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Improving the resolution in soft X-ray emission spectrometers through photon-counting using an Electron Multiplying CCD

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Improving the resolution in soft X-ray emission spectrometers through photon-counting using an Electron Multiplying CCD

D.J. Hall,^{a,1} M. Soman,^a J. Tutt,^a N. Murray,^a A. Holland,^a T. Schmitt,^b J. Raabe,^b
V.N. Strocov^b and B. Schmitt^b

^a*e2v centre for electronic imaging, Planetary and Space Sciences Research Institute,
The Open University, Walton Hall, Milton Keynes, MK7 6AA, U.K.*

^b*Paul Scherrer Institut,
Villigen PSI, Switzerland*

E-mail: d.j.hall@open.ac.uk

ABSTRACT: In 2007, a study of back-illuminated Charge-Coupled Devices (CCDs) for soft X-ray photon detection demonstrated the improvements that could be brought over more traditional micro-channel plate detectors for X-ray spectrometers based on diffraction gratings and position sensitive detectors. Whilst the spatial resolution was reported to be improved dramatically, an intrinsic limit of approximately 25 micrometers was found due to the spreading of the charge cloud generated in the CCD across several pixels. To overcome this resolution limit, it is necessary to move away from the current integrated imaging methods and consider a photon-counting approach, recording the photon interaction locations to the sub-pixel level.

To make use of photon-counting techniques it is important that the individual events are separable. To maintain the throughput of the spectrometer for high intensity lines, higher frame rates and therefore higher readout speeds are required. With CCD based systems, the increased noise at high readout speeds can limit the photon-counting performance.

The Electron-Multiplying CCD shares a similar architecture with the standard CCD but incorporates a “gain register”. This novel addition allows controllable gain to be applied to the signal before the read noise is introduced, therefore allowing individual events to be resolved above the noise even at much higher readout rates.

In the past, the EM-CCD has only been available with imaging areas too small to be practical in soft X-ray emission spectrometers. The current drive for large area Electron-Multiplying CCDs

¹Corresponding author.

is opening this technology to new photon-counting applications, requiring in-depth analysis of the processes and techniques involved. Early results indicate that through the introduction of photon-counting techniques the resolution in such systems can be dramatically improved.

KEYWORDS: X-ray detectors; Spectrometers; Photon detectors for UV, visible and IR photons (solid-state) (PIN diodes, APDs, Si-PMTs, G-APDs, CCDs, EBCCDs, EMCCDs etc); Photon detectors for UV, visible and IR photons (solid-state)

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1 Introduction

The use of a Charge-Coupled Device (CCD) in an energy dispersive spectrometer is discussed with regards to the Super Advanced X-ray Spectrometer (SAXES) and Resonant Inelastic X-ray Scattering (RIXS) by Ghiringhelli et al. [1] with the improvements that the CCD offers over the more traditional micro-channel plate detectors detailed by Dinardo et al. [2]. The current SAXES set-up is limited by the dominant resolution component of the detector spatial resolution (that of the CCD), a common problem for all RIXS instruments currently in operation and under design. In RIXS, one of the main goals is to achieve a very high energy resolution.

This study aims to demonstrate the performance that could be possible if the CCD was to be replaced with an EM-CCD. An experimental study into the use of centroiding on soft X-ray images acquired using an EM-CCD feeds into simulations of the impact of these results on the SAXES instrument performance. With the current drive for larger area EM-CCDs, this technology, previously limited by small detector imaging areas, is opening up to new applications.

2 The super Advanced X-ray spectrometer

Soft X-rays (several hundred eV) are of great importance for resonant spectroscopy techniques, incorporating the absorption edges of many important elements (silicon, carbon, nitrogen, oxygen, *3d* transition metals and lanthanides). With the increasing availability of third generation synchrotron sources, there is a push for higher energy resolution in inelastic X-ray scattering spectroscopy [1]. At the Swiss Light Source (Paul Scherrer Institut, Switzerland), the ADvanced RESonant Spectroscopies (ADDRESS) beamline offers a high-performance soft X-ray undulator beamline, for 300 eV to 1.6 keV [3]. The beamline hosts two endstations: Angle-Resolved Photoelectron Emission (ARPES) and Resonant Inelastic X-ray Scattering (RIXS).

