Removal of the Continuum of X-Ray Spectra Using Morphological Operators

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***Abstract*— In energy dispersive X-ray fluorescence analysis, the estimation and removal of the continuum on which the X-ray spectrum is superimposed is a primary requirement. The algorithms commonly used are either complex, or in the case of, e.g., neural network algorithms, computation-intensive. They usually require strong constraints and/or hypotheses on the data or the shape of the continuum. Moreover, if the continuum amplitude is comparable to or bigger than the peak amplitudes, some of these algorithms can lose peaks. A new approach to continuum removal based on mathematical morphology is proposed here. The new algorithm permits fast continuum elimination without peak deterioration. Other than a rough estimate on the widths of the peaks, the new method does not require additional information about the spectrum. The method can also be applied without modification to background elimination from gamma ray spectra. This new method is described and results obtained from real and simulated spectra are discussed and evaluated.**

***Index Terms*— Continuum removal, morphological operators, spectroscopy, X-ray spectra analysis.**

I. Introduction

QUANTITATIVE spectrum analysis requires techniques for extracting information about the peaks, such as position, energy, amplitude, and width, as accurately as possible. The first step toward this goal is continuum removal. Several algorithms have been reported in the literature and the most common ones are described by Thomsen *et al.* [1], Gerasimov [2], Maxwell *et al.* [3], and a complete review can be found in [4]. The first of these performs continuum removal using two models based on second- and third-order splines. The polynomial coefficients are calculated using previously established points localized at the minimums placed on either side of the peaks. Of course this method requires *a priori* estimates of peak position and requires also two general parameters: the full-width at half-maximum (FWHM) of the peaks and the noise level in the spectrum. The results reported in [1] are very good, but the method shows a strong dependence on the FWHM parameter.

The Gerasimov method is a five-step recursive filter based on a previously developed filter [5] with stabilization improvements. It requires knowledge of two spectral parameters: the FWHM of the peaks and an empirical parameter which Gerasimov denotes by α. The latter is chosen empirically between zero and one, depending on the FWHM values; α must be large for wide peaks and small for sharp ones. This method is superior to others in that peak positions are not required. For good continuum removal more than 30 iterations are generally required.

The algorithm of Maxwell *et al.* is based on Schamber's top-hat filter [6]. It is a zero-area digital filter that does not make assumptions about the continuum, except to suppose that it changes more slowly than the peaks. Gerasimov [7] suggests that it can be used when the peak forms are not gaussian. We have used it on some spectra, but the quality of continuum removal appears lower than in other methods.

The algorithm proposed here is based on mathematical morphology. It permits one to relax the constraints on continuum and peak shape. It requires just about the same assumptions as the filter developed by Maxwell, but with superior filtering performance. For the sake of completeness, a comparison with one of the previously described filters will be reported. Maxwell's filter would be the best of the candidates for a comparison with ours, but considering the quality of the filtering operation it is better to compare our morphological filter (MF) with the Gerasimov filter (GF), because the latter is, both as to its performance and as to the constraints it requires, the nearest to MF.

II. Mathematical Morphology

Mathematical morphology was developed in 1964 by Matheron and Serra as a nonlinear approach to image processing [8]. In this field it has shown robust performance in noise cancellation while conserving signal characteristics. It can be thought of as an interaction of a signal set with one or more other sets, called structural elements, containing shape information. This interaction changes the original data to a new form which is intended to be more expressive for the user. An MF is a local operator defined in terms of intersection, union, difference, max, and min. It is easy to apply morphological operators to one-dimensional signals such as spectral data. Such applications to electromedical signals can be found in [9] and [10]. Because the signals of interest here are one-dimensional, the discussion will be restricted to that case. See [8] for a complete treatment of mathematical morphology. The morphological language is based on two basic operations: dilation and erosion.

