Developing a CCD camera with high spatial resolution for RIXS in the soft X-ray range

Matthew Soman

A brief outline

- What is Resonant Inelastic X-ray Scattering (RIXS), why is it useful, and how can the performance of a RIXS spectrometer be improved?

- Background and results of experimental work investigating a linear centroiding algorithm

- Initial results from investigating non-linear centroiding algorithms

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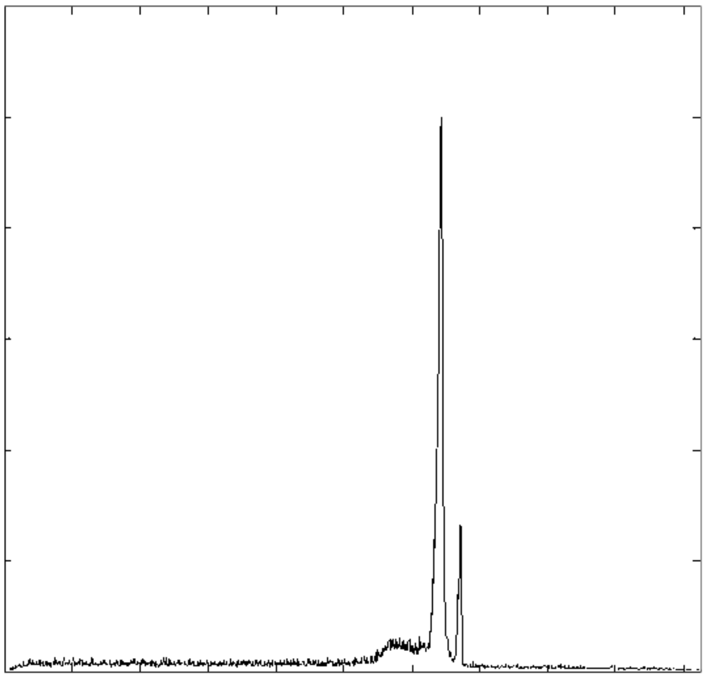
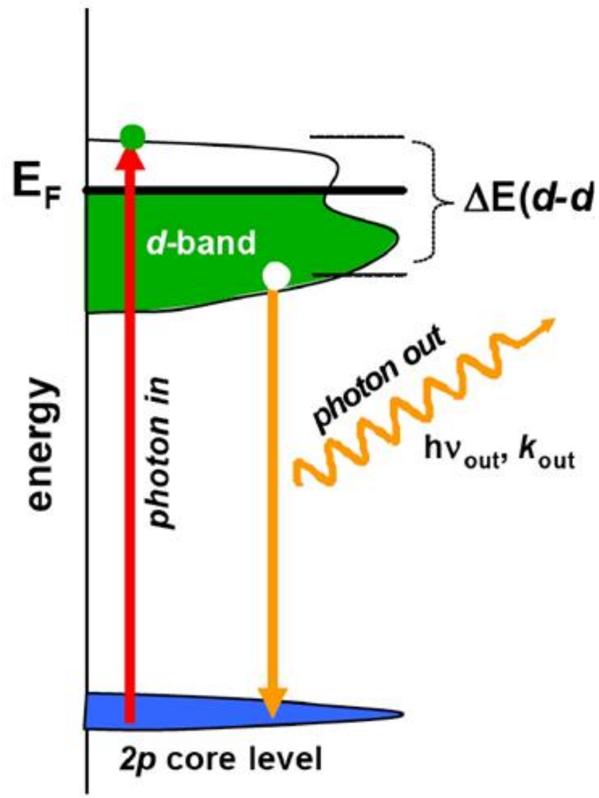
Resonant Inelastic X-ray Scattering

Measure spectrum and momentum change of photons scattered by a sample



Sample RIXS spectrum, from D.J. Hall (2012)



Example RIXS scattering for a 3d metal, from Moncton (2005).

Why is RIXS useful?

Nature 485, 82–85 (03 May 2012)

LETTER

doi:10.1038/nature10974

Spin–orbital separation in the quasi-one-dimensional Mott insulator Sr_2CuO_3

J. Schlappa[1,2], K. Wohlfeld[3], K. J. Zhou[1]†, M. Mourigal[4], M. W. Haverkort[5], V. N. Strocov[1], L. Hozoi[3], C. Monney[1], S. Nishimoto[3], S. Singh[6]†, A. Revcolevschi[6], J.-S. Caux[7], L. Patthey[1,8], H. M. Rønnow[4], J. van den Brink[3] & T. Schmitt[1]