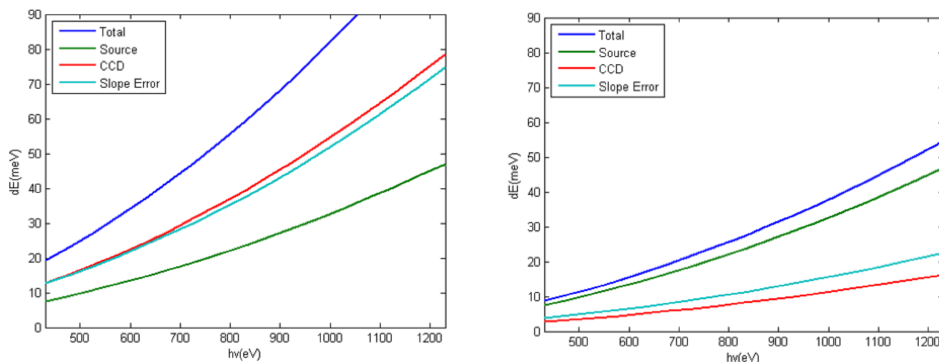


Figure 1. The spectrometer energy resolution is formed from a combination of the detector, photon source size and slope error. With the current system, the detector component dominates. *Left:* Present 3200 lines/mm grating and present CCD (slope error: $0.67 \mu\text{rad rms}$, CCD: $24 \mu\text{m}$). *Right:* Predicted response for an improved 3200 lines/mm grating and improved detector (slope error: $0.2 \mu\text{rad rms}$, detector: $5 \mu\text{m}$) [3].

Resonant Inelastic X-ray Scattering (RIXS) is a “photon-in photon-out” X-ray spectroscopy technique, designed to probe the electronic structure of molecules and materials. The Super Advanced X-ray Emission Spectrometer (SAXES), an evolution of the Advanced X-ray Emission Spectrometer (AXES), is a high resolution instrument installed on the ADDRESS beamline and designed for RIXS [1, 4, 5]. The main components of SAXES include a slit, mask, Variable Line Spacing (VLS) grating and CCD.

The grating disperses the emitted photons by energy, producing a spread of photons across the CCD where the spatial position of the photon detection is directly related to the energy of the photons. In this way the energy resolution of the spectrometer is directly related to the spatial resolution achieved with the CCD camera.

The energy resolution of the SAXES system is built, with the optical aberrations reduced to negligible due to the VLS grating parameters, from several main components, namely the detector, the photon spot size on the sample (source size) and the grating slope error, figure 1 (left). The component of the energy resolution from the detector in the current arrangement accounts for approximately 50% of the uncertainty in the energy measurements. The spatial resolution of the CCD camera is currently the limiting factor on the energy resolution of SAXES. This problem is common for all RIXS instruments currently operating and under design. If the component of the energy resolution due to the detector is reduced through an improvement of the spatial resolution to $5 \mu\text{m}$, the slope error from the grating becomes the dominant factor in the resolution. If an improved grating was installed along with a detector capable of a $5 \mu\text{m}$ spatial resolution, the energy resolution could be improved by a factor of two, figure 1 (right). In the experimental part of this study, the suitability of the EM-CCD detector to bringing this improvement is investigated.

3 Charge spreading in a Charge Coupled Device (CCD)

When an X-ray interacts in the silicon of a CCD, a large number of electron-hole pairs are created: one electron-hole pair for approximately every 3.65 eV of energy deposited by the incident X-

ray. There are three basic layers in a back-illuminated CCD: the electrode structure, the depletion region and the field-free region. Under back-illumination, X-rays are incident on the field-free region of silicon. For soft X-rays, the absorption length is typically short compared to the depth of the field-free region; charge when generated does not experience a field and will “migrate slowly by diffusion” [6]. The charge cloud expansion leads to the spreading of the signal across multiple pixels, leaving a wider spatial FWHM and degrading the spectral performance [6].