A. Erosion

Let f be the signal data and k the structural data. Then erosion can be written as

$$(f \Theta k)(m) = \min_{n=0,\cdots,N-1} \{f(m+n) - k(n)\}, \quad \text{for } m = 0, \cdots, M-N \tag{1}$$

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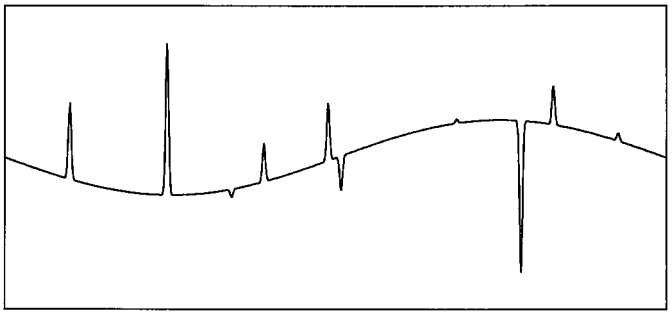
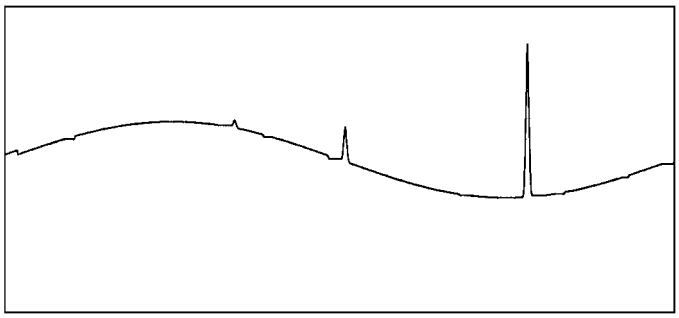


(a)



(b)

(c)

Fig. 1. (a) Sinusoidal curve with positive and negative amplitude gaussian pulses; (b) signal after opening operation; and (c) signal after opening and closing operations. In (c), flat zones corresponding to some peaks (hence distortion with respect to the original sinusoidal shape) are clearly visible.

where m, running from zero to $M-N$, indexes the spectral data of length M and n, running from zero to $N-1$, indexes structural data of length N.

B. Dilation

This is the complement of the erosion operation. Using the notation of the previous case

$$(f \oplus k)(m) = \max_{n=0,\cdots N-1} \{f(m-n) + k(n)\}, \quad \text{for } m = N-1, \cdots, M-1. \qquad (2)$$

Performing an erosion followed by a dilation provides a new operator, the opening, while an erosion after a dilation builds a closing operator. The opening operation cancels small components of the signal and smooths internal contours. Closing magnifies little components and smooths external contours. These operators can be used for continuum removal as shown in the example of Fig. 1. Fig. 1(a) represents a sinusoidal curve with positive and negative gaussian peaks. Let the structural element be a horizontal segment S. More precisely, let the structural element be given with zero intensities, i.e., $k(n) = 0$ for $n = 0, \cdots s-1$. The width of the structural element is taken as the base width of the gaussian peaks. If an opening operation is performed on the signal, the positive impulses with base narrower than S will be cancelled, as seen in Fig. 1(b). Subtracting the filtered data from the original data will extract the positive peaks. Next, if a closing operator is applied to the filtered data, the negative impulses narrower than S will be cancelled as indicated in Fig. 1(c). Note the distortion of the sinusoidal shape in Fig. 1(c) due to the structural element's horizontal slope. In general, using structural elements with different shapes or sizes will produce different distortions in both amplitude and shape. But, the distortion being local, it will be possible to partially eliminate it by interpolation, as is explained later. In principle, the interpolation could be performed with a specially shaped structural element. For example, in the case of Fig. 1(c), a sloping segment with varying slope could be used as the structural element to perform a linear interpolation. In this way, changing the structural element, it is possible to accomplish interpolation to any order.

