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Version: Version of Record

Link(s) to article on publisher’s website:
http://dx.doi.org/doi:10.1088/1748-0221/8/01/C01046
http://stacks.iop.org/1748-0221/8/i=01/a=C01046

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2013 JINST 8 C01046
(http://iopscience.iop.org/1748-0221/8/01/C01046)

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Abstract: The Super Advanced X-ray Emission Spectrometer (SAXES) is an instrument at the Swiss Light Source designed for Resonant Inelastic X-ray Scattering with an energy resolution \((E/\Delta E)\) better than 12000 at 930 eV. Improvements to the instrument have been predicted that could allow the energy resolution to be improved by a factor of two. To achieve this, the spatial resolution of the detector (currently a Charge-Coupled Device, CCD) over which the energy spectrum is dispersed would have to be improved to better than 5 \(\mu\)m.

X-ray photons with energies between a few hundred to a few thousand electron volts primarily interact within the field-free region of back-illuminated CCDs, where each photon forms an electron cloud that diffuses isotropically before reaching the depleted region close to the electrodes. Each photon’s electron cloud is likely to be detected as an event with signal split across multiple pixels. Analysing these split events using centroiding techniques allows the photon’s interaction position to be determined to a sub-pixel level.

PolLux is a soft X-ray microspectroscopy endstation at the Swiss Light Source that can focus 200 eV to 1200 eV X-rays to a spot size of approximately 20 nm. Previous studies using data taken with a linear scan across the centre of a pixel in 3 \(\mu\)m steps predicted an improved resolution by applying centroiding techniques and using an Electron-Multiplying CCD (EM-CCD). In this study, a full 2D map of the centroiding accuracy in the pixel is presented, formed by rastering in two dimensions across the image plane in single micron steps. The improved spatial resolution from centroiding events in the EM-CCD in all areas of the pixel over the standard CCD is attributed to the improved signal to noise ratio provided by the multiplication register even at high pixel readout speeds (tens of MHz).

Keywords: X-ray detectors; Spectrometers; Solid state detectors; Data processing methods

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doi:10.1088/1748-0221/8/01/C01046
1 Improving the Super Advanced X-ray Emission Specrometer

The Super Advanced X-ray Emission Spectrometer (SAXES) [1] is a soft X-ray emission grating spectrometer that disperses the energy spectrum across the surface of a Charge Coupled Device (CCD). The energy resolution of the spectrometer is therefore dependent upon the spatial resolution of the detector. Initial studies by Dinardo et al. [2] verified the advantages of thinned back-illuminated CCDs over microchannel plates, showing factors of improvement of greater than 3 in spatial resolution and approximately 40 in quantum efficiency. Following this study SAXES was built to use a thinned back-illuminated CCD42-40 from e2v technologies plc. [3], operated in a charge pile-up mode with a spatial resolution dominated by the electron cloud size formed from the X-ray interactions in the device. Ghiringhelli et al. [1] measured the Full Width Half Maximum (FWHM) of the electron cloud size in the current setup to be approximately 24 µm at 930 eV in both row-wise and column-wise dimensions. A preliminary study [4] has shown that the overall spectrometer energy resolution can be improved by a factor of 2 by developing the spatial resolution of the detector to be better than 5 µm (FWHM) together with upgrading the grating.

Previous work [5] has achieved a spatial resolution better than 5 µm for 530 eV to 1000 eV energy X-rays with an e2v technologies plc. thinned back-illuminated CCD42-10 [6]. The device has 13.5 µm square pixels and was operated at a 60 kHz pixel readout rate, resulting in a total background noise of approximately 6 electrons rms. The CCD42-40 currently operating in SAXES has the same pixel structure and is operating with a similar total noise performance at 100 kHz pixel rate. Although the results meet the requirement for the SAXES upgrade of better than 5 µm spatial resolution, they were achieved at a slow read-out rate to minimise the read noise: a dramatic decrease in spectrometer throughput would be required to implement centroiding at the current readout speed and photon flux at SAXES (reducing the number of photons recorded by a factor of approximately 2.2).

In a conventional CCD, readout noise is added during the conversion of signal from the charge to voltage (and then to digital) domains. The readout noise increases as the readout rate is increased, causing signals just visible above the noise floor at low readout rates to be lost in the noise at higher readout rates. Electron-Multiplying CCDs (EM-CCDs) have an additional register that can multiply signal in the charge domain by accelerating electrons through a potential difference in
the order of 20 V to 50 V. When operated at high gain, EM-CCDs increase the electron signal to which the readout noise floor is applied, effectively reducing the level of readout noise. Effective readout noise levels can be reduced below 1 electron rms, even when operated at high readout rates. However, the stochastic nature of the avalanche gain process contributes noise to the signal which can outweigh the benefits in certain applications [7].

