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Early Design Stage of the MsAa-4 Mössbauer Spectrometer

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Entirely new Mössbauer spectrometer MsAa-4 is currently under design and construction. New features as compared to the basic features of the previous generation MsAa-3 spectrometer could be summarized as follows. Completely digital processing of the γ-ray detector signal beyond the Gaussian shape filter/amplifier is to be implemented. The spectrometer is going to be able to accommodate external multiple detector heads. One could collect simultaneously up to 128 γ-ray spectra in 16384 channels of 32-bit each and up to 512 Mössbauer spectra in 4096 channels of 32-bit each provided the proper external multiple detector head is used. The count-rate per single detector is limited to about 10^5 counts per second total. Improved precision of the reference function from 12-bit to 16-bit is to be provided. The reference function is stored in 8192 channels per complete cycle. Addition of the random noise to the reference corner prism of the Michelson–Morley calibration inteferometer is to be introduced to avoid spurious fringes due to the phase lock-up. Integrated universal temperature controller being able to use variety of the temperature sensors is to be interconnected with the proper spectrometer. The spectrometer is now a stand-alone network device as it is equipped with the Ethernet connection to the outside world. Modular design and use of the strict standards allows easy reconfiguration for other applications than the Mössbauer spectroscopy.

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1. Introduction

The Mössbauer spectrometers in the energy domain evolved from some simple electro-mechanical devices. High quality instruments are based on the stable

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and linear transducers and operate in the scanning mode. The multi-scaler arrangement has been finally adopted due to the negligible dead time for sorting pulses beyond the single channel analyzer (SCA). It is advantageous to use linear velocity scales, and therefore modern spectrometers use this mode with the increased demand on the transducer quality in comparison to the simple sinusoidal mode. Symmetric triangular reference function is currently the best choice as modern memories have very large volumes [1–8]. Stand-alone units of the modular design are rather preferred in comparison with the computer-based designs. The latter arrangements were preferred for some time due to their relative simplicity [2, 5, 7]. It is important to integrate with the spectrometer some auxiliary units, e.g. temperature controllers. Some of the older spectrometers had some rudimentary control of the external environment [8], but more intelligent interface with the integrated temperature controller has been developed in some simple form for the MsAa-3 spectrometer [9]. Usually old spectrometers were capable of collecting only few spectra at once [5], but the most of them could not collect more than two spectra simultaneously. Usually, the velocity is calibrated by using the standard absorbers, but the optical methods have been developed as well. The very stable Michelson–Morley interferometer with the separated beams has been developed for the MsAa-1, MsAa-2 and MsAa-3 spectrometers [10–12]. It is sometimes important to have ability to collect spectra at several SCA windows. Only few spectrometers have this ability currently, and those are very specialized units like the MIMOS II [13].

The vital parts of the spectrometer are: medium to high quality γ-ray spectrometer, transducer driving system including transducer, multi-scaler data acquisition system and a variety of the auxiliary devices including the data transmission system. The spectrometer MsAa-3 has been equipped for the first time with the TCP/IP 100 Mbaud twisted pair Ethernet link [9]. Such arrangement makes it completely independent stand-alone unit in the Internet web.

This contribution reports on the planned modifications and improvements while upgrading into the MsAa-4 version from the previous MsAa-3 version. The MsAa-3 spectrometer was described in detail in Ref. [9].

2. Nuclear module

Classical nuclear module consists of the radiation detector with the associated high voltage supply, preamplifier, Gaussian shape filter/amplifier, SCA and analog to digital converter (ADC) used to collect γ-ray spectra (or other equivalent spectra). The output from SCA (or several SCA units) is fed to the multi-scaler system synchronously with the transducer motion. The output from ADC is fed to the γ-ray spectrum memory in coincidence and anti-coincidence with the respective SCA pulse. The sum of coincidence and anti-coincidence spectra makes direct γ-ray spectrum, while either coincidence or anti-coincidence spectrum is used to visualize respective SCA window. All signals prior to SCA and ADC are analog. The ADC signal is based upon maxima of the respective pulses and one is able to apply some analog pulse shape recognition systems to reject distorted and overlapping pulses. The rejection rate gives some information about the current dead time of the nuclear channel. The analog nuclear channel is the most vulnerable and costly part of the electronics.

The MsAa-4 nuclear channel is going to operate on quite different principle. The analog signal just behind the Gaussian filter/amplifier is to be digitized by the fast ADC of 12–14 bits with the rate of 60–85 mega-samples per second. The digital signal could be analyzed on-line by flexible adaptive algorithms based on the constant pulse shape and results sorted in real time according to their meaning. Due to the fact that each event has unique address corresponding to the pulse amplitude one can dispense entirely with the SCA, and it is sufficient to collect solely the direct γ-ray spectrum.

2.1. Correction for the overlapping pulses

For the analog system there is little to be done to correct for the overlapping pulses except application of the high order Gaussian-filter. One has to rely on the peak amplitude detection without any possibility to determine the real pulse amplitude against the variable background. The situation is much better for the digital signal. One of the possible correction algorithms based on the invariant pulse shape is outlined in some detail below.