III. METHODS

Since X-ray and gamma-ray spectra do not contain negative peaks, for continuum removal only the opening is required. One possible difficulty is that the FWHM changes with energy. The GF uses a fixed FWHM value, chosen as the largest in the spectrum under study. The MF, instead, permits one to change easily, during the run, the size of the structural elements as the channel, i.e., energy, changes. In this way it is possible to tune it to every FWHM. This can be relevant if one has *a priori* knowledge of the spectrum. In fact, small structural elements follow the continuum better than big ones, thus permitting more efficient noise removal. The best structural element for spectrum filtering is the segment with zero amplitude values because it does not distort the amplitude values of the data. The width of the segment can be decided according to Fig. 2, which shows the patterns that may be found after an opening operation. The left side is a schematic representation of a peak superimposed on four different continuum shapes, the central column reports application of a segment shorter than the peak base, and the column on right shows the effect of a segment wider than the peak base. These patterns are formed by the intersection of the two extremes of the structural element with the data shape: the narrower the structural element is compared to the peak base, the more of the peak remains in the modified signal. This holds also for the continuum without peaks. In any case, the result of this kind of structural element application is a pedestal superimposed on the continuum. So, if one has a rapidly variable continuum, false peaks could be detected, but they can be eliminated by calculation of the area over the peak. In fact, if the peak is not a true one, the area will be very small and it can be canceled in the final filtered data. Moreover, these false signals will be found only if one has both a wide structural element and a nasty, i.e., rapidly varying, continuum. After the application of the structural element, and after

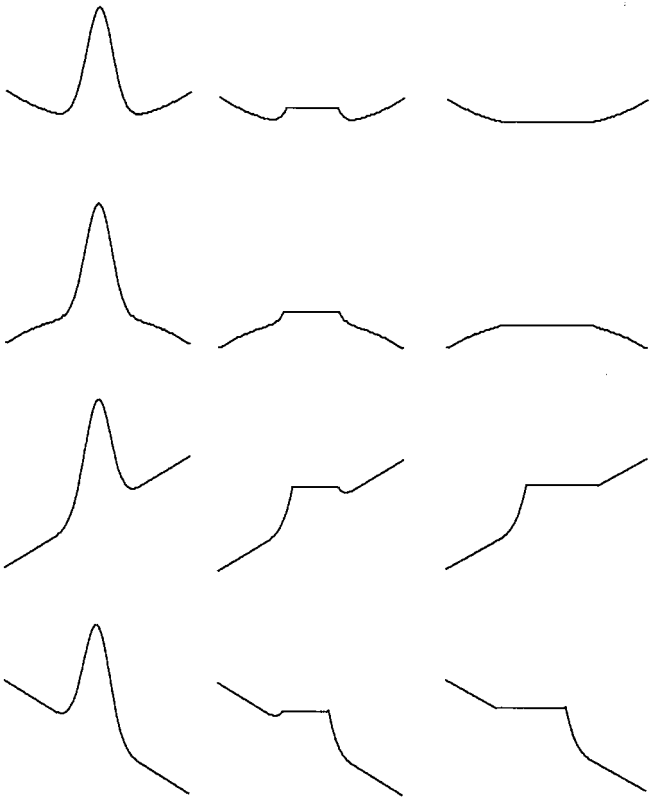


Fig. 2. Effects of the application of a segmental structural element to spectra. Background slopes here have been chosen larger than usual for clarity of representation. Left column, principal cases of background and peak superposition; central column, structural element narrower than peak pedestal; and right column, structural element wider than peak pedestal.

subtracting the resulting estimate of the continuum from the original signal, as described above, a raw filtering is obtained but with peak amplitudes somewhat reduced. The errors are amplitude dependent, and they will be high for very small peaks (say less than 100 counts). These errors can be corrected by interpolation under the peaks. This operation requires the estimation of both of the extremes of the peak. Estimates of these extremes are obtained using the structural element action again. First, the type of peak pedestal, classified as in Fig. 2, must be determined. This can be easily done by observing the values of the points neighboring and external to the pedestal; in the case of the central column in Fig. 2 the minimum points or slope changes must be found. This can be done using again the structural element action. In fact, in real data, between adjacent channels, there is little oscillation. In the low, i.e., continuum, part of the spectrum, the structural element will cancel it, producing little flat zones. These will be external to peak area and thus can be used as extremes points. The cases in the right column can be subdivided in three categories:

- values at points near the pedestal smaller than the pedestal value;
- values at points near the pedestal smaller than the pedestal value on the left, but larger on the right, or vice versa;
- values at points near the pedestal larger than the pedestal value.