When viewed as an elementary particle, the electron has spin and charge. When binding to the atomic nucleus, it also acquires an angular momentum quantum number corresponding to the quantized atomic orbital it occupies. Even if electrons in solids form bands and delocalize from the nuclei, in Mott insulators they retain their three fundamental quantum numbers: spin, charge and orbital[1]. The hallmark of one-dimensional physics is a breaking up of the elementary electron into its separate degrees of freedom[2]. The separation of the electron into independent quasi-particles that carry either spin (spinons) or charge (holons) was

separate itself completely from the holon. When instead of creating a hole, as typically is done in a photoemission experiment, an electron is excited from one copper 3*d* orbital to another, the phenomenon of spin–orbital separation can in principle occur (Fig. 1a). The orbiton created in this manner may also deconfine after exciting a spinon, thus splitting the electron into its orbital and spin degrees of freedom[8].

Here we use high-resolution resonant inelastic X-ray scattering (RIXS) to search experimentally for spin–orbital separation in the quasi-1D copper oxide Sr_2CuO_3 (for material details, see Supplementary Information, section 1). We observe deconfinement of the spinon

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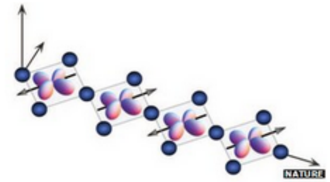
Electron 'split-personality' seen in new quasi-particle

Researchers have discovered another way that electrons - one of the Universe's few fundamental particles - can undergo an "identity crisis".



The structure of the material permits careful study of electrons as they only have one way to move in it

Electrons can divide into "quasi-particles", in which their fundamental properties can split up and move around like independent particles.

Two such quasi-particles had been seen before, but a team reporting in Nature has now confirmed a third: the orbiton.

These orbitons carry the energy of an electron's orbit around a nucleus.

Generally, these properties are not independent - a given electron has that set of properties, maintaining them as it moves around, while a nearby electron has a different set.

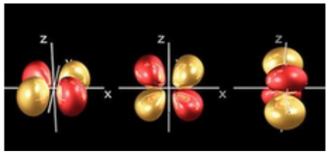
But the idea of quasi-particles allow these properties to split and move around independently, granting them to nearby electrons.

An analogy of this slippery idea is a traffic jam on a one-lane road - it is as if one blue car, pointed west and running at 1,000 RPM, passes on its blueness, its engine speed and its direction to adjacent cars.

The cases in which such strange behaviour can be induced are rare, but an international team of researchers turned to a material called strontium cuprate to investigate it.

The arrangement of atoms in the material is much like the one-lane road: electrons can only move in one direction along it in what is called a spin chain.

The team used the Swiss Light Source at the Paul Scherrer Institut in Switzerland to shine intense X-ray beams into the material, catching



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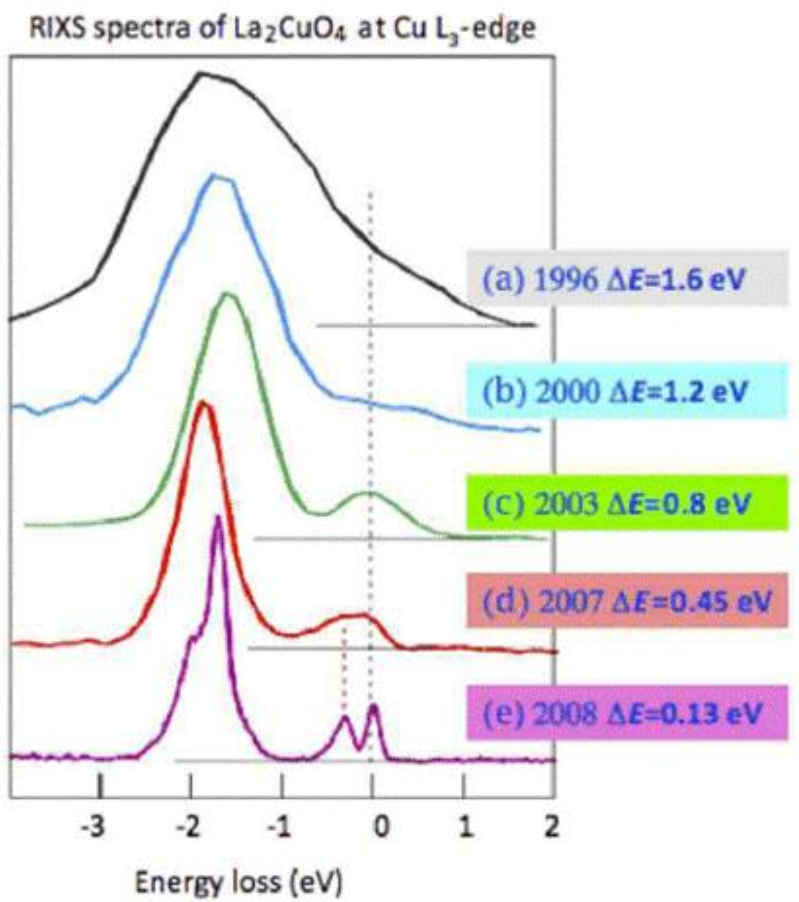
Past energy resolution improvement



