Software based digital signal processing and spectrum deconvolution in X-ray spectroscopy

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Approaches for software based digital signal processing and numerical deconvolution of measured signals which overcome limitations of state-of-the-art systems are described. The basic technical equipment for digital signal processing consists of an energy resolving detector with a preamplifier followed by a fast sampling analogue-to-digital converter (ADC). The main idea is the numerical decomposition of the measured signal into contributions caused by single photon absorption using standard pulses. The latter can be obtained by measurements under definite conditions. The maximum pulse rate is then limited only by the ratio of sampling time to the time between two pulses which should be attributed to single events. Thus pulse overlaps do not require pulse rejection. At sampling rates of 10^8 samples per second theoretically a comparable photon rate can be detected at throughputs of 100%.

Beyond that it is outlined that in a comparable manner a numerical deconvolution of measured energy spectra (statistic distribution functions of single events) into combinations of standard spectra, which can likewise be determined by measurement, offers outstanding possibilities, too. On the one hand the energy resolution attainable for individual events for a given detector can be improved drastically by the statistical treatment of spectra. On the other hand an energy resolving work principle becomes possible for certain detectors, which do not permit this conventionally due to their poor signal to noise ratio.

Keywords: X-ray spectroscopy, digital signal processing, X-ray detector, Gamma-ray detector

1. Introduction

Contemporary advances in the field of signal processing in gamma- and X-ray spectroscopy profit from rapid developments of digital electronics. Today commercial products working on the base of digital signal processing of electrical charge pulses from gamma- and X-ray detectors are available. In these systems the pulse shaping is accomplished by using digital signal processing circuits which offer the possibility of continuous tuning of corresponding parameters. The next stage to the preamplifier in such systems is a sampling ADC which repeatedly samples the analogue signals resulting in a numerical reflection of the signal by values taken in equidistant time intervals. Mostly the sampling ADC is followed by digital filter and signal processing components which process numerical information according to dedicated algorithms.

One important advantage of digital signal processing is the elimination of influences of temperature, time and other operating conditions to the stability of the signal after this stage. Beyond that this strategy is the basis to reach the best possible resolution at any digital setting of rise time for the detector in use.

A strategy basing on an iterative reconstruction of the primary undistorted charge distribution of detector signals by a deconvolution of the measured signal with the transmission function of the preamplifier was suggested by Gast *et al*. (1992). The entire charge can be obtained by considering a time interval for deconvolution which covers typical pulse lengths eliminating influences of noise accomplished using a time discrimination and control unit. Because of limitations concerning pulse spreading in time the strategy in (Gast *et al*., 1992) gives at comparable values of noise discrimination a throughput 20% higher than that of other state-of-the-art combinations of switched integrator and successive approximation ADC.

Already practically realised devices on base of a measurement of the preamplifier output signal with subsequent digital signal processing are described for instance in (Farrow *et al*., 1995) and (Skulski *et al.*, 2000). These systems permit a real time processing of the signals with a throughput clearly higher compared with similar systems, however they still depend on timely isolated events. Limitations in throughput following from it can be eliminated by applying software strategies for decomposition of ADC signals (Meyer, 1996/97).

Until quite recently the available computing power has limited practical use of software strategies. In a former work (Meyer & Gawlitza, 1997) it was shown that measurements of several minutes can be practically realised using state-of-the-art personal computers. This measuring strategy is interesting e.g. for measurements of dynamical processes such as chemical reactions running over comparable time intervals. Since one can expect a dramatic increase of computing power and accessible memory capacity in the next years the measuring time mentioned is of current relevance only. Additionally we refer to modern radiation sources such as synchrotrons and X-ray lasers which emit extremely high photon intensities. For practical use of their capability today first of all the throughput of detectors at given parameters as energy resolution and pulse amplitude stability is the limiting factor. While in (Meyer & Gawlitza, 1997) the use of software based numerical decomposition of the measured signal using standard pulses was described for a detector with pulses having a large overlap on time scale, we now present its applicability to a popular thermoelectrically cooled solid state detector (KEVEX PSI with KEVEX PULSE PROCESSOR 4561A). We found a dramatic improvement of throughput at an energy resolution comparable with that achievable at low throughputs using standard analogous signal processing.

2. Experimental setup and numerical deconvolution of measured signals

Our experimental setup was based on a 12-Bit ADC (NATIONAL INSTRUMENTS PCI-MIO-16E-1 multifunction I/O card in conjunction with a Pentium MMX 233-MHz personal computer). Actual characteristic times for data transfer via PCI-bus and writing on hard disc memory enabled continuous measurements at highest possible sampling rate of the ADC card of 1.25 Msamples / s. The input range of the ADC card can be configured from -10 V to +10 V down to -50 mV to +50 mV.