The preliminary study [4] proposed that an EM-CCD could replace the CCD42-40 currently used in SAXES: spatial resolutions better than 5 µm could be achieved with an EM-CCD at high readout rates by photon counting and centroiding, using the multiplication gain to effectively reduce the readout noise, without reducing the spectrometer throughput. Initial tests focussed 1000 eV X-rays into the corner and centre of an EM-CCD’s pixel, with the device operated between $-30^\circ$C to $-10^\circ$C with an effective background noise of 1.9±0.1 electrons rms (read noise, stray light and dark current). Here, a full two dimensional map of the spatial resolution across an EM-CCD’s pixel is presented for both 850 eV and 1000 eV energy photons, with the device operating at sub-electron effective readout noise levels.

2 Centroiding a soft X-ray “spot”

The PolLux spectromicroscope [8] at the Swiss Light Source, Paul Scherrer Institute, is capable of focussing monochromatic soft X-rays to a minimum spot size of 20 nm with a Fresnel Zone Plate (FZP) arrangement. The standard sample holder mounted on three translational stages can be replaced by a CCD, allowing the X-ray spot to be rastered in two dimensions in the plane of the detector surface. Focussing can be achieved by translating normal to the surface, as shown in figure 1.
Figure 2. Left: A single 1000 eV photon is seen in the central focussed spot of an image (row 7, column 8), with signal from other 1000 eV X-ray interaction events visible in the other regions of the image. Right: The average of pixels’ signals across all images captured at 1000 eV shows the distribution of X-rays across the device. The X-rays focussed from the 1st order FZP diffraction ring are detected in the central spot and contribute signal mainly confined within a 3 × 3 pixel region. X-rays from the 0th order FZP diffraction ring are detected in the surrounding pixels with an overall distribution given by the optics of the beamline before the FZP.

The focal distance can be estimated by maximising of the proportion of signal appearing in a single pixel in the centre of the focussed spot. More accurate focussing can be achieved by determining the focal distance at which the oversampled average X-ray event has a minimum width, and therefore has a minimum contribution from the width of the focussed spot. The occurrence of images captured containing a single photon interaction in the central focussed spot can be maximised (limited by Poisson statistics to a maximum of 36.8%) by adjusting both the entrance slits to the spectromicroscope and the integration time of the CCD.

The CCD97 used in this work is a thinned back-illuminated device from e2v technologies plc. with 16 µm square pixels [9]. In this experimental work it was operated at a total background noise between 0.35 and 0.6 electrons rms, with stray light from the chamber’s translational stage interferometers being the major component of this noise. The system was first focussed from its arbitrary initial distance between the CCD and FZP using 1000 eV photons. At this energy, the spot was rastered across an 18 × 18 grid (1 µm steps), capturing 2000 images at each position before the focus was automatically tracked to collect an identical data set with 850 eV photons. A typical image containing a single 1000 eV photon in the central focussed spot and the average 1000 eV image collected are shown in figure 2.

3 Results with an electron multiplying CCD

The images in the data sets have been sorted to identify those with single photon interactions in the focussed spot and discard images with photons detected in pixels close to the focussed spot (whose signal may split into the pixels of the central focussed spot). The average number of images kept at each grid position was 255 and 345 images for 850 eV and 1000 eV photons respectively. Single photon events in the focussed spot are centroided over a 3 × 3 pixel area using the following Centre
of Mass’ (COM) algorithm, equation (3.1), where $\text{row}_{\text{COM}}$ is the centroid location (along the row), $\text{row}_i$ is the location of the $i^{th}$ pixel along the row and $S_i$ is the signal.

$$
\text{row}_{\text{COM}} = \frac{\sum_{3 \times 3} \text{row}_i S_i}{\sum_{3 \times 3} S_i}
$$

(3.1)

The sums are over all nine pixels in the $3 \times 3$ pixel area, which is centred on the pixel with maximum signal. A similar equation is used to determine the centroid location along the column, $\text{col}_{\text{COM}}$. At each grid position the centroid locations were binned in both the row and column dimensions and fitted by a Gaussian profile using ROOT [10]. The centre of the Gaussian profile for a distribution of $\text{row}_{\text{COM}}$ values determines the mean row-wise centroid location and FWHM determines the row-wise spatial resolution (similarly a Gaussian profile fit of a distribution of $\text{col}_{\text{COM}}$ positions determines the column-wise attributes). All the spatial resolution measurements presented here include an unknown contribution from the focussed X-ray beam width (between 0.02 $\mu$m and the spatial resolution measurement).

