpha_{0,1}$	$\alpha_{0,1}$	$\alpha_{0,0}$
Library [34,35]	A	11.87 ± 0.03	17.14 ± 0.04	70.79 ± 0.10	27.16 ± 0.19	72.74 ± 0.18
	μ	5105.81 ± 0.21	5143.82 ± 0.21	5156.59 ± 0.14	5123.6 ± 0.2	5168.13 ± 0.15
L'Hoir [6]	A	$\mathbf{14.2 \pm 0.3}$	$\mathbf{16.2 \pm 0.6}$	$\mathbf{69 \pm 1}$	$\mathbf{28.2 \pm 0.4}$	$\mathbf{71.7 \pm 0.8}$
	μ	$\mathbf{5104.9 \pm 0.8}$	5142.9 ± 0.8	5156.6 ± 0.8	5123.9 ± 0.8	5168.8 ± 0.8
	σ	3.76 ± 0.01	3.76 ± 0.01	3.76 ± 0.01	3.76 ± 0.01	3.76 ± 0.01
	τ	9.17 ± 0.02	9.17 ± 0.02	9.17 ± 0.02	9.17 ± 0.02	9.17 ± 0.02
Bortels and Collaers [11]	A	12.1 ± 0.4	17.3 ± 0.6	70 ± 1	27.8 ± 0.4	72.1 ± 0.8
	μ	5105.1 ± 0.8	5143.1 ± 0.8	5156.8 ± 0.8	5124.1 ± 0.8	5168.2 ± 0.8
	σ	3.91 ± 0.01	3.91 ± 0.01	3.91 ± 0.01	3.91 ± 0.01	3.91 ± 0.01
	τ_1	8.05 ± 0.03	8.05 ± 0.03	8.05 ± 0.03	8.05 ± 0.03	8.05 ± 0.03
	τ_2	116 ± 1	116 ± 1	116 ± 1	116 ± 1	116 ± 1
	η	0.0804 ± 0.0007	0.0804 ± 0.0007	0.0804 ± 0.0007	0.0804 ± 0.0007	0.0804 ± 0.0007
Koskelo [14]	A	$\mathbf{13.9 \pm 0.4}$	$\mathbf{16.3 \pm 0.6}$	70 ± 1	$\mathbf{28.4 \pm 0.4}$	$\mathbf{71.5 \pm 0.8}$
	μ	$\mathbf{5104.4 \pm 0.8}$	5143.2 ± 0.8	5156.9 ± 0.8	5124.2 ± 0.8	5168.3 ± 0.8
	σ	4.77 ± 0.1	4.77 ± 0.1	4.77 ± 0.1	4.77 ± 0.1	4.77 ± 0.1
	T	2.40 ± 0.01	2.40 ± 0.01	2.40 ± 0.01	2.40 ± 0.01	2.40 ± 0.01
Garcia-Torano [16]	A	$\mathbf{12.6 \pm 0.4}$	$\mathbf{16.1 \pm 0.6}$	71 ± 2	27.8 ± 0.4	72.1 ± 0.9
	μ	$\mathbf{5104.8 \pm 0.8}$	5144.4 ± 0.8	5156.6 ± 0.8	5123.8 ± 0.8	5168.7 ± 0.8
	σ_r	4.60 ± 0.02	4.60 ± 0.02	4.60 ± 0.02	4.60 ± 0.02	4.60 ± 0.02
	σ_l	6.69 ± 0.04	6.69 ± 0.04	6.69 ± 0.04	6.69 ± 0.04	6.69 ± 0.04
	n	1.021 ± 0.004	1.021 ± 0.004	1.021 ± 0.004	1.021 ± 0.004	1.021 ± 0.004
Gaussians	A	$\mathbf{37 \pm 1}$	$\mathbf{9 \pm 1}$	$\mathbf{54 \pm 3}$	$\mathbf{25 \pm 1}$	75 ± 3
	μ	$\mathbf{5135.2 \pm 0.8}$	$\mathbf{5155.9 \pm 0.8}$	$\mathbf{5168.5 \pm 0.8}$	$\mathbf{5135.2 \pm 0.8}$	$\mathbf{5179.6 \pm 0.8}$
	σ	30.4 ± 0.2	5.0 ± 0.2	7.1 ± 0.2	4.63 ± 0.08	4.42 ± 0.05

similar comparison was performed by Bland [18], who reported the spectral deconvolution of a mixed-Pu spectrum by using peak shapes proposed by Bortels and Collaers [11] and Koskelo et al. [14]. Here, the comparison also includes L'Hoir [6] and García-Toraño [16] peak shapes and the spectral deconvolution is performed for three spectra with different spectral resolution, number of counts, and background noise. Finally, a sensitivity analysis is carried out for testing the robustness of the results by changing the initial values of the peak shape parameters in the spectral deconvolution process.

2. Model and data

2.1. Peak shapes

The four peak shapes to be compared were proposed by L'Hoir [6], Bortels and Collaers [11], Koskelo et al. [14], and García-Toraño [16]. The details of their definitions are reported in Appendix A. These four peak shapes can be considered representative of the different alternatives proposed by other authors.

L'Hoir [6] adopted an exponential function to describe the low-energy tail of the energy distribution along with a Gaussian on the high-energy side, as previously suggested by Baba [8] and Watzig and Westmeier [9]. Bortels and Collaers [11] suggested a Gaussian on the high-energy side and two, or more, exponential functions for the tail on the low-energy side and represent the typical case of the use of multiple exponential functions in the definition of a peak shape. A similar approach was followed by Westmeier and Van Aarle [13] and Pommé and Caro Marroyo [17]. Both in L'Hoir [6] and Bortels and Collaers [11] the exponential functions are joined to the Gaussian at its center. Koskelo et al. [14] still used one exponential function to take into account the tail, but introduced the joining point between the Gaussian and the exponential function as an independent free parameter in the spectral deconvolution process, similarly to Lozano et al. [15]. The same approach was followed by García-Toraño [16] where the exponential function slope is also modified by making it dependent on the square root of the energy, an approach previously proposed by García-Toraño and Aceña [10].

Each of these solutions introduces a number of parameters to define the function characterizing the alpha peaks. Generally, s shape parameters are common for all the peaks depending on the sample, the measurement geometry, and the spectrometer, while 2 parameters are specific for each peak (i.e., the transition probability A and the energy of the peak μ). If n is the number of alpha peaks identified in the measured spectrum, the total number of parameters in the fitting procedure will be $2n+s$ (Appendix A).