The cases in the second category use, as the first interpolating point, the last pedestal point on the high side and, as the second interpolating point, the location of the minimum. The minimum is located using the same technique as for the central column cases. So long as the width of the structural element is reasonable, i.e., not much bigger than the FWHM, peaks from the first and third categories generally do not require correction because near such peaks the continuum is usually changing relatively slowly and the error is small. But the previous techniques can be used if needed.

Once the extreme points of the peak are determined, a linear or higher order interpolation can be performed.

In our experience, if the spectrum has isolated or short tail peaks, a linear interpolation has always worked well. To the contrary, if the spectrum presents large overlapping peaks structures, then the assumption that the continuum is varying slower than what is in this case a group of the peaks is no longer true. So, in this case it is better to use an interpolation of order higher than one. However, in general, if a small amplitude peak is near to stronger neighboring peaks and a precise estimate is required, it is better to use higher order interpolation. If the peaks have long tails, the interpolation method does not always work well. This is not due to the order of interpolation, or at least this is not principally, but fundamentally to the method of choosing the extremes points, which can produce a cut of the tail. This happens only when a tail is superimposed upon another peak. In this paper, where the principal purpose is to demonstrate the effectiveness of our method, only linear interpolation is used and the problem of long tail peaks is neglected. Regarding the action of the MF on other peak shapes, such as the lorentzian, it will be much the same.

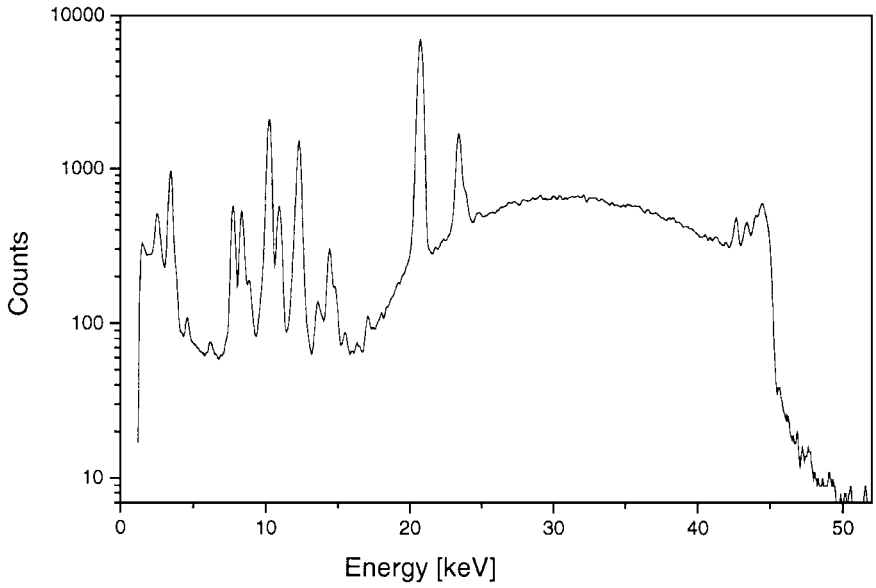
After this general discussion one practical point must be underlined: until now, statistics permitting, this filtering method has never lost peaks. That cannot be said of other methods. In regards to the structural element, it is preferable, in accordance with the above discussion, to choose its width to approximately match the FWHM.

IV. Algorithm

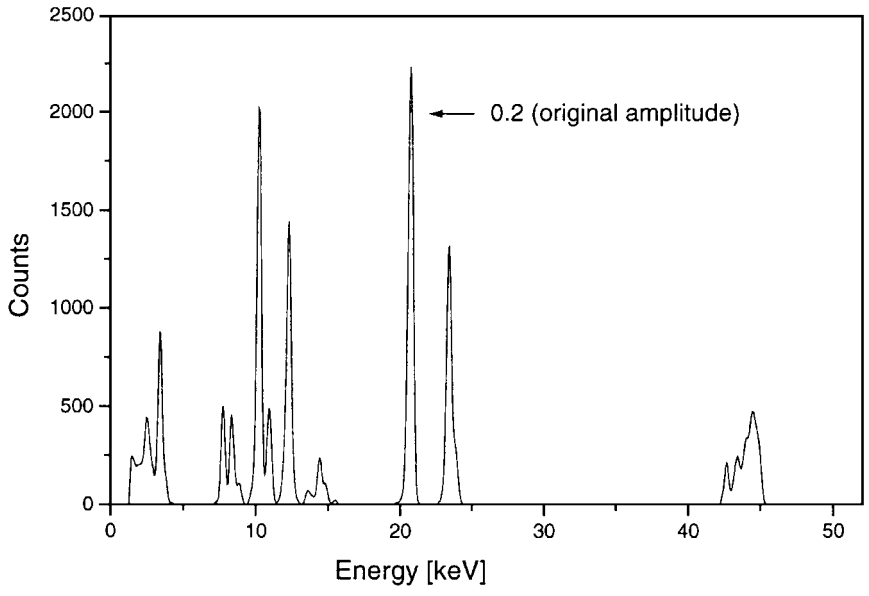
From the previous paragraph, the following algorithm can be extracted.

