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Advanced signal separation and recovery algorithms for digital x-ray spectroscopy

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ABSTRACT

X-ray spectroscopy is widely used for in-situ applications for samples analysis. Therefore, spectrum drawing and assessment of x-ray spectroscopy with high accuracy is the main scope of this paper. A Silicon Lithium Si(Li) detector that cooled with a nitrogen is used for signal extraction. The resolution of the ADC is 12 bits. Also, the sampling rate of ADC is 5 MHz. Hence, different algorithms are implemented. These algorithms were run on a personal computer with Intel core TM i5-3470 CPU and 3.20 GHz. These algorithms are signal preprocessing, signal separation and recovery algorithms, and spectrum drawing algorithm. Moreover, statistical measurements are used for evaluation of these algorithms. Signal preprocessing based on DC-offset correction and signal de-noising is performed. DC-offset correction was done by using minimum value of radiation signal. However, signal de-noising was implemented using fourth order finite impulse response (FIR) filter, linear phase least-square FIR filter, complex wavelet transforms (CWT) and Kalman filter methods. We noticed that Kalman filter achieves large peak signal to noise ratio (*PSNR*) and lower error than other methods. However, CWT takes much longer execution time. Moreover, three different algorithms that allow correction of x-ray signal overlapping are presented. These algorithms are 1D non-derivative peak search algorithm, second derivative peak search algorithm and extrema algorithm. Additionally, the effect of signal separation and recovery algorithms on spectrum drawing is measured. Comparison between these algorithms is introduced. The obtained results confirm that second derivative peak search algorithm as well as extrema algorithm have very small error in comparison with 1D non-derivative peak search algorithm. However, the second derivative peak search algorithm takes much longer execution time. Therefore, extrema algorithm introduces better results over other algorithms. It has the advantage of recovering and measuring over 21,941 peaks. Although, 1D non-derivative peak search algorithm has better extraction of peak height than other algorithms.

1. Introduction

X-ray spectrometers (XRSs) are used in several fields in both fundamental research and industrial applications [1]. These are elemental mapping of sample composition, medical diagnostics, environmental monitoring, and works-of-art investigation. It employs dedicated systems for high-resolution x-ray spectroscopy [1].

Atomic x-rays are emitted during electronic transitions to the inner shell states in atoms of modest atomic number [2]. These x-rays have characteristic energies related to the atomic number. However, the ideal detector in x-ray spectroscopy detects all incident x-rays, absorbs all of their energy, and generates output pulses with height proportional to the absorbed energy. Thus, ideal output pulse is based on full-energy deposition, no escape of secondary x-rays, and no carrier trapping [3]. On other hand, an ideal detector pulse does not exist. Therefore, correction for spectral distortion must be applied to realize a quasi-ideal detector. The main causes of distortion in measured x-ray signal are in [3]. Additionally, the peak areas of x-ray signal represent the information of interest [4]. However, signals overlapping cause spectral distortion towards the higher energy region [3].

The effects of signals overlapping include reduced throughput [5], system dead-time and degradation of energy resolution [6]. These effects can significantly affect the overall performance [7]. The photons hitting the detector are randomly spaced in time. Therefore, two pulses are sufficiently close to be read as a single pulse by the data-acquisition system. The result is a waveform whose peak amplitude is not proportional to the energy of the detected photons [1]. Consequently, signal overlapping distortion is a common problem for pulse-height measurement at high counting rates [8–11]. Electronic pulse overlapping is an unavoidable source of distortion. The composite signal may be interpreted by the analyzing system as

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corresponding to a fictitious event. Furthermore, the analog to digital converter (ADC) assigns to it an erroneous energy value [12]. All x-ray spectroscopy systems exhibit pulse overlapping and dead time losses arising in the signal processing electronics [13,14]. Therefore, one must determine and correct for these losses in order to accurately determine the true incoming count rate and spectrum. A discussion of some of the earlier attempts at digital pulse processing for x-ray signal can be found in [15]. This paper is organized as follows: Section 2 presents the implemented algorithms in x-ray spectroscopy. However, Section 3 introduces comparison between the considered algorithms. Effect of signal separation algorithms on spectrum drawing and assessment is demonstrated in Section 4. Section 5 is devoted for conclusion of this work.