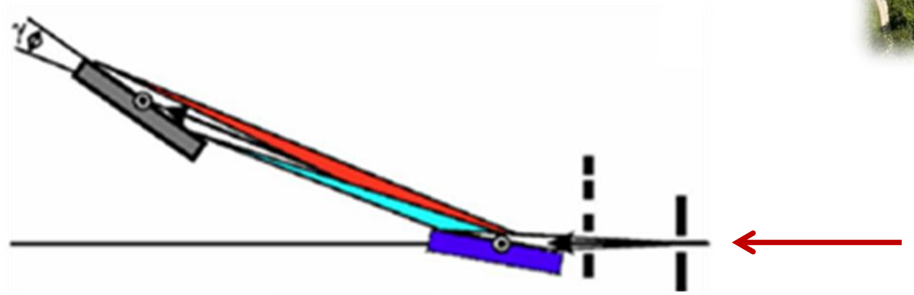
RIXS spectra improvement, from G. Ghiringhelli and L. Braicovich

Improvements in the resolution of spectrometers used for RIXS have allowed smaller spectral features to be resolved in the past 15 years.

The experimental results included in the example publication in Nature (previous slide) were taken with an energy resolution of 0.14 eV at SAXES.

SAXES: spectrometer at the SLS

A dispersive spectrometer at the Swiss Light Source, Paul Scherrer Institute



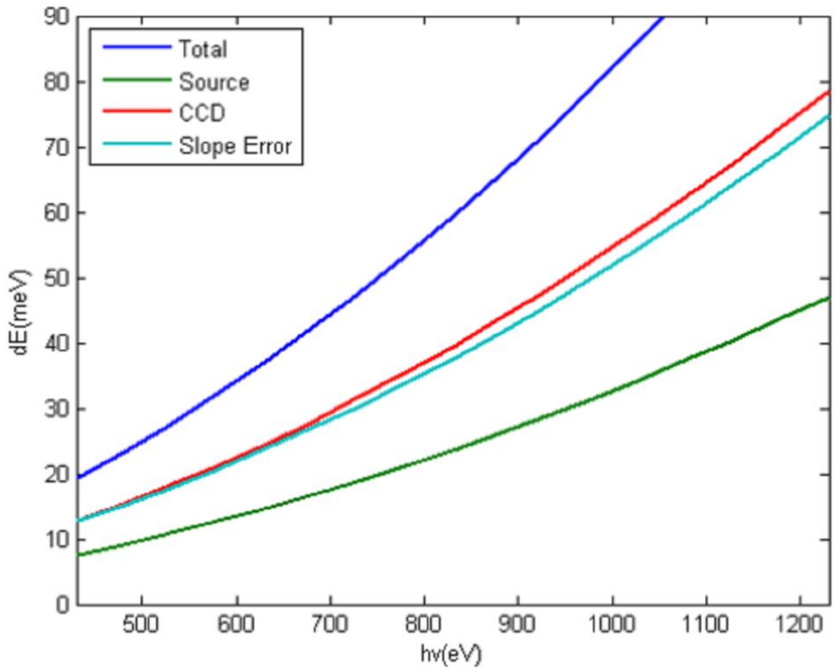
Detector: a CCD

Grating

X-rays scattered from sample (400 to 1600 eV)

G. Ghiringhelli *et al.* (2006)

SAXES: current energy resolution



Current setup:

3200 lines/mm grating

Present CCD (24 µm)