Although high resistivity devices allow deeper (or full) depletion, thus minimising the field-free region and reducing the spreading to provide a higher proportion of single pixel events [7], if one wishes to improve the FWHM of the PSF beyond the limit of the pixel dimensions, the spreading of the charge can be used as an advantage. With the charge spread across multiple pixels, centroiding algorithms can be used to improve the spatial resolution to the sub-pixel level. Measurements carried out in [1, 2] suggest a PSF of the charge clouds with FWHM of 24 μm and 25-28 μm respectively.

4 Current imaging system

The CCD currently implemented in SAXES is a Princeton Instruments Digital Spectroscopy System, comprising of a liquid nitrogen cooled e2v CCD42-40 camera head [8]. The e2v CCD42-40 is a 13.5 μm pixel device, with an imaging area of 27.6 \times 27.6 mm (2048 \times 2048 pixels). The CCD has a typical read noise of 5-6 electrons rms at 100 kHz (varying with readout system). The readout system comprises of a dual speed controller, offering 16-bit readout at 1 MHz and 100 kHz.

The system is currently operated at 100 kHz for low noise readout (quoted: 3.48 e^- rms, total measured: 4.7 e^- rms). Reading out the full device takes 42 seconds; 5-10 minutes are required for sufficient data to be integrated to generate a spectrum. Pile-up of events, figure 2, prevents the use of a single 5-10 minute frame with centroiding techniques. To avoid decreasing the throughput of the spectrometer, a higher readout rate is required and to this end, the system can be operated at 1 MHz (full-frame readout in 4.2 seconds). The noise specification at 1 MHz is quoted at 10.8 electrons rms, although interference (banding) offers a minimum noise of 14 electrons rms (18 electrons rms across the whole device). At 10.8 electrons rms, the signal in the pixels surrounding the central pixel is lost below the read noise and centroiding is not possible. To enable centroiding, the readout speed must be sufficiently high whilst maintaining a sufficiently low noise level.

5 The electron multiplying CCD

The Electron Multiplying CCD (EM-CCD) was developed following experiments in the mid 1990s at e2v technologies to show that a process called “impact ionisation” could be used to provide a controllable gain process [9]. The high signal-to-noise ratio provided by the detectors allows detection of low level signals that would otherwise be lost in the read noise of the standard CCD. The probability of impact ionisation occurring increases as the strength of the electric field increases (as the applied voltage is increased). The signal is multiplied before the read noise is added, effectively allowing the reduction in read noise to the sub-electron level in comparison to the signal level [10].

