

The necessity of recognizing all events in x-ray detection

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Abstract

In our work in studying properties of inner shell ionization, we are troubled that the experimental data used to determine the basic parameters of x-ray physics have a large and unexplainable scatter. As we looked into the problems we found that many of them contradict simple logic, elemental arithmetic, even parity and angular momentum conservation laws. We have identified that the main source of the problems, other than the human factor, is rooted in the signal processing electronics. To overcome these problems we have developed a fully digital signal processor, which not only has excellent resolution and line shape but also allows proper accounting of all events. This is achieved by processing all events and separating them into two or more spectra (maximum sixteen), where the first spectrum is the accepted or good spectrum and the second spectrum is the spectrum of all rejected events. The availability of all the events allows one to see the other part of the spectrum. To our surprise the total information explains many of the shortcomings and contradictions of the x-ray database. The data processing methodology cannot be established on the partial and fractional information offered by other approaches. Comparing Monte Carlo detector modeling results with the partial spectra is ambiguous. It suggests that the metrology of calibration by radioactive sources as well as other x-ray measurements could be improved by the availability of the proper accounting of all events. It is not enough to know that an event was rejected and increment the input counter, it is necessary to know, what was rejected and why it happened, whether it was a noise, a noisy or disturbed event, a retarded event or a true event, or any pile up combination of these events. Such information is supplied by our processor reporting the events rejected by each discriminator in separate spectra. Several industrial applications of this quality assurance capable signal processor are presented.

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Introduction

If we look at the experimental data there are strong contradictions in almost all the parameters necessary for x-ray analysis. A detailed discussion is given in [1,2]. Since that time we have seen additional problems that will be elaborated upon in separate papers. Here we will briefly mention some of the warning signs and analyze a few examples.

From the point of view of making an x-ray measurement, the simplest measurement to perform is an angular distribution measurement, as absolute calibration is not necessary with results given by the ratio of the number of x-rays collected from different directions. Many transitions, depending on the excitation mode, present strong angular distribution [3]. Yet such a methodologically simple exercise has led to very disturbing results such as strong violation of parity and angular momentum conservations [4,5].

These inconsistencies are also strongly reflected in the L-shell Coster-Kronig transition and fluorescence yield data [6], which defy simple arithmetic. But maybe this should not be surprising, as the appropriateness of the experimental equipment is usually not properly investigated. One of the first works applying synchrotron radiation to determine L-shell Coster-Kronig data was the work of Jitschin et al [7]. If we look at even the simplest spectrum in that paper, the gold L3 shell x-ray spectrum, we see immediate problems. Quasi monochromatic radiation in energy between the L2 and L3 shells' binding energy ionizes the L3 shell only and the fluorescent radiation contains only L3 shell X-rays, therefore the x-ray groups are well separated, and the spectrum is almost background free. Yet the ratio of the $L\beta$ to $L\alpha$ groups deviate by 20% from the Scofield data of DHFS calculation [8]. The detector efficiency in this energy range is almost constant and absorption was considered but is small, therefore such a discrepancy could not be explained. In our view the remaining possibility, one that we have seen in many cases, is that the signal processor signal detection efficiency was strongly energy dependent.

Similar effects are frequently seen in the $K\beta/K\alpha$ ratios. In addition to the energy dependent signal recognition capability another significant issue is the pile up recognition. As it was demonstrated for some signal processing electronics the pile up recognition is a serious problem even at what are apparently low (a few thousands counts per second) input rates [9].

Another example is the experimental ionisation cross sections for particle impacts. They have a large scatter of the order of a factor of three, while each individual measurement accuracy is reported as better than twenty per cent [10]. This implies large unrecognized systematic errors. One approach that has been used, is to take a statistical average of all measurements, and accepting this value, although this would yield a wrong value for the physical parameter determined unless by fortuitous circumstance the systematic error yields results that are centered about the true value. The reason is simple. With an unidentified source of error the average value will be different from the true value by the average size of the error and thus will likely bear no relation to the true value of the physical parameter being studied. Thus we believe that a better approach would be to identify the source of the scatter with the different approaches used, cataloging the different techniques and establishing a correlation that would lead to a better recognition of the systematic errors and thus to better measurements. Using different detectors each with its own associated electronics can be considered as a different approach.