Slope error of 0.67 µrad rms

Simulation by V. Strocov

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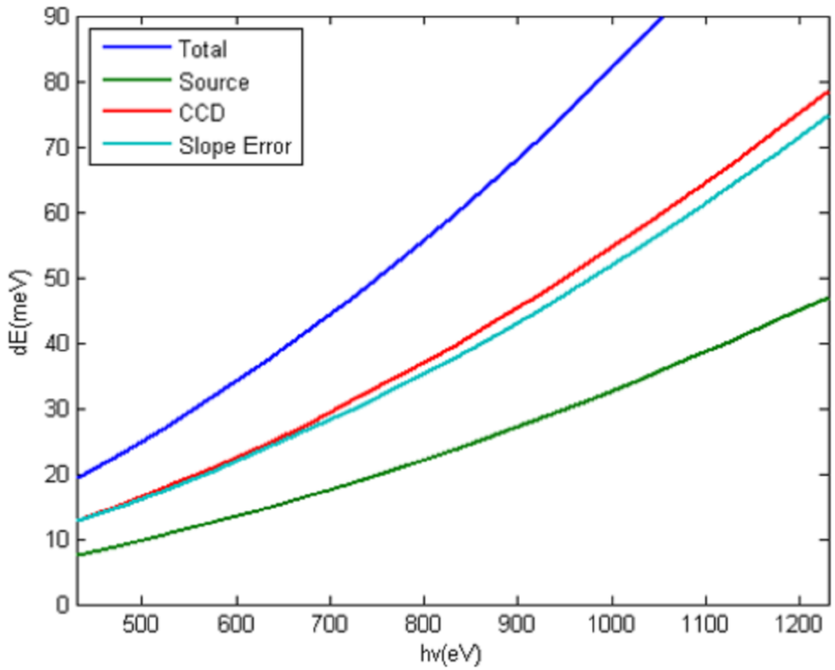
SAXES: potential energy resolution



Current setup:

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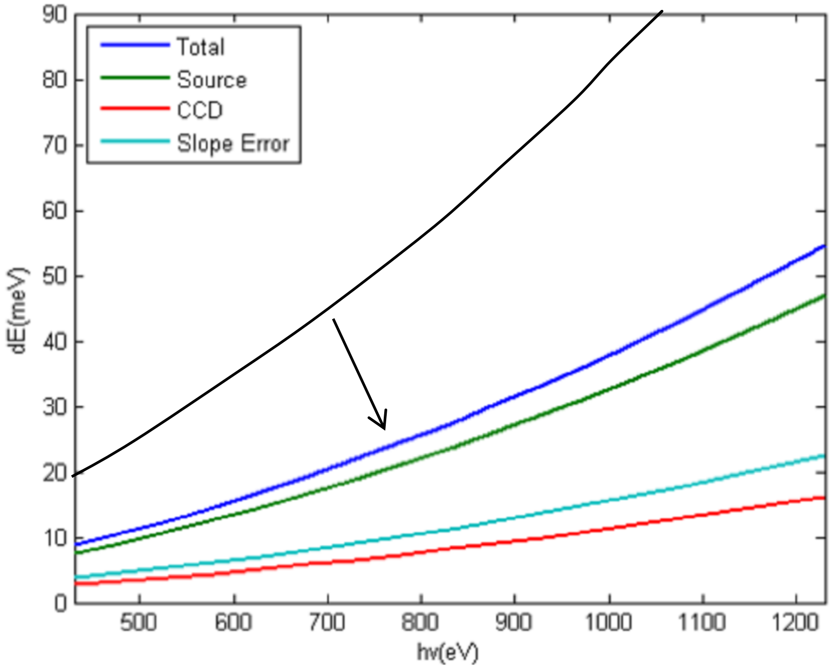

Predicted response from upgraded setup:

Improved 3200 lines/mm grating

Improved detector (5 µm)

