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A DIGITAL COINCIDENCE DOPPLER BROADENING SYSTEM IN LAMAR

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A simple digital Coincidence Doppler Broadening Analysis (CDBA) of the 511 keV γ line system developed in the Laboratory for Measurement and Applications of Radiation (LaMAR) is presented and tested. It uses a 14-bit digitizer card, directly sampling signals from the preamplifier, and acquires data triggerless in listmode, with dedicated software-based offline coincidence analysis. Performance of the new approach is compared to that of its analogic counterpart.

Keywords: digital spectrometer, doppler broadening, coincidence data

1. Introduction

Doppler broadening of the annihilation radiation is one of the basic methods of positron annihilation spectroscopy used for the investigation of defects in materials [1][2]. It is used to probe the momentum distribution of the annihilating electron-positron pairs, which in turn reveals information on the nature of the electrons from the material under investigation. Positron annihilation with low-momentum valence or conduction electrons leads to a small Doppler shift, whereas, tightly bound core electrons, with higher momenta, will contribute to a large shift in tails of the 511 keV γ line [2][3][4]. Since the chemical environment and crystal bonding have virtually no effect on the core electrons, analysis of the higher-momentum tails of the 511 keV line helps to identify the chemical elements around the point of annihilation.

Conventional 1-detector setups examine only one of the two photons emitted after pair annihilation, thus prone to background contamination, affecting the low-energy side of the annihilation peak important for information on core electrons from the sample. The 2-detector coincidence setup proposed by Lynn *et al.* [5] proved that significant improvements to the peak-to-background ratio and the energy resolution (by a factor $\sqrt{2}$) can be achieved [5].

Classical Coincidence Doppler Broadening Analysis (CDBA) setups make use of spectroscopic (shaping) amplifiers, logical units, time pick-off units and, finally, a Multi-Channel Analyzer (MCA). The current setup available at the

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LaMAR laboratory at the Department of Physics of University POLITEHNICA of Bucharest uses a complex albeit analogic pulse processing chain for CDBA studies. The past decade, however, has seen the advance of digital electronics and the highly-integrated digital acquisition cards (digitizers), with a consequent adoption in the fields of positron annihilation-based material studies : CDBA, in particular [6][7][8][9], as well as Positron Annihilation Lifetime Spectroscopy (PALS) [10][11].

We now present a simplified digital version of the CDBA setup at LaMAR, and compare it to its analogic counterpart.

2. Experimental Setups

A ^{22}Na source encased in Kapton foil, with an activity of approximately 26.26 kBq, was used for both analogic and digital setup measurements, with two mechanically-cooled coaxial HPGe detectors of 25% and 30% relative efficiency, respectively. The detectors were placed in a face-to-face geometry, with the source in the center, on the common axis of the detectors. The distance between the source and detectors was adjusted in order to have a count rate of less than 2000 counts/second in singles mode per detector in order to avoid any skewing effects. No reference sample was used for these measurements, only the ^{22}Na source, hence the annihilations are due to the Kapton foil only. Both analogic and digital sets of data were calibrated using a standard ^{152}Eu source.

2.1. Analogic Approach

The block-diagram of the existing analogic CDBA setup at LaMAR is presented in Figure 1. Such a setup is called a *fast-slow coincidence setup* [12][13], since it combines pulse-height selection (slow branch) and coincidence determination (fast branch).

The slow branch consists of a first set of signals from the charge-sensitive preamplifiers of each HPGe detector which pass on to a Ortec 671 Spectroscopic (Shaping) amplifier, afterwards being fed to the Multichannel Analyzer (Ortec ASPEC-927). The spectroscopic amplifiers also provide logical Pile-Up Rejection (PUR) signals used to prevent analysis of any distorted signals by the MCA.