Pulses from the γ-ray detector are defined versus constant background and deviation from the background could be defined for the isolated pulse originating at time $t = 0$ as the following function of time t:

$$S(t) \equiv 0 \quad \text{for} \quad t \leq 0 \quad \text{and} \quad S(t) = A\left(\frac{y(t)}{y(t_0)}\right). \tag{1}$$

Here the symbol $A > 0$ stands for the pulse amplitude and it may vary from pulse to pulse depending upon the γ-ray photon energy. The function $y(t)$ is defined for $t \geq 0$ and it does not depend upon the photon energy. The latter function could be approximated by the following expression for the Gaussian-type filter/amplifier:

$$y(t) = [1 - \exp(-\alpha t)]^{n-1}\left[(n\alpha + \beta)\exp(-(\alpha + \beta)t) - \beta\exp(-\beta t)\right]. \tag{2}$$

The parameter n takes on the values $n = 2,\ 3, \ldots$ with the $n = 2$ value being rather crude approximation. Remaining two parameters are defined as $\alpha = 1/\tau_0$ and $\beta = 1/\tau_1$, where $\tau_1 > \tau_0 > 0$ stand for the characteristic time constants. The function described by Eq. (2) has positive maximum at time $t_0 > 0$, it goes through zero at time $t_1 > t_0$, and it has negative minimum at time $t_2 > t_1$. These times could be determined according to the following algorithm:

$$t_0 = -\tau_0 \ln(z_2), \qquad t_1 = -\tau_0 \ln\left(\frac{\beta}{n\alpha + \beta}\right), \qquad t_2 = -\tau_0 \ln(z_1),$$

$$z_1 = \frac{n\alpha^2 + 2n\alpha\beta + 2\beta^2 - \sqrt{\Delta}}{2(n\alpha + \beta)^2}, \qquad z_2 = \frac{n\alpha^2 + 2n\alpha\beta + 2\beta^2 + \sqrt{\Delta}}{2(n\alpha + \beta)^2}$$

$$\text{and} \quad \Delta = n^2\alpha^4 + 4n^2\alpha^3\beta + 4n\alpha^2\beta^2. \tag{3}$$

Overlapping pulses add algebraically. It is assumed that two adjacent pulses could overlap at most. It is further assumed that pulses separated by less than $0 \leq T_{\rm D} < \frac{3}{2}t_0$ are indistinguishable one from another and that such events are rejected. For the delay time interval $T_{\rm D} \geq \frac{3}{2}t_0$ the second (later) pulse is strongly distorted unless the delay time interval is large enough. However, it could be corrected by subtraction at the second (later) maximum $S(t_{\rm M})$, where the signal subtracted refers to the previous pulse at time $t_{\rm M} > 0$. A time interval $t_{\rm M}$ is the time interval from the beginning of the previous pulse till the second maximum occurrence. For digital processing of the detector signal such correction could be calculated on-line. Figure 1 shows two overlapping pulses calculated for the following parameters: $n = 3$, $\tau_0 = 50$, $\tau_1 = 1000$, and common amplitude of both pulses $A = 1$. Here time and amplitude are expressed in arbitrary units. It is assumed that the first pulse starts at $t = 0$, while the second (later) starts at $T_{\rm D} = 83$. For the pulses described by the above parameters one obtains: $t_0 = 52$, $t_1 = 206$ and $t_2 = 359$.

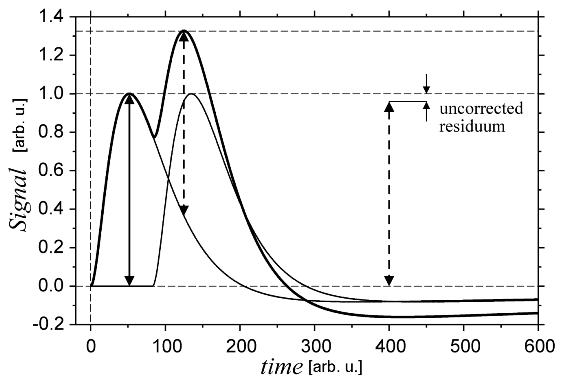

Fig. 1. Signal generated by two overlapping pulses.

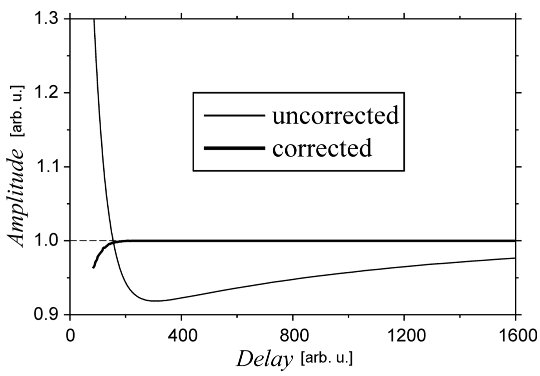

Fig. 2. Relative amplitude versus delay time interval.