Slope error of 0.2 µrad rms

Simulation by V. Strocov

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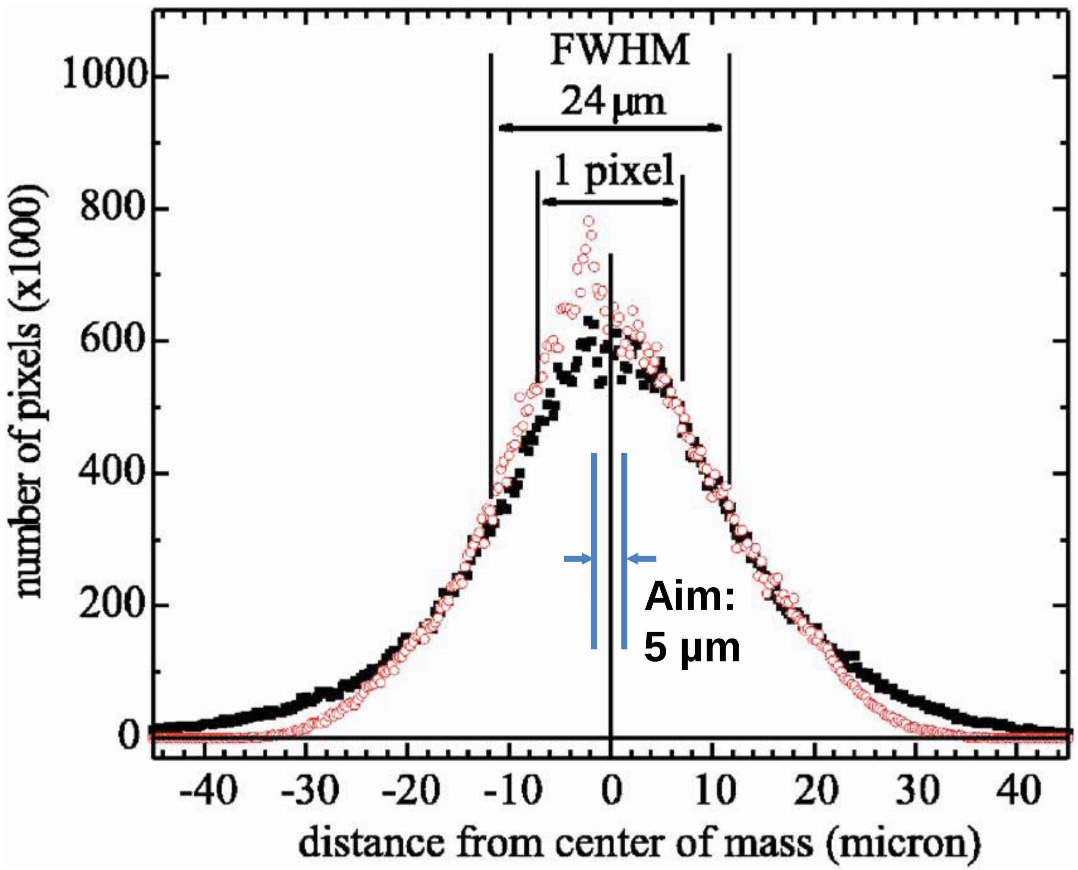
SAXES: detector spatial resolution

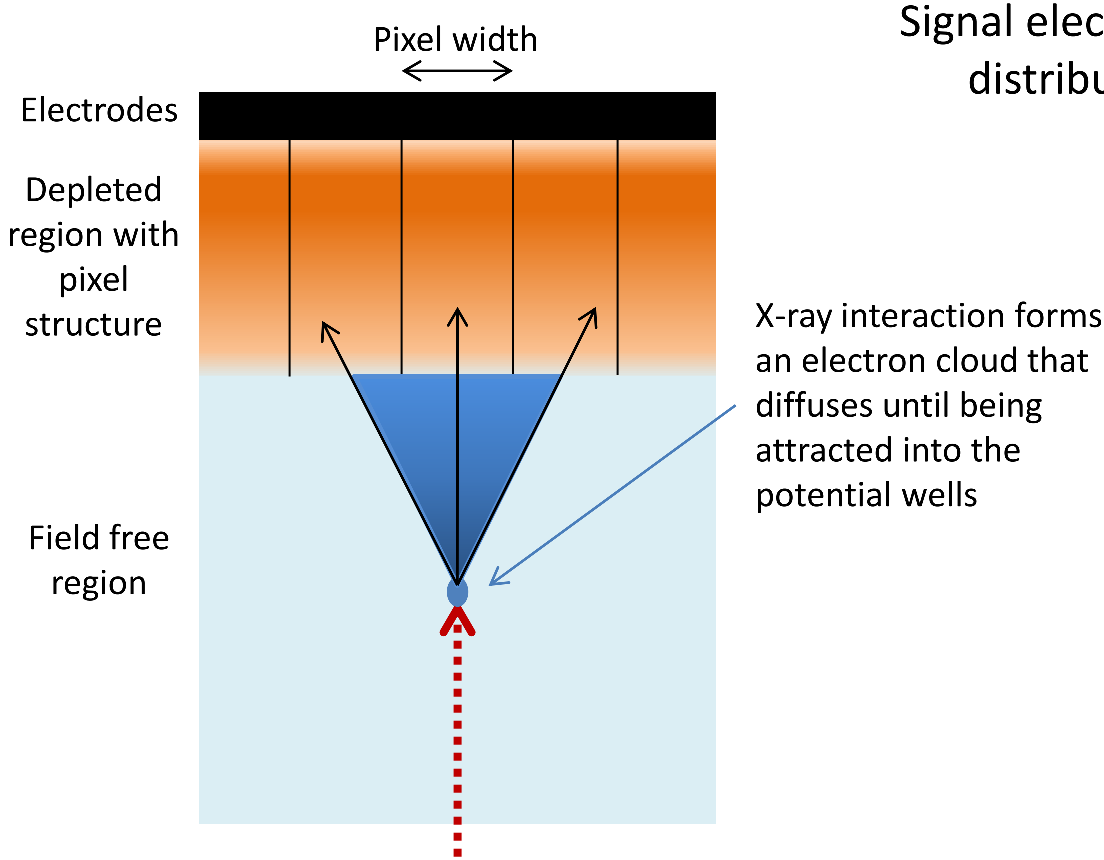


The current spatial resolution of the CCD is given by the width of Gaussian-like charge cloud distribution.