1) Estimate the base width of the peaks.
2) Choose the width of the structural element segment based on the results of Step 1).
3) Open the data using the structural element.
4) Linearly interpolate with the techniques described in the previous paragraph (or other techniques.)
5) Subtract the result of the previous step from the original data.
6) Eliminate false peaks and noise by area estimation.

The first and second steps determine the structural element. The choice of width is important, but, as can be seen by examining Fig. 2, no very great precision is needed. Care must be taken to choose the structural element width shorter than the characteristic length of variations in the continuum. Here, the continuum is intended to mean the slowly varying continuum which one observes by studying the entire data set and is not intended to include rapidly varying noise fluctuations, for example random errors varying from channel to channel.



(a)



(b)

Fig. 3. Example of MF applied to a fluorescence spectrum: (a) original data (semilog scale) and (b) background removal using the MF (linear scale with the highest amplitude peak attenuate by a factor of 0.2 for clearer visual presentation). The sample is a palladium powder. However, other peaks are also present, due to collimator and X-ray tube anode contamination. Pb, Cu, Zn, and Ca characteristic lines are visible.

In Step 3) the algorithm executes the row filtering of the spectrum. The outcome of this step is a continuum with various superimposed pedestals. These pedestals are eliminated in Step 4).

Step 5) leaves the estimated peaks with a lots of false peaks and noise fluctuations. The false peaks can be eliminated by finding the maximum of every zone and calculating the area. Then each area value is compared to a gaussian peak with the same FWHM and peak amplitude as the presumed peak. If the estimated area is considerably less then the simulated area then the peak is considered to be a false peak; otherwise, it is accepted as a true peak. Before this step it is convenient to eliminate the noise. This operation could be performed by the false peak detection procedure, but as explained next, the algorithm will be faster if a different procedure is used. In fact, the noise removal can be performed by a zero-amplitude segment covering exactly three channels. This is effective in eliminating the rapidly fluctuating noise which arises from random differences in counts from one channel to the next. The filtering is performed using both opening and closing operations. Using a structural element wider than three elements will strengthen the filtering operation, extending it to fluctuations regarding more than two channels, but the drawback is that the high parts of true peaks will be cut off. The effect of the three-element noise filter on the peaks depends generally on the amplitude and FWHM of the peaks. For example, for a gaussian peak which an amplitude of 10 000 counts and a FWHM of ten channels, the variation of the area