It has long been held that some level of quality control can be achieved by properly characterizing the response function of the detector and if it is unchanged then this can guarantee

that the detector-signal-processing-electronics system is in the same condition. We have strong reservations about such an approach, as it requires a series of very rigorous measurements and even more importantly it is related to the accepted spectrum only and has no information about the rejected events. It is difficult to know what fraction have not met the criteria prescribed by the discriminators for any given measurement. For instance we have observed with various optimized detector systems (Si(Li) [11], HPGe, Si PIN [12]) that the most striking feature is the shape of the low energy tailing in the response function that includes a step at low energies and is readily explained on the basis of the escape of x-rays and energetic electrons from a finite sized detector as explained in [12]. However, with other systems, possibly in the presence of a great deal of noise these features are swamped by tailing that is orders of magnitude higher so that the response function can vary significantly [13].

We have used various detector systems, and it has been our experience that even the $K\beta/K\alpha$ ratios were varying, and with some systems were dependent upon the setup of the parameters, or the potentiometer positions. It is not uncommon, and in fact is usually desirable, to use various discriminators to improve the spectrum quality. Such an example is well presented for CZT detectors in [14]. Similar approaches are used for Si and Ge based detectors as well. It can be seen in figure 4 of ref [14] as a very good example, that the discriminator acts very differently for the different energy x-rays. This very clearly indicates an electronic efficiency. However, the noise on a signal also can be different for high and low energy x-rays, which makes a reasonably accurate measurement difficult and very high quality measurements impossible, as the supplied information is not sufficient. Therefore we decided to develop a system with quality assurance capability. This is realized in such a way that all events are processed, and the signal complying with the conditions set by the discriminators are collected in one spectrum and the events failing the discriminators are processed and collected in a second spectrum. The second spectrum allows one to identify the origin of the rejected events and thus make corrections for energy efficiency, varying noise conditions etc.

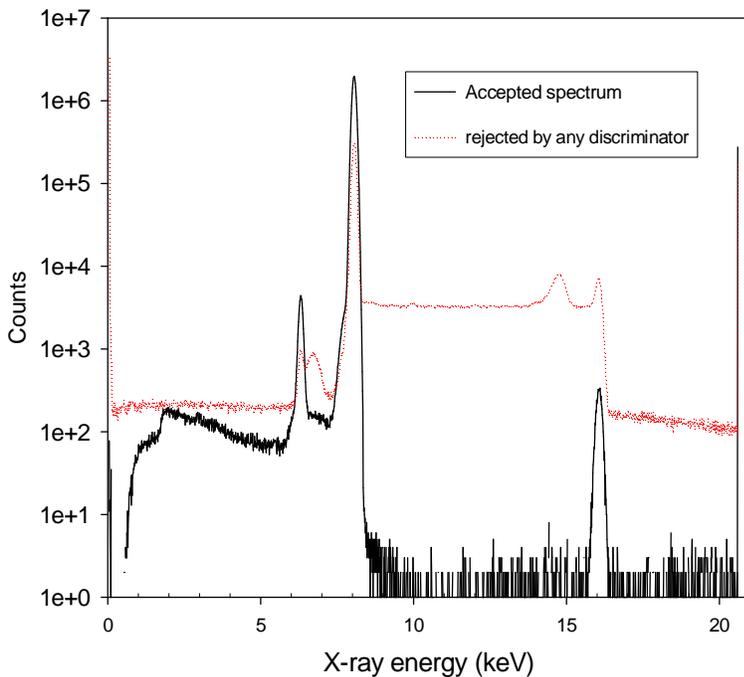
The concept of a quality assurance capable signal processing

Pile up and dead time treatment are difficult issues and several approaches have been implemented to address them. These techniques were developed for gamma ray detectors where the deposited energy in the detector is significantly larger than for x-ray detectors. For x-ray detectors we have to additionally consider that the noise and electronic disturbances can also generate events that the signal processor has to be able to identify and reject. This rejection is necessary as it is advantageous to use a detection system with good line shape, peak resolution and low detector tailing.

Furthermore not only true events are present in the preamplifier signal. Some area of the detector produces degraded events. In many cases it is the side of the detector, where the field uniformity is not always guaranteed. Such events produce unwanted contribution to the spectrum, and we call them degraded events. Rejecting such events can improve the quality of the spectrum, and increase the information that can be derived. Often rise time discrimination can eliminate such events. Other events caused by the ballistic deficit and slow trapping and detrapping processes can be identified as having a differently shaped signal that can be identified by a shape discriminator.