The goal is a spatial resolution of better than 5 µm (FWHM).

Figure from Ghiringhelli et al. (2006)

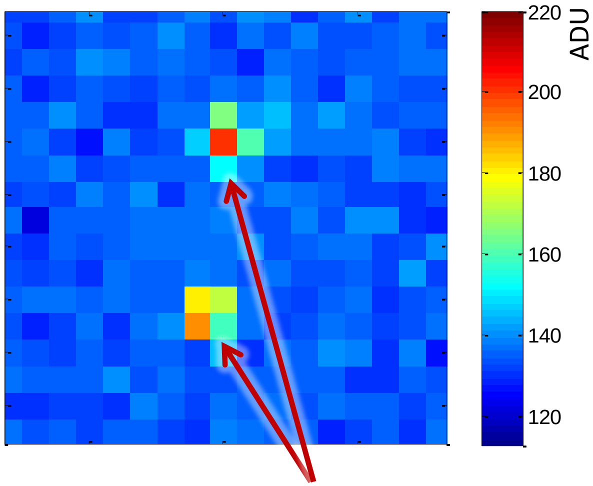
CCD soft X-ray detection



Soft X-ray is incident on 'back surface' of Back Illuminated device

Signal electrons are spread in a 2D Gaussian-like distribution that is sampled by the pixels.

SAXES data, from T. Schmitt



Single X-ray photons events with their total signal spread over multiple neighbouring pixels

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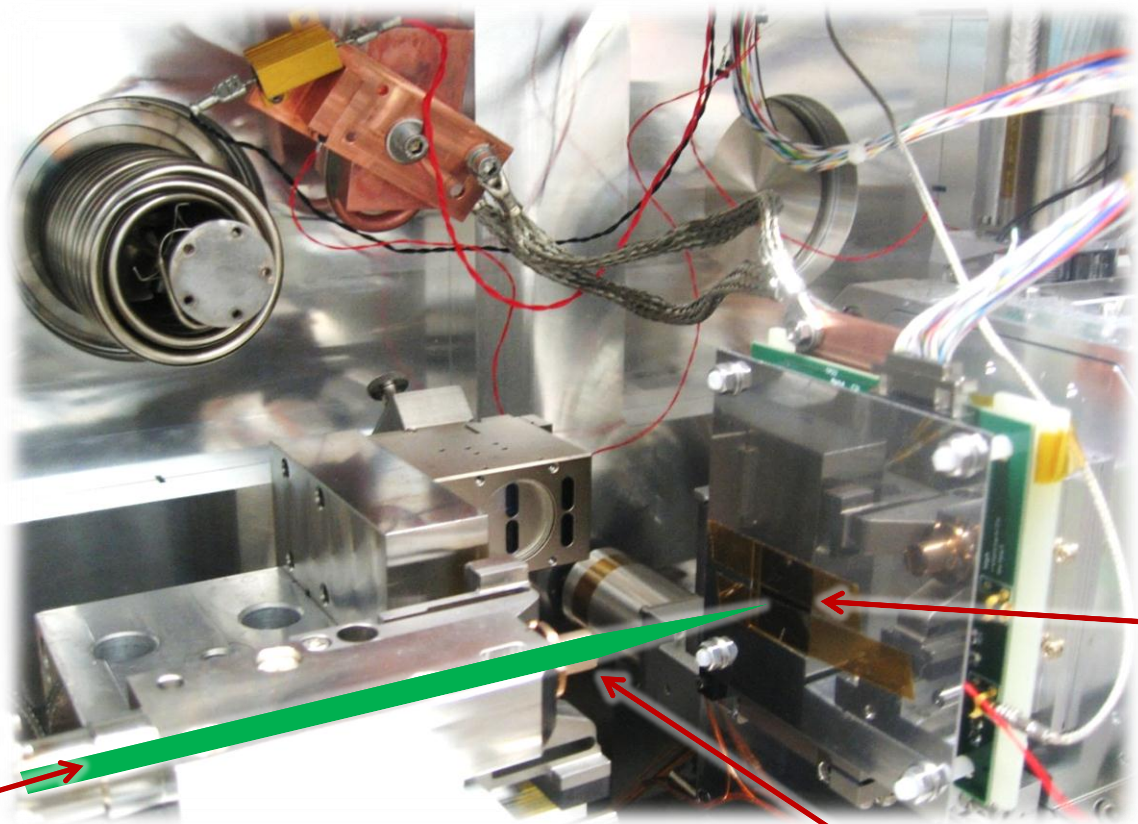
Setup in PolLux microspectroscope



