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2011 J. Phys.: Conf. Ser. 262 012014

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Digital setup for Doppler broadening spectroscopy

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Abstract. New digital spectrometer for measurement of the Doppler shift of annihilation photons was developed and tested in this work. Digital spectrometer uses a fast 12-bit digitizer for direct sampling of signals from HPGe detectors. Analysis of sampled waveforms is performed off-line in software. Performance of the new digital setup was compared with its traditional analogue counterpart. Superior energy resolution was achieved in the digital setup. Moreover, the digital setup allows for a better control of the shape of detector signals. This enables to eliminate undesired signals damaged by pile-up effects or by ballistic deficit.

1. Introduction

Doppler broadening (DB) of the annihilation peak is very important observable frequently used in defect studies with slow positron beams. The Doppler shift in energy of annihilation photons can be precisely measured using HPGe detectors. A scheme of a traditional analogue DB spectrometer is shown in Fig. 1A. Signals from a charge sensitive preamplifier coupled with HPGe detector are amplified and shaped by a spectroscopy amplifier. Shaping into a pseudo-Gaussian form is performed by passing detector signals through active high-pass CR and low-pass RC frequency filters. Finally amplitudes of shaped pulses are converted to numbers by an analogue-to-digital converter.

Novel digital setup for DB spectroscopy developed in this work is shown in Fig. 1B. The analogue modules used in the traditional setup were replaced by a fast 12-bit digitizer which directly samples detector signals in the *real time*. Sampled waveforms are stored in computer and analyzed *off-line* in software. New digital setup has several advantages compared to the traditional analogue configuration: (i) sampled detector signals do not suffer from random noise added by analogue modules in the spectroscopic track, (ii) all detector signals are accessible for the analysis, i.e. the amount of recorded information is much higher than in the analogue setup, (iii) data analysis can be performed repeatedly in order to find the optimal strategy how to derive the required physical information, (iv) time consuming adjustment of analogue nuclear instrument modules is not necessary anymore. Performance of the digital setup was compared with performance of its analogue counterpart.

2. Experimental details

A $^{22}\text{Na}_2\text{CO}_3$ with activity of 1 MBq deposited on a 2 μm thick mylar foil was used as a positron source. A well annealed pure Al (99.99999%) was used as a reference sample. Both digital and analogue setup were tested using a HPGe detector Canberra GC 3519 with relative efficiency of 35 %.

In the traditional analogue configuration shown in Fig. 1A detector pulses are shaped in a spectroscopy amplifier Canberra 2020 and their amplitudes are converted to numbers by an analogue-to-digital converter Canberra 8713.

In the digital setup shown in Fig. 1B detector pulses are directly sampled by a 12-bit digitizer Acqiris DC440 (Agilent Technologies U1066A) with sampling frequency of 16.7 MHz (sampling period 60 ns). The digitizer is externally triggered by slow positive logic SCA signals from a constant fraction discriminator Ortec 473A fed by detector signals appropriately shaped in a delay line amplifier Ortec 460. Although external triggering is in principle not necessary, it has an advantage that position of pulse maximum occurs always at similar time. Moreover, uninteresting low-energy signals can be suppressed by adjusting the lower discrimination level of the constant fraction discriminator.

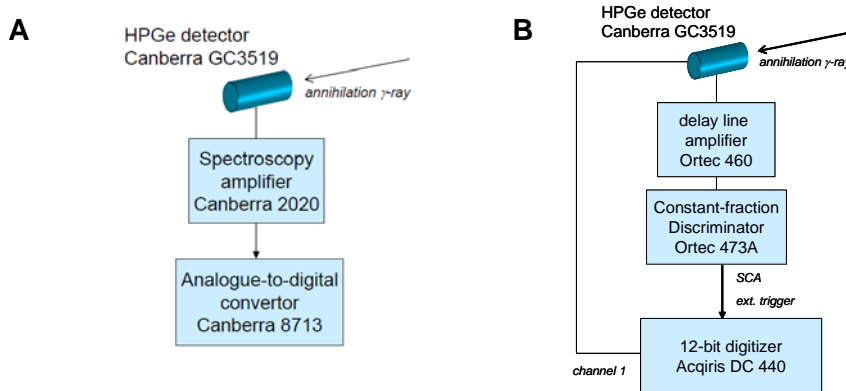


Figure 1. Scheme of (A) traditional analogue configuration for DB spectroscopy and (B) new digital setup.