The number of rejected events might be considered to be implied from the input rate indicator. However, the multitude of signal processors do not provide information on what basis the event was rejected. If it was a noise event, we have to incorporate it into the dead time, but it should not be considered as an x-ray event. The noise distribution can be very different from the x-ray event, therefore there isn't sufficient information to decide whether the rejected event is a false trigger by noise or electronic disturbances, a noisy real event that can be considered as an event and noise pile up, or a pile up of two real events. Since the spectrum contains only fractional information we expect that the x-ray data derived from such spectra will have large unexplained scatter. In the next section we demonstrate that indeed we are facing such a situation. We do not claim that the signal processor is responsible for all the discrepancies, as all the elements are important in the measurement e.g. the primary x-ray spectrum (scattered structures, background), the detector (manufacturing details), the preamplifier, the signal processor and the human factor (responsible for ground loop elimination, microphonics reduction, noise environment selection, signal processor set up, spectrum evaluation and data treatment). However, the effect of the signal processor is usually not mentioned in research papers as the researcher usually has little information on the workings of the unit.

To offer a solution, more information is necessary. It is offered by our processors, via processing all events and sorting them to events that have passed or failed the discriminators' criteria. Such a spectrum is presented for a quasi monochromatized Cu K α 1 x-ray peak from an x-ray monochromator in figure 1. The signal processor can also be used in a mode where the events rejected by each discriminator alone are presented in a separate spectrum. For simplicity



we have presented here all the rejected events in a single spectrum. The low energy tailing in the accepted spectrum has the expected shape [12].

Figure 1. A spectrum of a quasi monochromatized Cu K α 1 x-ray peak from an x-ray monochromator is shown. The measured spectrum contains two spectra, one for the accepted spectrum (continuous line) and one for the rejected spectrum (dashed line) The lower side tailing frequently called the plateau, has the expected slope, demonstrating the excellence. This plateau is the lowest ever seen and it's size is limited by the preamplifier design approach. The rejected spectrum

allows the analyst to identify the origin of the event, whether it was noise, noisy event degraded event, electronic disturbance or any combination.

Application of quality assurance capable signal processors

It is typical to use radioactive sources for detector efficiency calibration. They are also frequently used in measuring x-ray and gamma ray radiations for establishing doses as well as in industrial process control. We have made comparative measurements of various sources to assess the performance of the Cambridge Scientific digital signal processor series, CSX2, CSX3, CSX4, via comparisons with the industry standard high quality analog signal processor. The measurements were made in parallel via splitting the preamplifier signal and feeding it to both processors simultaneously. One such measurement involved using a ^{65}Zn source irradiating an iron foil. We have observed that the CSX units show a significant improvement in the background, presented in figure 2.