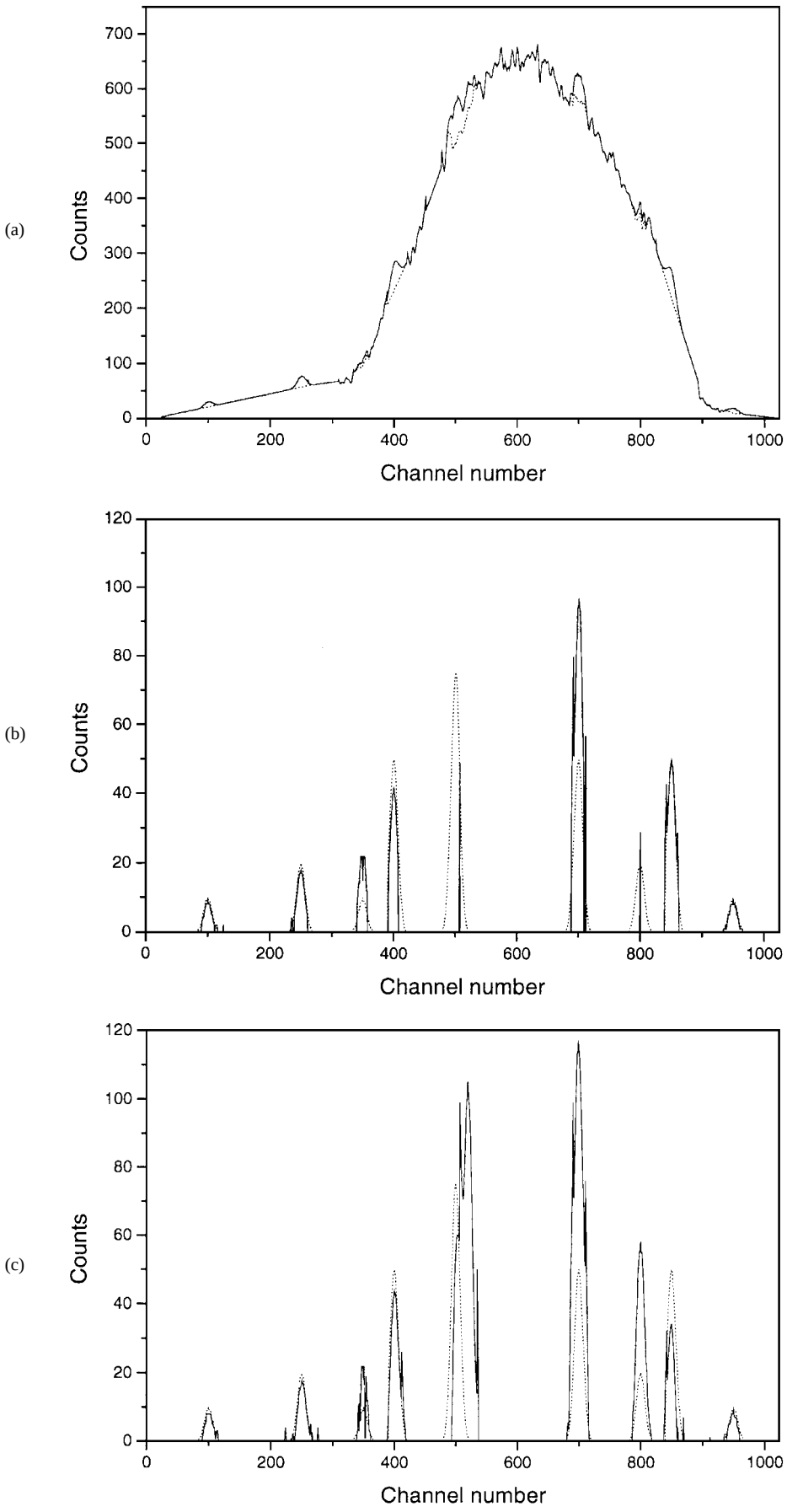


Fig. 4. Simulated spectrum. The peak amplitudes are always smaller than the background: (a) original spectrum (solid line). The continuum contribution is reported by the dotted line; (b) filtered by GF (solid line) and original peaks (dotted line); and (c) filtered by MF (solid line) and original peaks (dotted line).

TABLE I
SIMULATED GAUSSIAN PEAKS SUPERIMPOSED UPON THE BACKGROUND AS EXTRACTED BY GF FROM THE FLUORESCENCE SPECTRUM OF FIG. 3. THE AMPLITUDES ARE EXPRESSED IN COUNT UNITS

Peak position (ch#)	Amplitudes			Background/peak ratio
	"true" value	Gerasimov filter	Morphological filter	
100	10	1.9	8	8
250	20	2.8	19	18
350	10	13.6	0	9
400	50	4.7	55	40
500	75	10.3	94	101
520	45	15.3	0	85
700	50	12.4	104	90
800	20	20.3	30	41
850	50	4.7	50	36
950	10	1.2	9	9

of the peak is less ten counts over an area of 10^6 counts. If the FWHM goes down to four channels, the variation of the area is about 40 counts over 400 000 counts. For low amplitude peaks the error is practically zero.