3. Results and discussion

Examples of sampled detector pulses are shown in Fig. 2. Each sampled waveform consists of 2500 12-bit points. Fig. 2A shows the simplest case of a ‘clean’ pulse without any pile-up. More complex waveform consisting of a pile-up event, i.e. two overlapping pulses, is shown in Fig. 2B. Each waveform was fitted by a model function

$$f(t) = f_{main}(t - t_0) + f_{pile-up}(t - t_1) + f_{prec}(t) + b c g, \quad (1)$$

which consists of a main pulse $f_{main}(t)$, an overlapping random pile-up pulse $f_{pile-up}(t)$, an exponentially decaying base-line $f_{prec}(t)$ produced by some preceding pulse, and a constant base-line $b c g$. While $f_{main}(t)$ is always present, $f_{pile-up}(t)$ and $f_{prec}(t)$ are present only in complex waveforms, e.g. the waveform shown in Fig. 2B. The main pulse

$$f_{main}(t) = \left[\frac{1}{\beta_2 \sqrt{2\pi}} \exp\left(-\frac{t^2}{2\beta_2^2}\right) \right] * [\beta_0 H_s(t - t_0) \exp(-\beta_1(t - t_0))] \quad (2)$$

is approximated by an exponential decay function with origin at time t_0 and decay rate β_1 . Amplitude of the main pulse β_0 is the most important parameter because it is directly proportional to the energy of detected photon. The exponential decay function is multiplied by the Heaviside step function H_s and the product is subsequently convoluted (the symbol $*$ denotes convolution) with a Gaussian with standard deviation β_2 . This accounts for a finite energy resolution of HPGe detector. The pile-up pulse is modeled by a similar function as the main pulse

$$f_{pile-up}(t) = \left[\frac{1}{\beta_2 \sqrt{2\pi}} \exp\left(-\frac{t^2}{2\beta_2^2}\right) \right] * [\beta_3 H_s(t - t_1) \exp(-\beta_1(t - t_1))]. \quad (3)$$

There are two additional fitting parameters related to the pile-up pulse: amplitude of the overlapping pulse β_3 and its position t_1 . The tail of some preceding pulse is modeled by exponential decay function

$$f_{prec}(t) = \beta_4 \exp(-\beta_1 t), \quad (4)$$

where the fitting parameter β_4 represents amplitude of the preceding pulse. Fitting of waveforms by the model function (1) is performed by the Newton-Raphson method. Examples of fit of a simple and a complex waveform, respectively, are shown in Fig 2A and 2B.

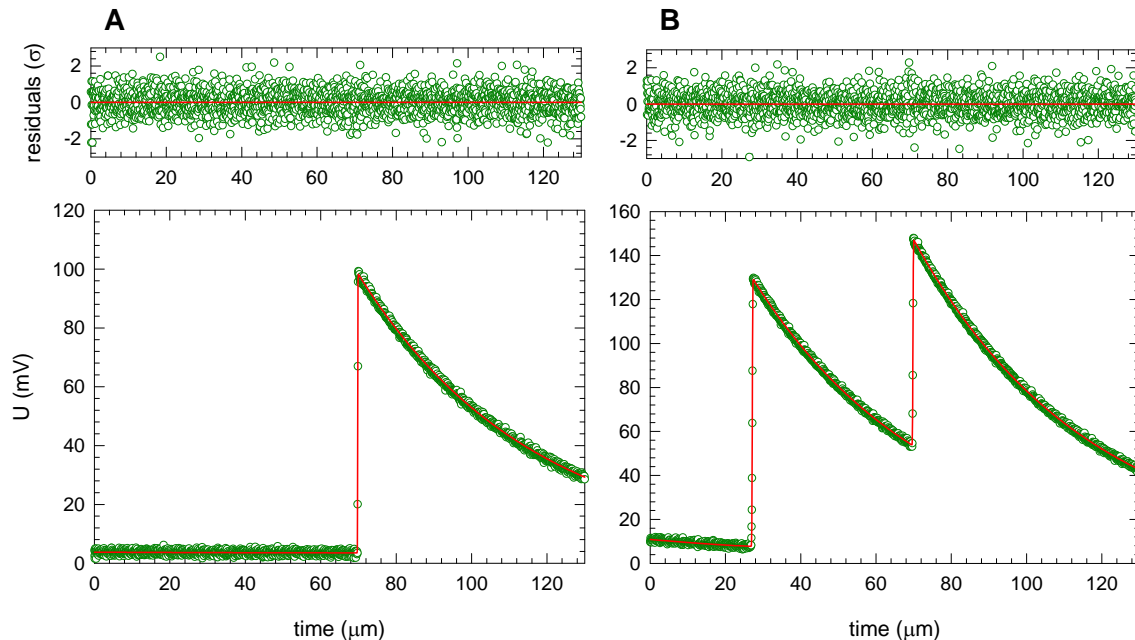


Figure 2. An example of sampled waveforms: (A) simple ‘clean’ pulse, (B) complex waveform consisting of a main pulse, an overlapping pile-up and an exponential tail from preceding pulse. Solid lines show a fit of waveforms by the model function (1). Residuals are shown in the upper panels.

The operations performed during analysis of each waveform can be summarized as follows:

1. read the waveform
2. fit the waveform by the model function (1)
3. perform χ^2 test to check if the waveform is well described by the model function (1). The waveform is accepted only if the calculated χ^2 value is smaller than a pre-selected value corresponding to the significance level of 0.01. Hence, distorted pulses damaged, e.g. due to ballistic deficit, do not pass the χ^2 test and are rejected at this point.
4. If the waveform was accepted, add the main pulse amplitude β_0 into histogram.