The fast branch uses the second set of preamplifier signals, processed by fast amplifiers (Ortec 474 Timing filter amplifiers) then by the time pick-off unit (Ortec 584 Constant Fraction Discriminator), and are connected in a Start-Stop configuration to a Time-to-Amplitude Convertor (TAC) unit (Ortec 567). The latter produces, on one hand, a signal proportional to the time difference between the Start and Stop detectors, on the other, it provides a Single Channel Analyzer (SCA) logical signal each time a valid (in this case, a coincident) event has occurred. By accurately setting the coincidence interval, the fast branch of the setup can be used to further condition the slow branch, hence, to acquire the pulse-height spectra of mostly those events that are correlated.

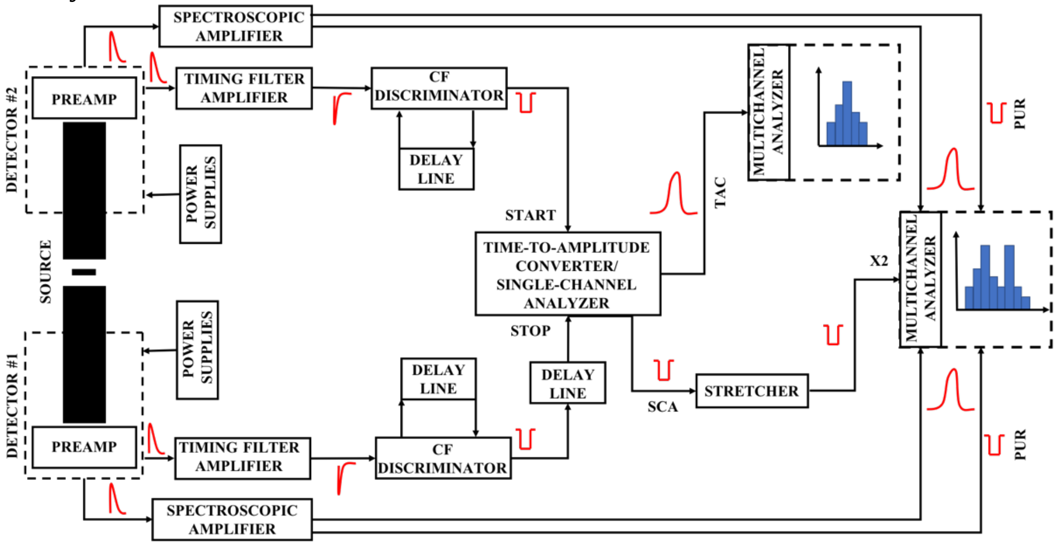

Fig. 1 – Block-diagram of the Analogic CDBA setup at LaMAR. Meaning of the abbreviations: SCA – Single Channel Analyzer logical output, PUR – Pile-Up Rejection logical output

Two separate MCA units are used to acquire data from both detectors as well as their coincidence curve on three *independent* channels. The recorded histograms result by continuously incrementing the digitized (after analogic pulse processing) pulse-height signals corresponding to valid events. However, these are *only hardware-correlated*, since the channels are independent. Further data analysis is restricted to these final spectra, without the possibility of performing any time matching offline.

2.2. Digital Approach

As previously stated, the current MCA mode of operation has the severe drawback of not allowing for Energy-Time correlation of the data offline, while at the same time requiring a large amount of electronics. We have thus tested the setup using 14-bit 80 MSa/s XIA DGF-4C rev. F [14] digitizers, eliminating the analog pulse processing part, and acquired data triggerless, with coincident events being constructed offline using a custom developed flexible Event Builder.

The digital approach is presented schematically in Figure 2. A previous study [15] conducted at LaMAR used standalone one-channel digitizers *without* the possibility of interconnecting. By contrast, DGF-4C rev. F digitizers used in this work can handle up to four input channels, each providing timestamped data, and several cards can be coupled in a master-slave configuration via a backpane distributed clock bus [14][16].