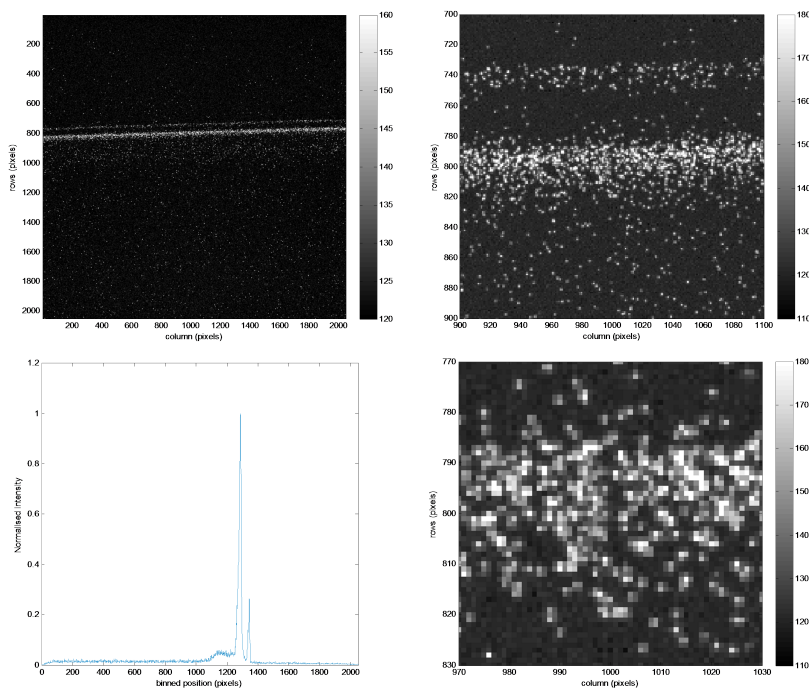


Figure 2. Example image taken on SAXES at 710 eV with readout set to 100 kHz. *Top left:* Full image. *Right:* Enlarged regions. The individual photon interactions in the CCD are seen to overlap, hence centroiding algorithms cannot be used efficiently whilst maintaining the same integration to readout time ratio. *Bottom left:* Spectrum taken from the summation of the signal across the energy spread direction (a few degrees from vertical). Pixel positions are inverted from the row numbers shown (top left)

Through the application of a “high” voltage to a series of gates in the readout register of the EM-CCD (nominally 40-50 V), a high electric field is created between adjacent electrodes. When an electron encounters the region of high-field it is accelerated and gains kinetic energy such that it effectively “slams” into the silicon crystal lattice. If the field is sufficiently high, then the collision can break the silicon-silicon covalent bonds, resulting in “impact ionisation” [11].

Due to the stochastic nature of the gain process, each signal charge packet will not undergo exactly the same level of gain. The noise introduced by the gain process is detailed in [12] for the optical case and in [13] for the detection of X-rays. In the case of dispersive instruments, the multiplication noise only affects the centroiding accuracy. Without the decrease in effective read noise through the use of multiplication gain it would not be possible to use centroiding.

Using the characteristics of data obtained from the experimental testing described below, simulations have been used to demonstrate the impact of the noise sources for spatially dispersed soft X-ray spectrometers, figure 3. With low read noise, events can easily be extracted from the background in both the CCD and EM-CCD. As the read noise increases, representative of increasing the readout speed, the events become lost in the background fluctuations and the gain from the EM-CCD becomes a necessity. One needs to be able to extract events from the noise floor, whilst the signal levels in the wings of the event profiles (determining the calculated centroid position) must not be lost within the noise floor. The increase in noise level not only affects the signal in

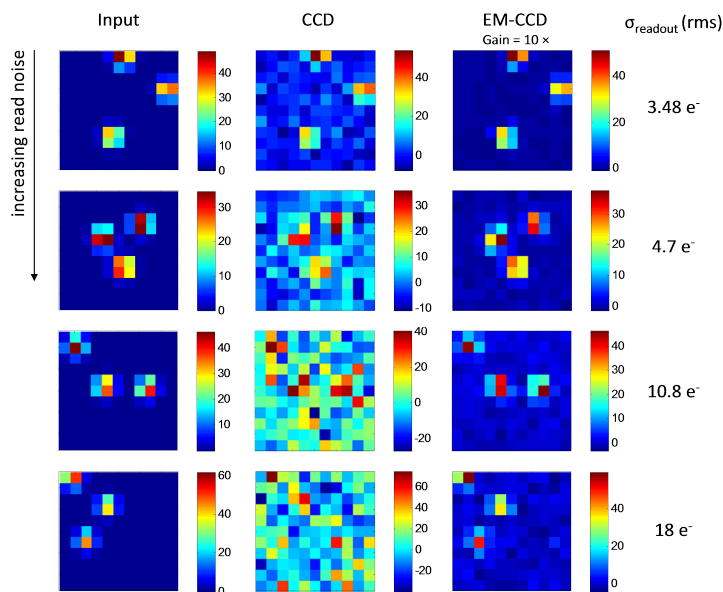


Figure 3. Example input images at 400 eV show random interaction positions using a profile based on experimental results, simulated for a gain of 10 (EM-CCD). Shot noise, noise on signal splitting, read noise and multiplication noise are included. From top to bottom: 100 kHz quoted read noise, measured noise, 1 MHz quoted read noise, measured noise. As read noise increases, events become harder to distinguish from background fluctuations (even with knowledge of their location); additional “events” may be attributed to spurious areas of higher signal. Taking the $18 e^-$ noise case for the CCD, with knowledge of where the events “should” be, one can process at the event locations. However, in reality the event positions are unknown and there are several positions (for example, two in the final row of the image) indistinguishable from the real events. These events are not “real” and are simply a consequence of the read noise.