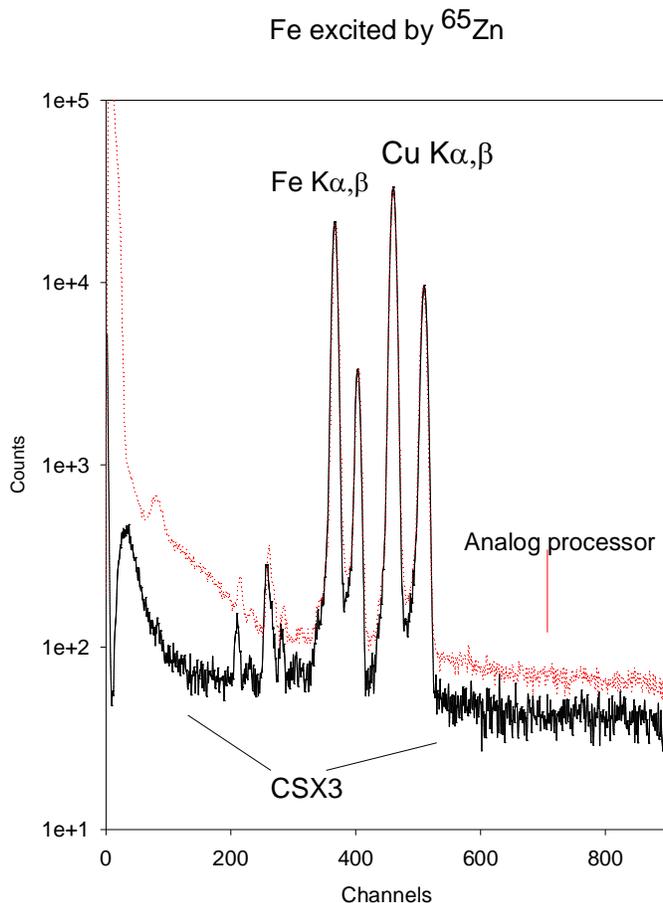


Figure 2. An Fe sample is irradiated with Cu K radiation from a ^{65}Zn source in transmission geometry, and measured with a Si(Li) detector. The background is substantially reduced using the CSX processors. The manufacturers analog processor (dotted line), and the Cambridge Scientific CSX digital processor (continuous line).

It remained to be decided whether the improvement is caused by the better noise recognition, thus the reduction is originating in the noise reduction, and the noise and event pile up reduction, or maybe from the degraded events. Measuring the source spectrum with the CSX3 processor we can see the rejected spectrum that is also presented in figure 3. From the rejected spectrum, it can be established that the background reduction is achieved by identifying and rejecting the background components originating from gamma ray scattering in the detector. Not

having the rejected spectrum available we would have to guess the meaning of the input rate indicator. Even if we would have strong experiences in this direction, and were able to identify that some of the events counted by the input counter are in fact coming from gamma rays, the magnitude of this contribution would be impossible to guess.

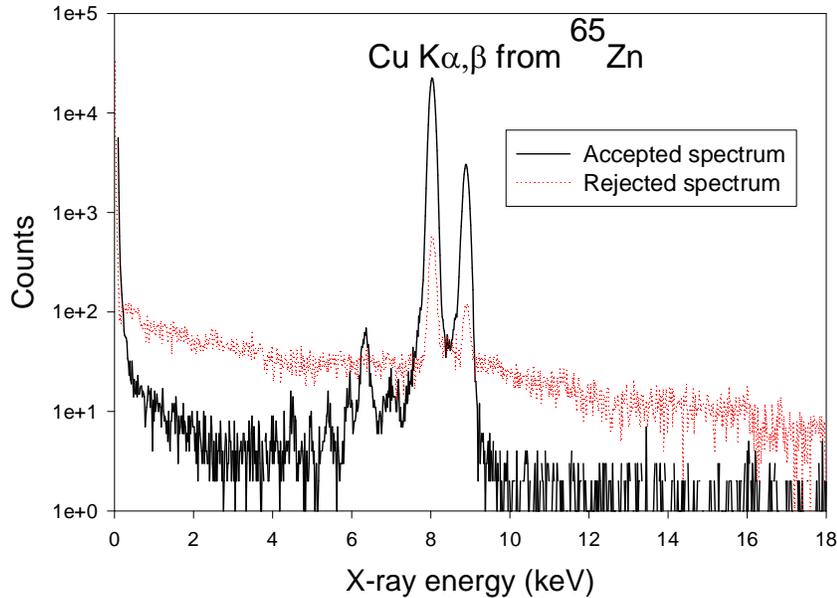


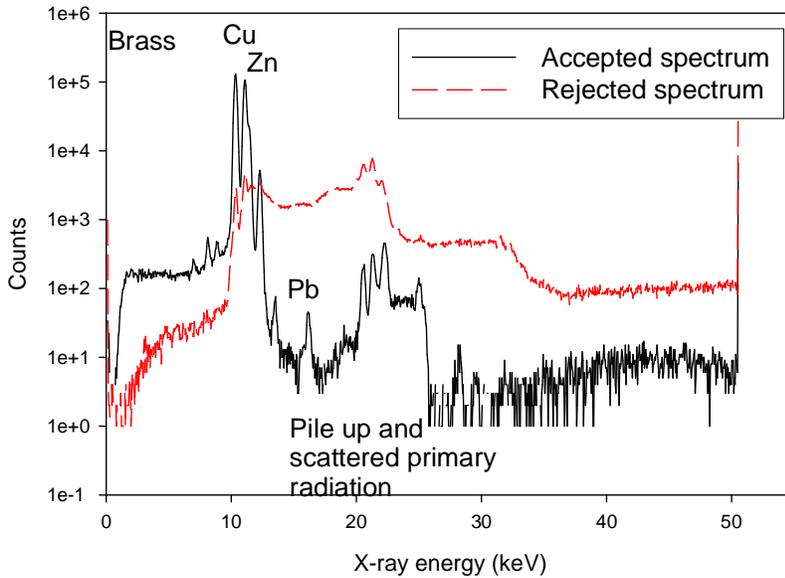
Figure 3. The copper K spectrum from a ^{65}Zn source measured with CSX3 processor, shows the accepted and rejected spectrum. It demonstrates that the rejected spectrum in this case was mainly nuclear background events. The rejected event spectra of several radionuclides have well defined low energy peaks which merit further investigations.