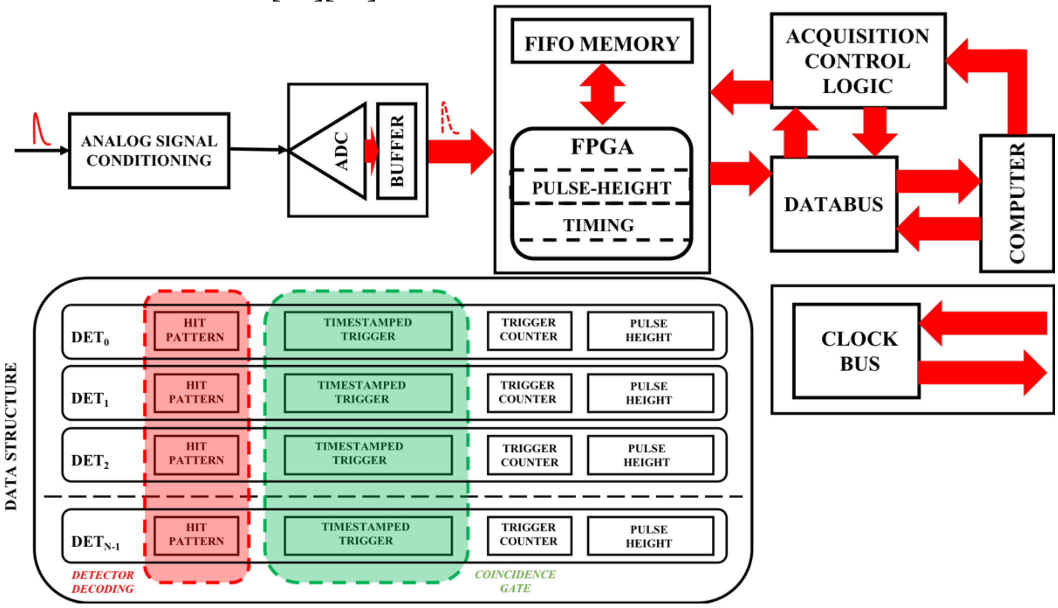

Fig. 2 – Schematic representation of the digital approach to the CDBA setup. The upper section shows a block-diagram of the digitizer and one of its channels. The clock bus allows to connect several digitizers in a master-slave configuration, increasing the number o possible detectors. The data structure and principle of offline coincidence is represented in the lower-left section. See text.

The new digital system uses the Linux-based command line control software initially developed for the MINIBALL array [17] with online spectra visualization via the Multi-channel Analyser software package [18], ensuring minimal use of acquisition computer resources.

It is thus possible to acquire listmode data from several detectors simultaneously and, using the procedure depicted in Figure 2, construct coincidence events offline through software gates applied on the timestamped triggers, eliminating virtually the entire analogic chain from Figure 1. The event builder decodes the hit pattern from the data, revealing which detectors have contributed to a raw event, after which constructs coincident events by filtering the timestamped triggers for each input channels (i.e. each contributing detector) within a given coincidence window. At this stage it is possible to create coincidences between virtually all of the input channels, in this case between only the two HPGe detectors of the CDBA system. The resulting data is then processed using the general-purpose spectrum analysis software package GASPWare [19] and the aforementioned Multi-channel Analyser, both providing advanced peak-fitting and background subtraction procedures, as well as the possibility of constructing two-dimensional arrays. The overall setup now enables us to construct coincidence matrices, feature previously unavailable using the analogic processing chain.

3. Results and discussion

The spectra of the analogic fast-slow coincidence system can be seen in the Fig. 3, in which a brief amount of time data was acquired with and without gating, using a ^{22}Na source.