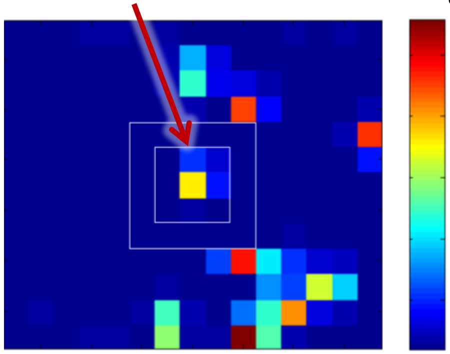
CCD

Beam of incident X-ray

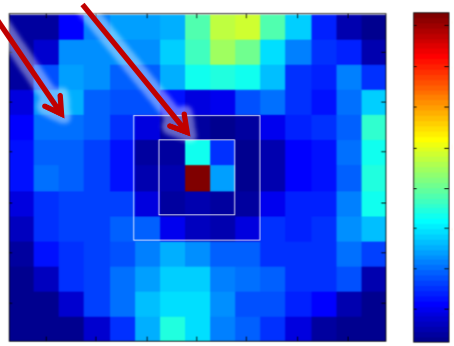
Focussing of X-rays by Fresnel Zone Plate

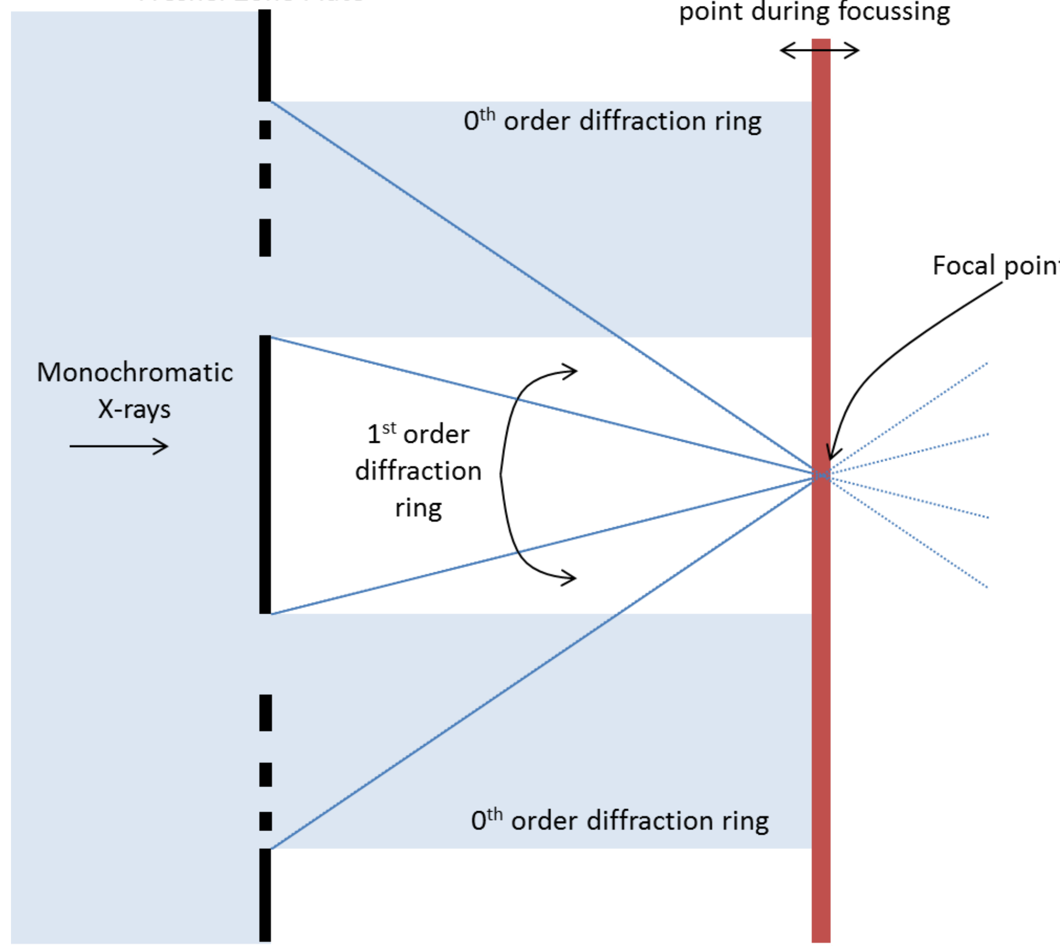
Testing at PolLux

Typical image with single photon detected from 1st order diffraction ring



Mean image showing signal from 0th and 1st order diffraction ring photons





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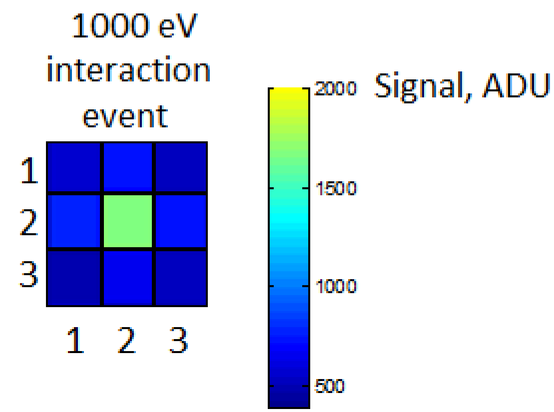
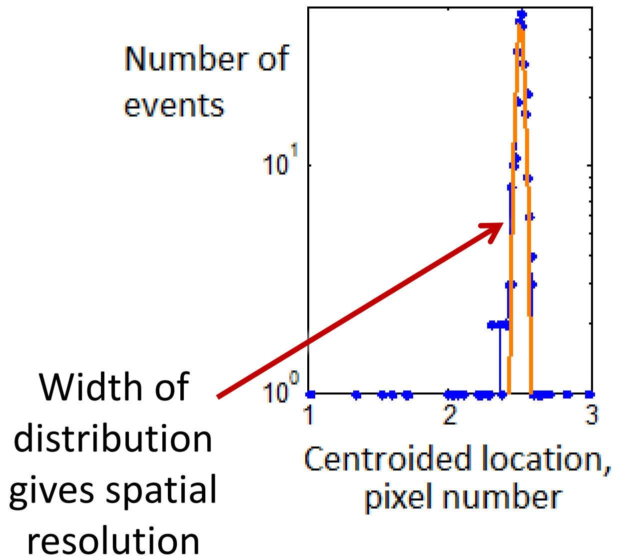
Investigating centroiding

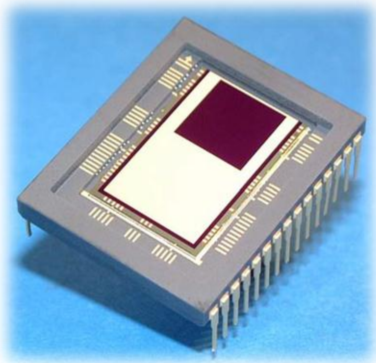