The number of rejected events might be considered to be implied from the input rate indicator. However the multitude of signal processors do not provide information on what basis the event was rejected. If it was a noise event we have to incorporate it into the dead time but it should not be considered as an x-ray event. The noise distribution can be very different from the x-ray event, therefore there isn't sufficient information to decide whether the rejected event is a false trigger by noise or electronic disturbances, a noisy real event that can be considered as a single lost event due to noise pile up, or a pile up of two real events. Since the spectrum contains only fractional information we expect that the x-ray data derived from such spectra could have large unexplained scatter.

Therefore the precise knowledge of many details of the excitation source spectra, including all the radiations, not only the x-rays and the geometry are necessary. These information should be supplemented also by the precise details how the signal processor handles the spectrum components with different origins. This difficulty is eased by the presence of the rejected spectrum. In the presented case the counts in the rejected spectrum is 25% of the accepted spectrum. Not having the rejected spectrum, we would have made 25% error in the detector calibration, if such or similar radionuclides would be used. Similarly we have seen the cautionary signs of what details are easily overlooked using ^{241}Am for calibration.

We do not claim that the signal processor is responsible for all the discrepancies, as all the elements are important in the measurement e.g. the primary x-ray spectrum (scattered structures, background), the detector (manufacturing details), the preamplifier, the signal processor and the

human factor (responsible for ground loop elimination, microphonics reduction, noise environment selection, signal processor set up, spectrum evaluation and data treatment).



However, the effect of the signal processor is usually not mentioned in research papers as the user usually has little information on the workings of the unit.

Figure 4. Lead inspection in brass in an industrial application. Although the information on the rejected event is always necessary, we recently realized its additional benefits in high rate, (105-106 cps) analytical measurements. From the rejected spectrum, the number of the pile up

events can be established.

We present a further application in an industrial XRF (X-Ray Fluorescence) analysis unit. One common application is the measurement of trace contaminants to ensure compliance with RoHS, WEEE. The spectrum of a brass sample is presented in figure 4. The excellent pile up recognition allows the analyst to identify contaminant elements at the ppm level. The rejected spectrum allows derivation of the true number of pile ups and thus the true input rate. In this measurement the input count rate was 260 kcps. The measurement equipment used a tungsten anode x-ray tube at 50 kV voltage and a primary filter combination, dominated by a Mo filter, to generate the excitation spectrum and an SDD (silicon drift detector) for detecting the x-rays. The continuous line is the accepted spectrum, while the dotted line is the rejected. Even at this high input rate the pile up recognition is quite excellent and the lead contamination is very visible. The rejected spectrum indicates that in this case the rejected spectrum is overwhelmingly pile up in origin and would easily have hidden the presence of the lead if not removed from the accepted spectrum.

Input rate output rate considerations

Usually systems have an input and output rate indicator. Ideally what one wants from the input rate indicator is a measure of the number of true events that have interacted with the detector in the measurement live time. In order to do that the input rate counter would have to be able to distinguish between, noise, real events, pile up of noise with noise, noise with real events, real events with one or more other real events etc. However the processor circuitry is not capable of making all of these distinctions in order to obtain the true number of real events and it is usually left to the analyst to deduce the necessary information from the input rate indicator and the visible spectrum.