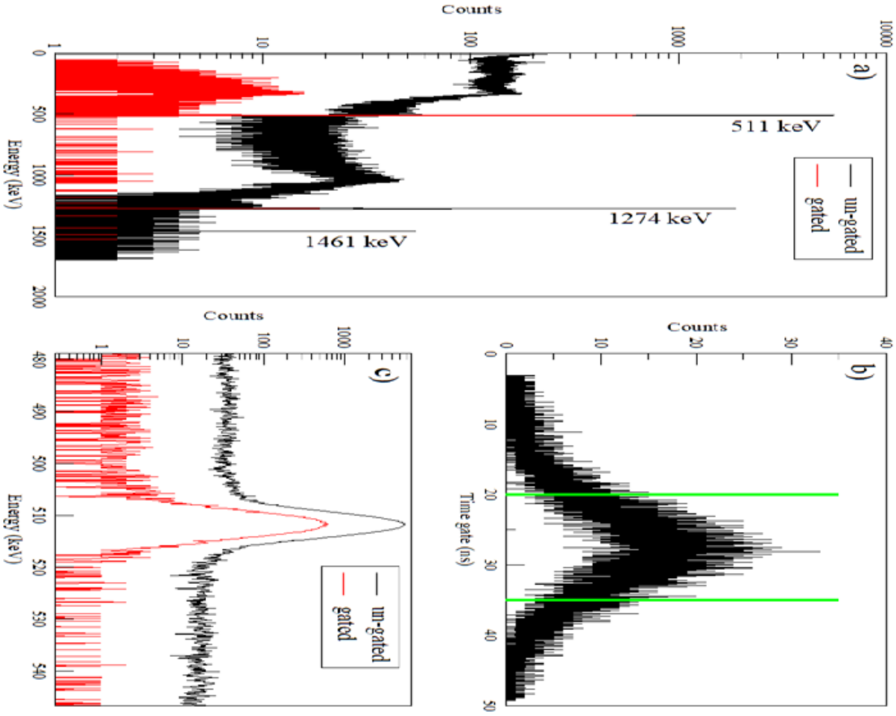

Fig. 3 – Sample spectrum of a ^{22}Na source acquired using the system described above. (a) shows the ungated singles spectrum in black and the result of using a coincidence gate via a SCA output (b) is shown in red. The lower-right panel (c) is a zoom-in of the 511 keV γ line.

The decrease in the peak count is due to the coincidence gating. Fig. 3a clearly shows that without gating (marked with black), background contribution from ^{40}K (1461 keV line) is present, and is significantly reduced afterwards (red). Optimization implies further constraints on the time spectrum to improve the quality of the data (marked with light green in Fig. 3b), resulting in a clean spectrum which preserves the lineshape of the 511 keV line (Fig. 3c).

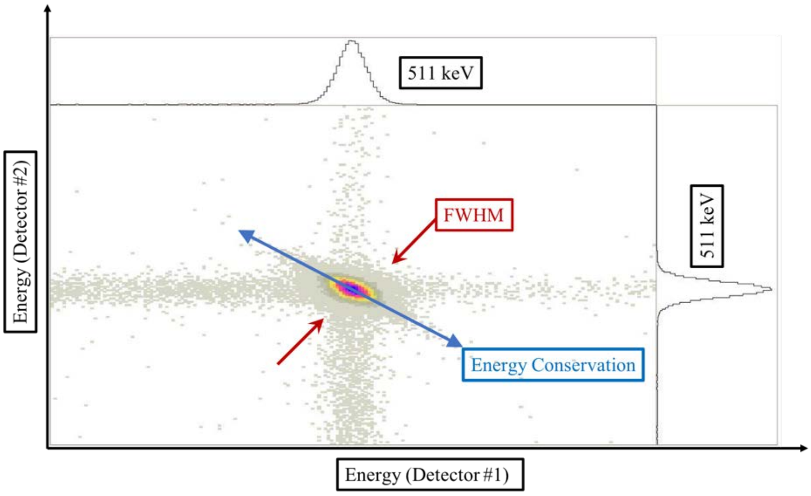

Fig. 4 – Coincidence matrix obtained using the digital setup (on a log-scale for visualization purposes). Focus is around the 511 keV line.

For such as system, special care must be taken when considering settings and calibration, as they influence the energy resolution and peak shape, the latter particularly important for Doppler Broadening-based techniques.