The row-wise spatial resolutions, obtained by centroiding 850 eV photon interaction events at each grid position, are plotted as a function of their location within the pixel (figure 3 (a)). The best resolution ($1.35 \pm 0.06 \mu$m) is achieved near the centre of the pixel, and the worst spatial resolution is measured at the edge ($2.85 \pm 0.16 \mu$m). However, the row-wise spatial resolution is constant (within the noise) as the position of the focussed spot is shifted up the pixel in the column-wise direction. The column-wise spatial resolution for 850 eV photons (figure 3 (c)) varies across a similar range, but the pattern across the pixel is orientated in the column-wise direction. The spatial resolutions achieved with 1000 eV photons (figure 3 (b) and 3 (d)) are similar. The observed pattern is due to the centroid location being biased towards the centre of the pixel by the COM algorithm, reducing the width of the centroid location distribution at the centre of a pixel. When interactions occur at the edge of a pixel, the location of the pixel with maximum signal (around which the $3 \times 3$ pixel centroiding area is centred) is most sensitive to the noise, broadening the distribution of centroid locations.

Each photon’s centroid location has been offset by the average position of the X-ray spot to construct the Point Spread Function (PSF) histograms shown for 850 eV and 1000 eV energy photons (figure 3 (e) and 3 (f)). A two dimensional Gaussian profile has been fitted to the PSFs, measuring the FWHM of the 850 eV (1000 eV) PSF at 2.21 $\mu$m and 2.03 $\mu$m (2.22 $\mu$m and 2.01 $\mu$m) in the column-wise and row-wise directions respectively. It should be noted that the PSFs are an average of the spatial resolutions at the $18 \times 18$ grid positions sampled within the pixel rather than a geometric average across the pixel, and that the PSFs contain contributions from the spatial resolution, X-ray spot width, and the error in the X-ray spot locations.

4 Conclusions

An X-ray spot has been focussed at 324 positions across the pixel of an electron multiplying CCD97. The COM algorithm has been applied to centroid interaction events from single 850 eV and 1000 eV photons, resulting in a spatial resolution map across the pixel for both energies and a PSF averaged across the sub-pixel locations that were sampled (figure 3). The widths of the 850 eV and 1000 eV PSFs were similar and the spatial resolution achieved was better in the column-wise
Figure 3. The spatial resolution is sampled at 324 positions across the 16 \( \mu\m\) square pixel at two X-ray energies. The positions deviate from the assigned 18\( \times \)18 grid due to inaccuracies in the translational stage movement, systematic errors in the centroiding algorithm (‘edge effects’) and errors in the fit parameter (maximum of \( \pm0.11 \mu\m\)). The resolution in the row-wise (a) and column-wise (c) directions is shown for 850 eV photons and in the row-wise (b) and column-wise (d) directions for 1000 eV photons. The 2D Gaussian-like PSFs for 850 eV (e) and 1000 eV (f) energy photons are constructed using the centroid locations obtained at the 324 sub-pixel positions.
direction \((2.0 \mu m \text{ FWHM})\) than the row-wise direction \((2.2 \mu m \text{ FWHM})\). Further work is required to explain the different spatial resolutions in the two directions, but it is believed to be an effect of the non-uniform distribution of grid positions across the pixel. There are significantly more grid locations with a bad column-wise resolution than positions with a bad row-wise resolution (comparing figure 3 (a) to 3 (c) and figure 3 (b) to 3 (d)). Alternatively, the asymmetry could be due to the linear polarization of the X-rays, or asymmetric charge collection of electron clouds produced in the field free region, due to the pixel structure. ‘Edge effects’, where centroid locations are biased towards the centre of the pixel by the linear centroid algorithm, have been observed in the map of the 2D spatial resolution across the pixel at both energies.

The results presented here demonstrate that the spatial resolution achievable with the electron multiplying CCD97 is better than the CCD42-10 measurements of 3.7 \(\mu m\) and 3.0 \(\mu m\) (FWHM) at 850 eV and 1000 eV respectively [5]. The improved performance is due to the gain register of the CCD97 allowing the effective readout noise to be reduced to the sub-electron level. The Electron Multiplying feature allows a faster readout rate whilst maintaining a low effective readout noise allowing the device to be operated in a photon counting mode without reducing spectrometer throughput.

Data sets collected with 530 eV and 680 eV photons are undergoing analysis to determine if the spatial resolution is better than 5 \(\mu m\) across the energy range required for SAXES. Correction algorithms to reduce the systematic biasing of centroid locations towards the centre of the pixel are under development and initial results have indicated that the overall spatial resolution remains significantly below 5 \(\mu m\) across the pixel of an electron multiplying CCD97.

Acknowledgments

With thanks to e2v technologies plc. for providing the CCDs used in the experimental work and Benjamin Watts for his help during PolLux experimental campaigns. This work was performed using the PolLux instrument at the Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland. The SAXES instrument at the ADRESS beamline was jointly built by Paul Scherrer Institut, Switzerland and Politecnico di Milano, Italy.

References


See also [http://root.cern.ch/](http://root.cern.ch/).