Thus one could try to sample the preamplifier output signals of the KEVEX detector of typically 4 mV/ keV at 250 ns rise time (setting for best energy resolution) directly. However a hardware stabilisation of the offset signal run with time is required because otherwise the average signal will soon exceed the range. This can be done by a continuous offset correction which may be achieved for instance by adding a corresponding voltage to a second input of the ADC configured for differential mode. From the plenty of strategies to work with preamplifiers directly we chose the position that most of the required components for the adjustment of the signal to the measuring range are included in the KEVEX PULSE PROCESSOR 4561A at a high level of quality. Hence the voltage signals sampled with the ADC typically range between 1 V and 10 V at rise times of up to 10 µs (selectable in certain intervals). This fits well to the limited sampling rate of our ADC and does not reduce the achievable throughput.

Typical signals are shown in Fig. 1 for the case of photons with energies in the range 4.5-20 keV obtained from the fluorescence spectrum of a multi-element compound. Note superposition of pulses on time scale caused by absorption of photons within time intervals comparable to pulse length. The second pulse in Fig. 1 follows the first one before it vanishes (so called pile-up pulse). For the shaping time used the typical pulse length amounts to 24µs, whereby approx. 18µs after the pulse maximum must go by until the amplitude vanishes and thereby can affect following pulses no longer. If only the pulse maximum is used to determine the energy of absorbed photons the maximum of the third pulse in Fig. 1 is not influenced in that way due to the time difference of about 14µs. Pile-up pulses for which the probability of occurrence increases rapidly with photon rate and which have to be rejected usually by hardware can be utilised by our method as described below.

Following the principles described in (Meyer, 1996/97) we aimed at decomposition of the measured signals into distributions caused by single photon absorption processes using standard pulses which were obtained by measuring signals under definite conditions. This allows in a more detailed procedure to achieve best energy resolution by correction of ballistic deficit, charge carrier trapping and pulse rate depending effects using typical pulses as

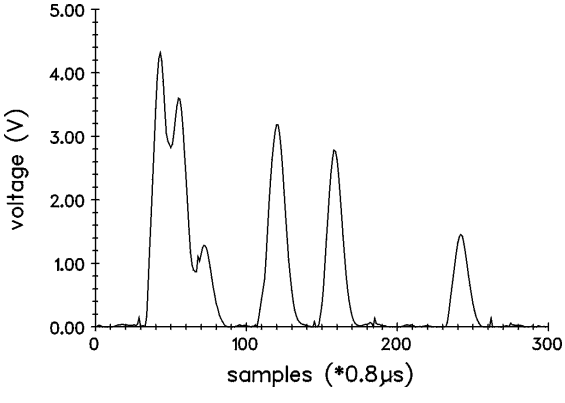

Figure 1
Typical signals at pulse processor output in dependence on time for photons with energies in the range 4.5-20 keV (isolated pulses are useful as standard pulses for numerical deconvolution). The average rate of absorbed photons amounted to approx. 30000 photons/s.

standard pulses in a basic system for numerical decomposition. The approach presented in (Meyer & Gawlitza, 1997) was based on the assumption that as a first approximation the measured signal can be described by a linear superposition of known standard pulses. Because this assumption agrees well with the physical background we chose the approach used for the present solid state detector similarly.

Dealing with the pile-up problem we have to consider two types of superimposed pulses. At first we notice a convolution of charge clouds caused by different photons absorbed in the detector medium. The well known probability of such coincidences depends on typical drift times of the charge clouds within the detection medium. Secondly we must pay attention to the pulse forming and pulse overlap caused by the processing time of the electronic stages following the detector. It is important to solve the pile-up problem numerically instead of throwing away those events. Our method of numerical deconvolution covers both effects. We emphasise at this point that we have achieved throughputs of genuine 100 % at a rate of 30000 absorbed photons per second (conventional analysis results in a throughput of approx. 30 % for that rate). The real absorbed photon rate was determined by purposeful enlarging the excitation power of X-rays (by changing the current of the X-ray tube) beginning from low rates with negligible influences of dead time. A rough examination is also possible by counting of pulses in a selected time interval. The investigated rate of 30000 absorbed photons per second is not a physical limit. In the given case we determined however, that for higher rates and thereby significantly more overlaps of pulses on time scale the resulting amplitude of the signal to be measured occasionally exceeded the input range optimised for precise sampling of single pulses of a certain energy range. In conclusion we argue that nevertheless for a given configuration a maximum rate exists. Exceeding that requires degradations of certain parameters to be taken into account.

Fig. 2 shows signals for the same situation as in Fig. 1 together with the sum of its software created deconvolution pulses (using only one standard pulse). A resulting histogram is shown in Fig. 3. Since in the limits of measuring accuracy in dependence on the photon rate no non-linear influences were found the numerical deconvolution could be done by applying a linear

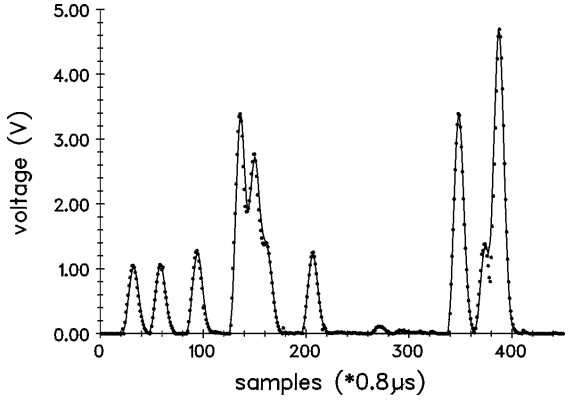

Figure 2
Measured signals at pulse processor output versus time (dots) for photons with energies in the range 4.5-20keV (rate approx. 30000 absorbed photons/s). They are compared to fitted values obtained from a superposition of single standard pulses (line).