Taking the parametrizations from [20][21] as starting points, the DGF-4C based system was optimized in order to achieve the best possible Full-Width-at-Half-Maximum (FWHM) and Full-Width-at-Tenth-Maximum (FWTM) [22][23], when compared to its analogic counterpart. Two second sets of data were

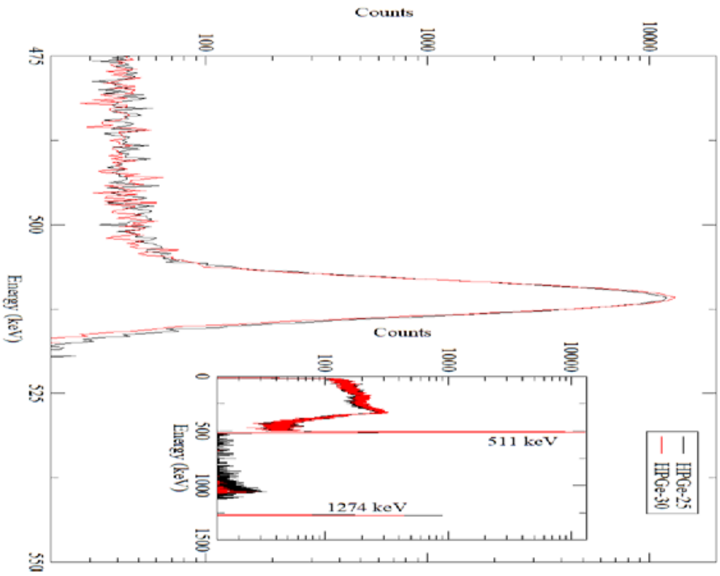

Fig. 5 – Projected spectra for both detectors from data acquired with the digital system, focused on the 511 keV line, with an inset showing the entire spectrum. A 1274 keV line is always coincident with the 511 keV from the pair-annihilation when using a ^{22}Na source.

recorded, for both analogic and digital setups, until the area under the 511 keV line reached 1E+06 counts in magnitude.

The data from the digital system was first passed through the Event-Builder, then sorted using gsort from the GASPW are package. It allowed to construct a 16k x 16k two-dimensional coincidence array using each detector as an axis (Fig. 4).

By further taking the projections along the axes from the coincidence matrix, focusing on the 511 keV line, two spectra were obtained and are presented in Fig. 5. These projected spectra were analyzed and compared to those from the analogic set, in terms of FWHM and FTWM of the 511 keV annihilation line (after background subtraction) as well as the ratio R=FTWM/FWHM, the results being summarized in Table 1.

Table 1

Indicators of peak shape quality

	HPGe-25			**HPGe-30**		
	FWHM (keV)	**FWTM (keV)**	**R**	**FWHM (keV)**	**FWTM (keV)**	**R**
Analogic	2.535	4.766	1.88	2.573	4.838	1.88
Digital	2.850	5.245	1.84	2.750	5.195	1.89

These measurements indicate that the resolution (FWHM) at 511 keV is slightly lower when using digitizers, and the peaks are always slightly skewed compared to a pure Gaussian, for both analogic and digital setups. On the other hand, considering [22][23], the peak quality is not affected.

4. Conclusions

A digital multiparametric Coincidence Doppler Broadening Analysis setup at the LaMAR laboratory has been tested against its analogic counterpart. By using a triggerless approach, the amount of electronics is minimized whilst allowing flexibility in offline data analysis. The energy resolution is slightly lower when using the digitizer, however, given proper optimization, the line shape maintains its quality.

Future developments will include the addition of several detectors in order to improve background reduction. Having multiple inputs available as well as the possibility of using several cards together, ensure that the additional detectors can be used in coincidence offline, moreover, will be treated as separate parameters for the HPGe, to maximize data analysis efficiency.

A separate analogic Positron Annihilation Lifetime System can also be added as an input to the digital system, resulting in a hybrid digital-analogic system, allowing both CDBA and PALS studies be carried out simultaneously.

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