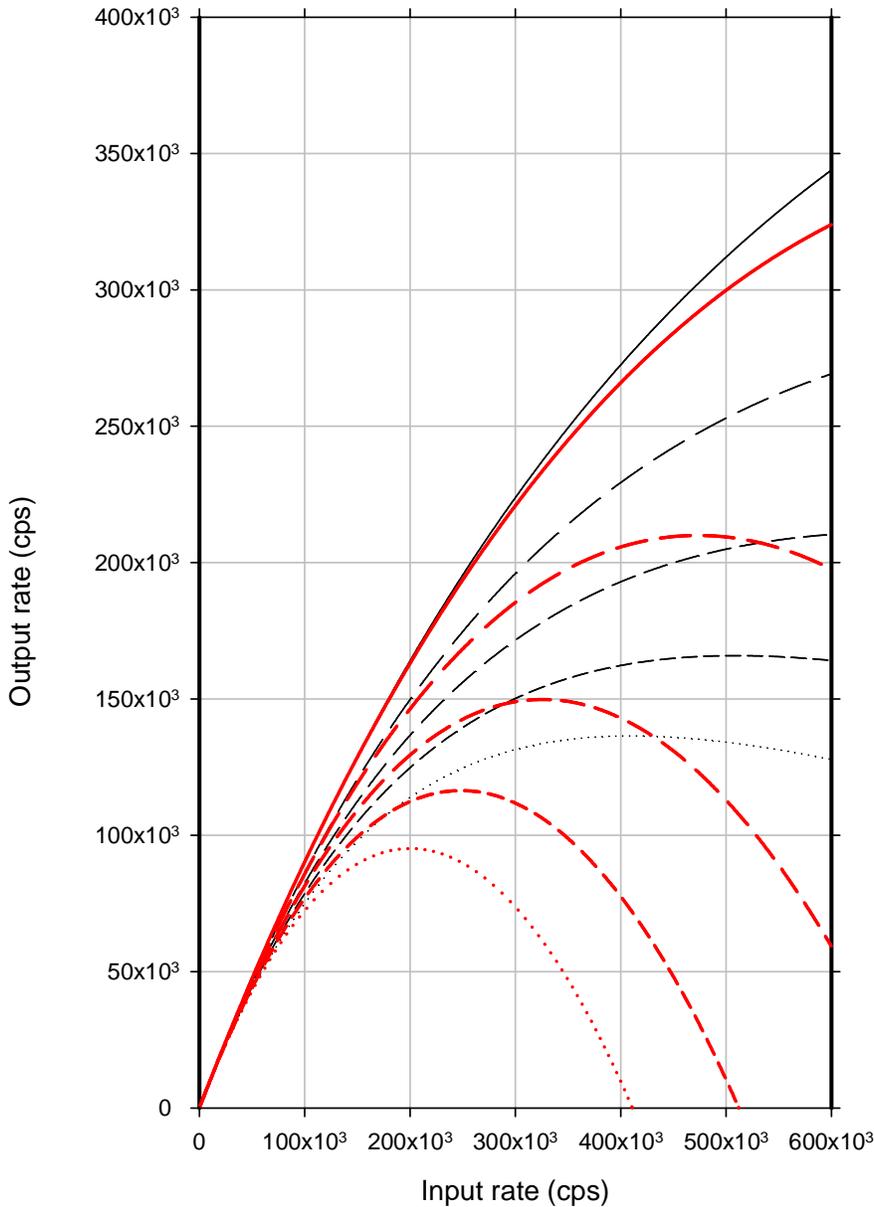


Figure 5. For the CSX2 processor the total OCR is given by the black curve. It was calculated for a preamplifier with 200 nanoseconds rise time, and a 40 nanoseconds ringing or overshoot time interval, which is excluded from the calculation of the energy of the x-ray event. The gray curve gives the OCR in the accepted spectrum, when maximum pile up rejection is applied. However, setting the parameters will effect the level of noise and disturbances that will be recognizable by the processor. This has a positive effect on the appearance of the spectrum but it must be emphasized that the ICR is the sum of all events both real and noise. The different curves are for 1.38, 1.86, 2.38, 2.82 and 3.3 microseconds TSP, where TSP stands for the time spent on a pulse, which includes the peaking time, excluded central region, rise time and processing dead time as well.

The input count rate (ICR) is an important indicator and is absolutely necessary for quantitative EDXRF analyses. Regardless of the number of events in the visible spectrum the input rate must be known for the proper corrections to the peak areas and system dead time.