The use of a three-coefficients structural element is therefore suggested for first noise removal, leaving further noise removal to the false peak detection procedure.

V. TEST DATA

Actually, when examining an X-ray spectrum, the location of a true peak may sometimes be used to calculate the expected position of some related peak, for example K_β using K_α. This circumstance does not hold for gamma ray spectra. Since one of the desiderata for the MF filter was that it could be applied to every kind of spectrum, it seems fair to test it in a situation where no *a priori* information on peak positions is available.

The simulated data (Fig. 4) were constructed by adding the continuum spectrum extracted by GF from Fig. 3(a) to a set of gaussian peaks with different intensities and equal FWHM of 16 channels. With this choice of continuum, the MF method should have no advantage with respect to the GF. The position of the peaks is quasi-random. The positions of the peaks are not, however, totally random because, in the interests of checking the results of MF on partially superimposed peaks, two peaks were placed on channels 500 and 520 [see Table I and Fig. 4(a)]. Note that the peak amplitudes are smaller than the continuum and, in some cases, the peaks are not visually identifiable [see Fig. 4(a)]. Thus, the simulated data presents the sort of situation where extraction methods are required. The continuum can be eliminated by eye when the peaks are easily distinguishable.

VI. RESULTS

Fig. 3 examines the fluorescence spectrum of a Palladium powder sample, acquired by a HPGe detector. In Fig. 3(a) the original data are shown, while in Fig. 3(b) the morphologically filtered data are shown. A structural element 60 points wide (7.5 times the FWHM) was used together with the interpolation method described in Section III. The filter's action and continuum removal are good. This example is included here to show the effect of the filter on genuine spectral data, but it does not allow careful study of how well the filter conserves the shape and amplitude of peaks. In Fig. 4(a)–(c), original simulated spectrum, GF element spectrum, and MF spectrum, respectively, are reported. In Table I the positions and intensities of the original peaks are reported, together with continuum/peak ratios and amplitude values extracted using GF and MF. GF found seven peaks plus two spikes corresponding to two other peak positions. MF extracted all ten peaks, considering the peak around the channel 500 as double because it is clearly larger than others. In the GF results the two adjunctive peaks (around 500 and 800 channels) appear only as two spikes which could be interpreted, if the original position of the peaks were unknown, as errors. In regards to the amplitude values extracted when the peak is found, GF is a little better than MF, but, once again, MF did not lose peaks. Moreover, using MF, once a peak's position is determined, then a more precise estimate of amplitude might be obtained by using a higher order interpolation.

VII. Conclusions

In this paper a new algorithm for removing continuum from X-ray and gamma-ray spectra is proposed. The algorithm is based on mathematical morphology. The techniques of mathematical morphology can be used to accomplish simple continuum removal. This filter is fast because it does not require the iterations which are common in other filters found in the literature. It is also versatile because it is easy to change the characteristics of the morphological operations according to the channel, i.e., energy. In this way variations of the measurement system's resolution can be taken into account. Such adjustments are not so easy to realize in the other algorithms and may not be possible at all. The performance of the MF has been tested on real and simulated spectra and compared to a good filtering method described in the literature. As a test case a very nasty simulated spectrum, with continuum bigger than peak amplitudes, was used. For this test case the superior performance of the MF over the reference method was verified. It must be stressed, once again, that in practice the morphological method has never lost a peak, and this is not necessarily true for the others algorithms. As a drawback, in particular cases, false peaks can be detected. Measuring the area under the false peak, they can be removed. For precise estimation of the amplitudes and shapes of the peaks, interpolation after the filtering is required. Linear interpolation using the algorithm described in Section III is useful in obtaining more precise estimates of the peak amplitudes. However, our choice can and should be adopted for all small amplitude peaks. The actual version of the algorithm, with linear interpolation, works well with isolated peaks or groups of peaks overlapping in a small region. When these conditions are not satisfied by spectrum errors in the amplitude area estimations will be made. We are currently studying how to improve the performance of the algorithm in these circumstances.

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