X-ray interaction events recorded by the CCD, but can lead to the “detection” of areas of higher signal caused by the noise and not by an X-ray interaction.

6 Improving the spatial resolution

The experiments detailed in this study were performed on the PolLux beamline at the Swiss Light Source, PSI, Villigen, Switzerland. Whilst the PolLux beamline was designed for Scanning Transmission X-ray Microscopy [14], the highly focussed (20 nm diameter) soft X-ray beam can be used to investigate the suitability of the e2v CCD97 [15] to the case of improving the energy resolution of energy dispersive X-ray spectrometers. Using a customised detector set-up to interface the detector with the mechanics of the beamline, a focussed beam (less than 100 nm in diameter) was scanned across the $16 \mu\text{m}$ pixel structure of a back-illuminated CCD97, figure 4.

An oversampled PSF of the event profile was obtained experimentally through the addition of photon events across the pixel, offering a representative illustration of the charge cloud size for the 1 keV photons interacting near the back surface of the CCD97, figure 5. The resulting PSF has a

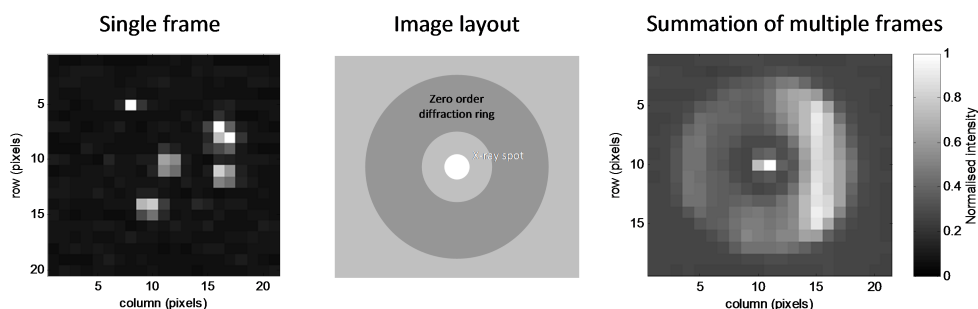


Figure 4. Single images (left) have a 37% chance of containing a single event in the central pixel (middle). Multiple images can be combined to provide an integrated image (right), showing clearly the diffraction ring. The standard methods for the removal of the diffraction ring could not be used with the EM-CCD in the standard ceramic package. Frames in which X-ray interactions from the diffraction ring interfere with the central “spot” are removed before processing.