On the other hand, Fig. 2 shows amplitude of the second pulse from the above sequence of pulses versus delay time T_{D}. Uncorrected amplitude is just the total signal at the second (later) maximum, while the corrected amplitude is derived according to the algorithm outlined above. Application of the correction results in the increased resolution at the high count-rates.

2.2. Multiple head detectors

The basic idea of the multiple detector-head is shown in Fig. 3. Such head is composed of some small area semiconductor detectors arranged in some matrix. Each detector has the high voltage supply, preamplifier, simplified Gaussian filter/amplifier or integral signal system with the discharge device, and fast ADC as described above. It is easy to calibrate velocity on each "pixel" either using

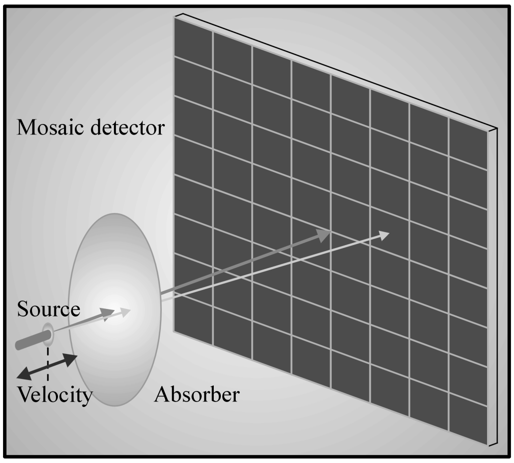

Fig. 3. Basic layout of the multiple detector-head used to map directional dependence of the spectra.

standard absorber or relying on the geometry and optical calibration on the axis. Such system could be used to map absorber inhomogeneity, to look upon directional dependence of the spectra in the absorber or to look upon similar behavior in the small size source. The latter application is particularly important while looking for the resonant atom diffusion in the single-crystal source. The MsAa-4 spectrometer would be able to accommodate up to 128 "pixels" with four non--overlapping "SCA" windows per "pixel", i.e., up to 512 Mössbauer spectra. Each Mössbauer spectrum consists of 4096 velocity channels and each channel has 32-bit capacity. The γ-ray spectrum from each "pixel" could consist of 16384 channels of 32-bit capacity each as well (4×4096 almost touching windows). Hence, the data memory of 16 Mbyte is required. It has to be very fast truly random access memory to accommodate data in the real time. For multiple head detectors data memory is to be located adjacent to the detector array in order to avoid extremely fast data transfers over long distances. Currently available memories could accept up to 10^5 pulses per second total from each "pixel". It seems that the ability to collect simultaneously multiple spectra at various orientations versus the beam is quite important in many cases and it remains rather poorly explored topic.

3. Other modifications

A transducer reference function is downloaded in all MsAa spectrometers. It is generated in 8192 channels per complete cycle and stored in the channels of 16-bit capacity. All versions of the MsAa spectrometer made until now used 12-bit of the above capacity. It is planned to improve this precision to full 16-bit in order to correct for the residual smooth contribution to the velocity error (see Fig. 4 of Ref. [9]).

Some random noise would be applied to the reference corner-prism of the Michelson–Morley interferometric optical calibration system in order to get rid off the spurious fringes. Such upgrade would allow using single longitudinal mode lasers. The optical calibration data are stored in 4096 channels with 32-bit capacity each. The power supply for the calibration laser would be operated from the same battery as the remainder of the spectrometer.

A digital oscilloscope would be installed on-board to watch various signals over the Internet and to dispense with the external oscilloscope.

The universal temperature controller is already installed for the MsAa-3 spectrometers and further integration of this unit with the spectrometer is envisaged. Already existing auxiliary board would be available to set various monitoring systems of the external parameters.

The proven Ethernet connection would be used to communicate with the outside world. Almost all analog signals used to set up various parameters internally would be replaced by the digital signals, e.g. setting of the detector high voltage would be performed by means of the local processor located adjacent to the detector.

A modular design and application of the strict standards makes this unit easy to reconfigure for other applications.

Remaining features of the MsAa-3 spectrometer would be retained. A detailed description of the spectrometer MsAa-3 properties could be found in Ref. [9].

The MsAa-4 spectrometer would be compatible with the MOSGRAF data processing system [14]. The MOSGRAF system has already program GMFPCOM capable to fit up to 128 spectra simultaneously with 2047 channels per spectrum. The latter number of channels is obtained upon having folded the raw spectrum. Hence, all spectra coming from within the single "SCA" window of the detector array could be processed correlating parameters between various spectra.

4. Summary of important modifications

1. Completely digital processing of the γ-ray detector signal beyond the Gaussian shape filter/amplifier.
2. Ability to accommodate external multiple-detector heads.
3. Increased number of channels per single γ-ray spectrum to 16384.
4. Improved precision of the reference function from 12-bit to 16-bit.
5. Addition of the random noise to the reference corner prism of the Michelson–Morley calibration interferometer.
6. Complete integration of the advanced temperature controller.

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