It should be noted that the reported ICR will include all events that trigger processing, both real events and noise. Although noise triggered events can be eliminated this does not eliminate pile up of real events with noise. If a real event triggers the processing it can still pile up with a later noise event and be eliminated but the number of such events will be unknown as the noise rate will not be known. Therefore analytical work based on the single accepted spectrum can be made only if there is no pile up or noise discrimination. In such a case all the events are accounted for but the overall spectrum is generally of poor quality. With the advent of the quality assured processor, with its rejected spectrum, it is possible to see how many real events have been rejected due to pile up with noise etc., making proper accounting possible while still maintaining a high quality spectrum for analysis. In figure 5 we present the input count rate (ICR) and output count rate (OCR) relation curves for the CSX2 processor equipped with a 50 MHz DSP processor chip. The OCR vs the ICR is presented for various TSP values where TSP is the time spent on a pulse that includes the peaking time and the processing dead time. The figure shows two curves for each TSP value. The higher curve represents a total output event rate that includes single events as well as piled up events, while the lower curve represents single events only. Although the total output is important for event accounting it is generally the single event spectrum that preferentially appears as the accepted spectrum.

It must be emphasized that the ICR is not the number of x-rays striking the detector but is instead the number of events that trigger the processor. In all processors it is desirable to have noise, pile up, line shape and other discriminators in order to produce quality spectra with good peak resolution and high peak to background values. Any disturbance, noise and or pile up that the processor identifies as a trigger event, even if recognized and rejected, is also an event. The ICR for the dead time and pile up correction is any signal that the processing method considers a signal. If the noise and noise pile ups are rejected then the sum of all the noise and all the event signals is the ICR. In real life it is even more complicated because there are not only noises present but also electronic disturbances. Therefore the signal suffered by the electronic disturbance is also part of the ICR although a good processor will usually reject it. Without the rejected spectrum it is a demanding task for the analyst to invent a method to justifiably estimate what part of the ICR is the x-ray event ICR. If the input rate counter represents the number of events that triggered the processor, both accepted and rejected, then the rejected spectrum allows the analyst to correct the ICR value to determine the number of real x-ray events that occurred during the measurements live time.

Conclusion

One job of a signal processor is to separate the noise, the noisy event, the event with electronic disturbances, the nuclear background, and the degraded events, from the clean event and to generate a good quality spectrum. For spectra of different origins, like radioisotope measurements, x-ray fluorescence, and particle induced x-ray emission, the primary signal from the preamplifier is so different, that the signal processor is facing very different challenges, and different metrological approaches are necessary in data processing.

This data processing methodology cannot be established on the partial and fractional information offered by other approaches. However, the maximum information utilization approach offered by our processor supplements the accepted spectrum with the rejected spectra of each discriminator and allows the development of a straightforward and accurate metrology. Having the extra information provided by the rejected spectra we were surprised to see how different conclusions and level of understandings are possible in detector characterization, detector efficiency, spectrum evaluation methodology, and how it explains many of the contradictions.

The magnitude of the observed Compton and nuclear background is highly dependent on the processor. Similarly the so called detector response function is significantly impacted by the signal processor. Studies that try to model this background by comparing model spectra to real spectra must be cautious as to the processor conditions with which the real spectra is collected. The interpretation of the spectra both the rejected and the accepted could be automated thus reducing the demand on the analyst, via offering quality assurance capability.

The CSX digital signal processor family with its great versatility and its ability to separate the events into good events and events that do not pass various inspection criteria is ideal for both high quality analytical and fundamental research measurements.

All of the control of the processor is digital, via the USB port, and therefore can be deployed in industrial settings for remote operation.

Many of the contradictions and discrepancies suggest that there would be benefits to using improved systems. Quality assurance is important at all levels of the measurement from sample preparation, to spectrum collection and analysis and data handling. Our CSX signal processor lines offer quality assurance at the signal processor level by providing additional information in the form of reporting all events sorted in accepted and rejected event spectra, the number of preamplifier resets, the number of x-ray energies outside of the selected energy range of the spectrum and the input rate.

Such an approach is beneficial in gamma ray spectroscopy as well, and has been developed for CdTe detectors at Cambridge Scientific. Specially should be mentioned it's immediate benefit for the determination of sum peak in and sum peak out count losses [15].

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