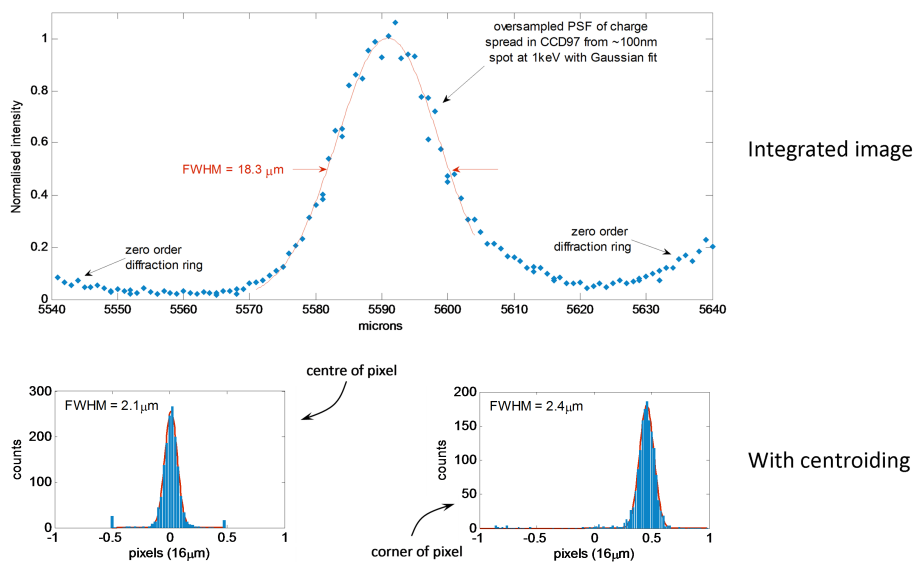


Figure 5. *Top:* The cloud size from this analysis follows a Gaussian profile with FWHM of 18.3 μm , the spatial resolution limit under integration. *Bottom:* The results from a simple centroid algorithm for two extreme positions in the pixel (*left:* centre of pixel and *right:* corner of pixel), with an average FWHM of 2.3 μm . Centroiding cannot be applied to readout at 100 kHz with the current system whilst maintaining the spectrometer throughput. At 1 MHz, the read noise of the current system is too high for the use of centroiding and an EM-CCD must be used to provide this dramatic improvement in resolution.

FWHM of 18.3 μm . Without the use of centroiding, this PSF represents the intrinsic limit on the spatial resolution of the device and therefore implies the current limit on the energy resolution.

Using a centroid algorithm, the centre of the events can be found to sub-pixel level and the effective FWHM of the detector dramatically reduced beyond the limit introduced by the charge

spreading as detailed above. With a simple algorithm for demonstration purposes, based on the “centre of gravity” approximation, the same events as used to generate the charge spreading PSF have been analysed. Taking two extreme examples (the centre of a pixel and the corner of a pixel), the centroid location was calculated across multiple events from the same spatial position. The variation in the calculated values represents the new PSF of the detector when using centroid techniques, figure 5, albeit here for a simple method only. The FWHM for the x and y directions show minimal differences (approximately 10%) and are within the measurement errors. In the centre of the pixel, the performance is slightly better, offering a FWHM of 2.1 μm . In the corner of the pixel, with the signal split such that each pixel contains a lower number of electrons, the FWHM has been calculated at 2.4 μm . It is expected that further significant improvements can be made in the values given through future calibration and optimisation of the centroid algorithms.

The component of the energy resolution from the current detector at 931 eV accounts for approximately 50% of the total energy resolution (see figure 1) [3]. With an improvement in the spatial resolution of the detector from 24 μm to below 5 μm , shown experimentally here to be possible using an EM-CCD, coupled with an improved grating, the energy resolution of the system could be improved by over a factor of two, figure 1 (right).

7 Conclusions

The resolution of a dispersive instrument for X-ray spectroscopy can be dramatically improved through the use of centroiding on the X-ray induced charge packets that are spread over a group of pixels in the CCD to provide sub-pixel positional information and remove the effective resolution limit defined by the charge spreading. In order to maintain the instrument throughput the readout rate of the CCD must be increased, causing an increase in read noise that must be overcome. The Electron-Multiplying CCD offers an alternative to the standard CCD and allows an effective read noise at the sub-electron level even at high frame-rates.

Through the use of an EM-CCD, our analysis has demonstrated that centroiding can be used to improve the spatial resolution FWHM by over one order of magnitude from 25 μm to 2.1-2.4 μm for 1 keV photons in soft X-ray spectrometers. Further study is required to investigate centroid algorithms for the optimal method and therefore the best spatial resolution. If the sum of the spatial components of the resolution can be reduced to below 5 μm then it has been predicted that the energy resolution could be reduced to 40 meV and below for 930 eV photons for the SAXES system currently installed at the ADDRESS beamline of the SLS. If such a system upgrade were to be implemented, the system would then be limited by the grating slope errors and photon spot size. For the implementation of a detector upgrade to make use of the improved performance of the EM-CCD as the availability of larger area devices increases, a balance in readout speed, detector area and incident flux must be achieved to avoid detrimental effects to the beamline throughput.

Acknowledgments

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and Politecnico di Milano, Italy, alongside experiments performed on the PolLux beamline at the Swiss Light Source, PSI, Villigen, Switzerland.

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