2. Implemented algorithms

The main purpose of the current x-ray spectrometer is elemental mapping of sample composition. It is used for in-situ applications for samples analysis. The ^{55}Fe radiation source was used. The acquisition system consists of a Silicon Lithium Si(Li) detector that cooled with a nitrogen followed by shaper amplifier and ADC. The resolution of the ADC is 12 bits. Moreover, the sampling rate of ADC is 5 MHz. The signal is acquired through a personal computer with Intel core TM i5-3470 CPU and 3.20 GHz. Therefore, different algorithms such as signal preprocessing algorithms, signal separation algorithms, and spectrum drawing and evaluation algorithms are described. Block diagram of the pulse height system analysis is depicted in Fig. 1. DC-offset, white Gaussian noise and overlapping problems complicate the x-ray signal. Therefore, different algorithms are provided that allows in conjunction with DC-offset correction, signal de-noising and overlapping corrections to be implemented.

The proposed algorithms have been tested using statistical measurements. Some parameters have been calculated for quantitative evaluation of the considered algorithms. These parameters are peak signal to noise ratio (*PSNR*), mean square error (*MSE*), root mean square error (*RMSE*), error, signal to noise ratio (*SNR*), and mean absolute error (*MAE*). *MSE* is the average squared difference between a reference signal and a distorted one. The sum of the mean square error (*MSE*) is used as a cost value to segment the difference signal computed by the absolute-valued log ratio [16].

$$MSE = \sum_{m=0}^{M-1} \sum_{n=0}^{J-1} \frac{(A(m,n) - B(m,n))^2}{MN} \tag{1}$$

where A, B, M and N denote the corrected signal, the input signal, the number of rows and columns of input signal, respectively. Therefore, the root mean square error (*RMSE*) is obtained by

$$RMSE = \sqrt{MSE}. \tag{2}$$

The *PSNR* represents a measure of the peak error. It is given by [16]

$$PSNR = 10\log_{10}\left(\frac{Max^2}{MSE}\right) \tag{3}$$

where *Max* denotes the maximum value of the signal. The *SNR* and the mean absolute error (*MAE*) are given by [16]

$$SNR = 10\log_{10}\left(\frac{P_s}{P_n}\right) \tag{4}$$

$$MAE = \sum_{m=0,n=0}^{M-1,N-1} \frac{|(A(m,n) - B(m,n))|}{MN} \tag{5}$$

where P_s and P_n denote the signal power and noise power, respectively. However, the error represents the absolute value of the difference between corrected and input signal. It is given by

$$Error = \sum_{m=0,n=0}^{M-1,N-1} |(A(m,n) - B(m,n))| \tag{6}$$

2.1. Signal preprocessing

X-ray signal should be processed without noise in order to determine the spectroscopy with high accuracy. Therefore, preprocessing steps include DC-offset correction and signal de-noising. These algorithms are described in the following sections.

2.1.1. DC-offset correction of x-ray signal

DC-offset is undesirable part of x-ray signal. It represents the offset of the signal due to electronics. The DC-offset correction is sometimes desirable to suppress very small noise pulses. Moreover, only pulses of known relative amplitude are required to test linearity and determine the zero offset [17].

This step is used to make the starting point above zero to remove signals before the measurements. The data acquisition system is usually turned on before the measurements process to guarantee the detection of the isotope data. In this experiment, the starting voltage is shifted by 0.0128 V. It means that the first 0.0128 V are removed. Therefore, the DC-offset of x-ray signal is corrected by applying the following formula:

$$C_m = O_m - B_m \tag{7}$$

where C_m, O_m, and B_m denote the DC-offset corrected signal, original signal that is depicted in Fig. 2(a), and minimum value of the original signal, respectively. The result of this step is shown in Fig. 2(b). Furthermore, a statistical measurement of corrected DC-offset signal is depicted in Table 1.

2.1.2. Signal de-noising

The problem of extraction of the signal from noise is common to almost any measurement using electronic systems [18]. The level of noise in a signal is commonly quantified in terms of the signal-to-noise ratio (*SNR*). It is defined as the ratio of the signal to the square root of the noise variance, σ [18]. Noise smoothing and filtering can be done through digital filters [18]. Therefore, we are concerned with elimination of the white Gaussian noise resulting from counting statistical noise. Four independent methods are used to eliminate this noise. These methods are described and compared in the following sections.

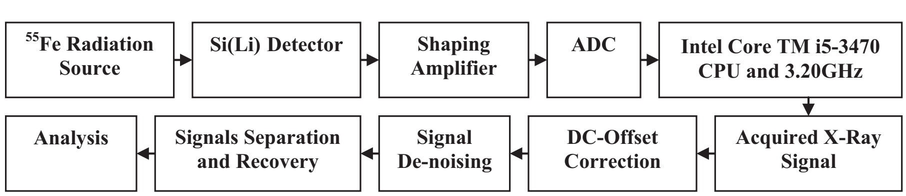

Fig. 1. Schematic diagram of the pulse height analysis of x-ray spectroscopy system.