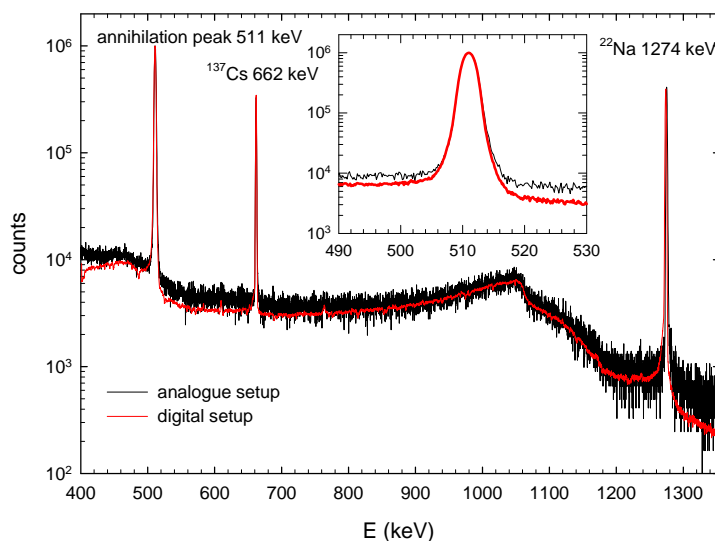


Figure 3.

Comparison of energy spectrum measured using the traditional analogue configuration and the spectrum obtained with the new digital setup. The inset shows a detail of the annihilation peak.

Accumulated histogram of main pulse amplitudes β_0 is calibrated using known energies of the annihilation γ -ray (511 keV) and the ^{22}Na starting photon (1274 keV). In order to improve the precision of energy calibration we used also γ -ray (662 keV) produced by auxiliary ^{137}Cs radioisotope. The calibrated energy spectrum obtained using this procedure is plotted in Fig. 3 together with the spectrum measured using the traditional analogue configuration. The inset in Fig. 3 shows a detail of the annihilation peak. One can clearly see in Fig. 3 that the digital setup suppresses background and improves the peak-to-background ratio compared to the traditional analogue configuration. This is due to a better control over the shape of sampled pulses which enables to reject events distorted by ballistic deficit or by pile-up effects.

Fig. 4 shows energy resolution (FWHM of γ -line) achieved using the analogue and the digital setup at various energies. It is well known that the width of a γ -line measured by a HPGe detector is directly proportional to the square root of energy deposited in detector by detected photon [1]. Indeed, points in Fig. 4 plotted versus the square root of energy fall on straight lines. Obviously γ -lines measured using the digital setup are narrower than corresponding lines measured by the traditional analogue configuration. The extrapolated energy resolution at 511 keV is (1.40 ± 0.05) keV and (1.21 ± 0.03) keV for the analogue and the digital setup, respectively. Hence, employment of digital technique leads to an improvement of energy resolution. This testifies that fitting of the whole detector pulse by a proper model function is the most precise way how to determine the energy of detected photons.

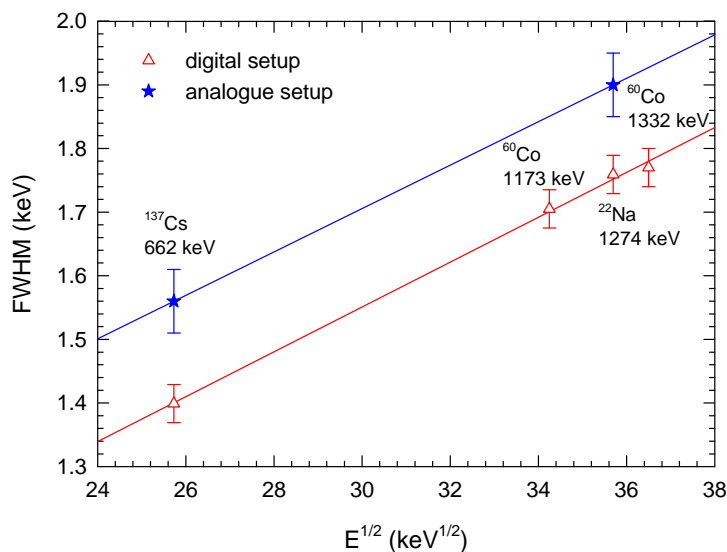


Figure 4.

Energy resolution obtained using the traditional analogue configuration and the new digital setup. FWHM of γ -lines produced by ^{137}Cs , ^{60}Co and ^{22}Na radioisotopes are plotted as a function of the square root of energy of detected photons.

4. Conclusions

New digital setup for Doppler broadening spectroscopy has been developed in this work. Detector signals are directly sampled using a fast 12-bit digitizer. Sampled waveforms are analyzed in software. Performance of the new digital setup was compared with its traditional analogue counterpart. It was demonstrated that the digital Doppler broadening spectrometer enables to achieve superior energy resolution and improved peak-to-background ratio.

5. References

- [1] Leo B W R 1994 *Techniques for Nuclear and Particle Physics Experiments* (Heidelberg: Springer)

Acknowledgments

This work was supported by the Academy of Science of the Czech Republic (project KAN300100801) and the Ministry of Schools, Youths and Sports of the Czech Republic (project MSM 0021620834).