combination of as many as desired (measured) standard pulses to the measured signals. The maximum number of standard pulses per time corresponds to the sampling rate. The coefficients of this linear combination are then determined and refined in several cycles by an adjustment according to the least square fit criterion. At present deconvolution of a signal course with a total measuring time of 1 second (sampling rate of 1.25 Msamples / s) requires some 10 minutes. However no special numeric algorithms were used, which suggests that a further reduction of the computing time by orders of magnitude may be possible.

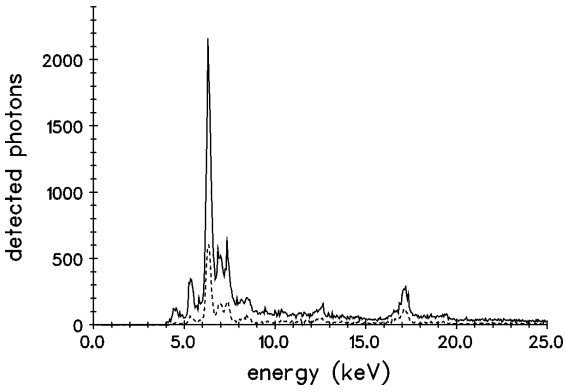

Figure 3
Histogram as derived from numerical deconvolution (line) compared to a histogram (dashes) determined by the conventional analogous way (only pulses without overlap on time scale) at the same time. Total measuring time was 2.0s. The throughput was 100 % for the case of numerical deconvolution (no losses of pulses due to absorbed photons) while for the analogous case it was 35 %, which is to be seen from the relatively smaller number of detected photons per channel. The histogram represents the fluorescence spectrum of a multi-element compound (containing Ti, Mn, Cu, Sr, Ag, Cs; excitation of fluorescence by irradiation with an X-ray tube with Mo anode).

In both cases – conventional and our standard pulse based deconvolution – we got an energy resolution of 3.5 % at 6.25 keV. A more sophisticated numerical deconvolution of the shape of pulses than applied up to now should result in a better energy resolution yet compared to conventional analogous pulse processing.

3. Numerical deconvolution of energy spectra into combinations of standard spectra

The idea of numerical deconvolution of functions into contributions of dedicated measured standard functions may be extended also to overlapping statistic distribution functions as energy spectra. These distribution functions of single events may also be deconvoluted into combinations of standard spectra, which can likewise be determined by measurement. While deconvolution into analytical model functions is usually used in this field, deconvolution into measured standard functions offers some outstanding possibilities in a comparable manner as discussed above for the case of single pulses. Beyond that we like to emphasise two important aspects. On the one hand the energy resolution attainable for individual events for a given detector can be improved significantly by the statistic treatment of spectra. On the other hand we see that an energy resolving work principle becomes possible for certain detectors, which do not permit this conventionally due to their low signal to noise ratio.

Energy spectrum deconvolution will always be of interest if high background contributions overlap the radiation components of interest. This is, for instance, the case for fluorescence XAFS experiments at samples with low content of the resonantly absorbing elements. On the other hand, for energies in the vicinity of absorption edges the necessary discrimination of pulses generated by elastically scattered photons often requires better energy resolution than practically achieved by solid state detectors.

4. Conclusions

Using a software based signal processing method we achieved at rates of about 30000 absorbed photons per second a throughput of 100 % at a comparable energy resolution as for analogous working principles which are limited to the analysis of single pulses, thereby exhibiting significantly lower throughputs (35 % in the present case). Numerical deconvolution of functions into contributions of dedicated measured standard functions can also favourably be used for overlapping statistic distribution functions as energy spectra. For certain detectors which do not permit an energy resolving work principle conventionally due to their poor signal to noise ratio it can become possible to differentiate certain energies.

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References

Gast, W., Georgiev, A., Stein, J., Bücher, A. (1992). *German patent application* DE4226175A1.

Farrow, R., Derbyshire, G.E:, Dobson, B.R., Dent, A.J., Bogg, D., Headspith, J., Lawton, R., Martini, M., Buxton, K. (1995). *Nuclear Instruments and Methods in Physics Research* **B 97**, 567-571.

Meyer, D.C. (1996/97). *German patent applications* DE19633301A1 (1996), DE19752122A1 (1997)

Meyer, D.C., Gawlitza, P. (1997). *Nuclear Instruments and Methods in Physics Research* **A 424** , 470-473.

Skulski, W., Momayezi, M., Hubbard-Nelson, B., Grudberg, P., Harris, J., Warburton, W. (2000). *ACTA PHYSIKA POLONICA B Vol.31, No 1,* 47-57.

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