Images containing single photon interaction events where the spot is focussed in the same area of the pixel are selected.

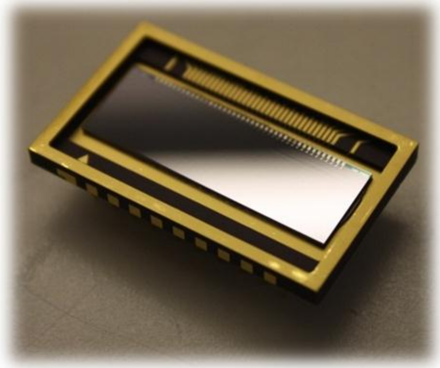


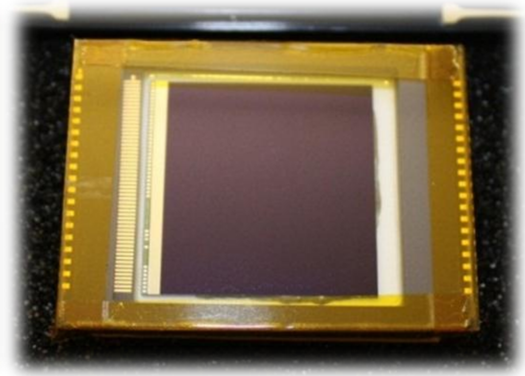
Applying centroiding algorithms to the interaction events allows the distribution of centroided positions to be determined.



Back illuminated CCDs investigated







	CCD97	CCD42-10	CCD207-40
Pixel size (square)	16 µm	13.5 µm	16 µm
Image area (pixels)	512×512	2048×512	1632×1608
Effective overall noise (electrons rms)	< 1	5 (at 100 kHz pixel readout rate)	< 1
Detector type	EM-CCD	CCD	EM-CCD

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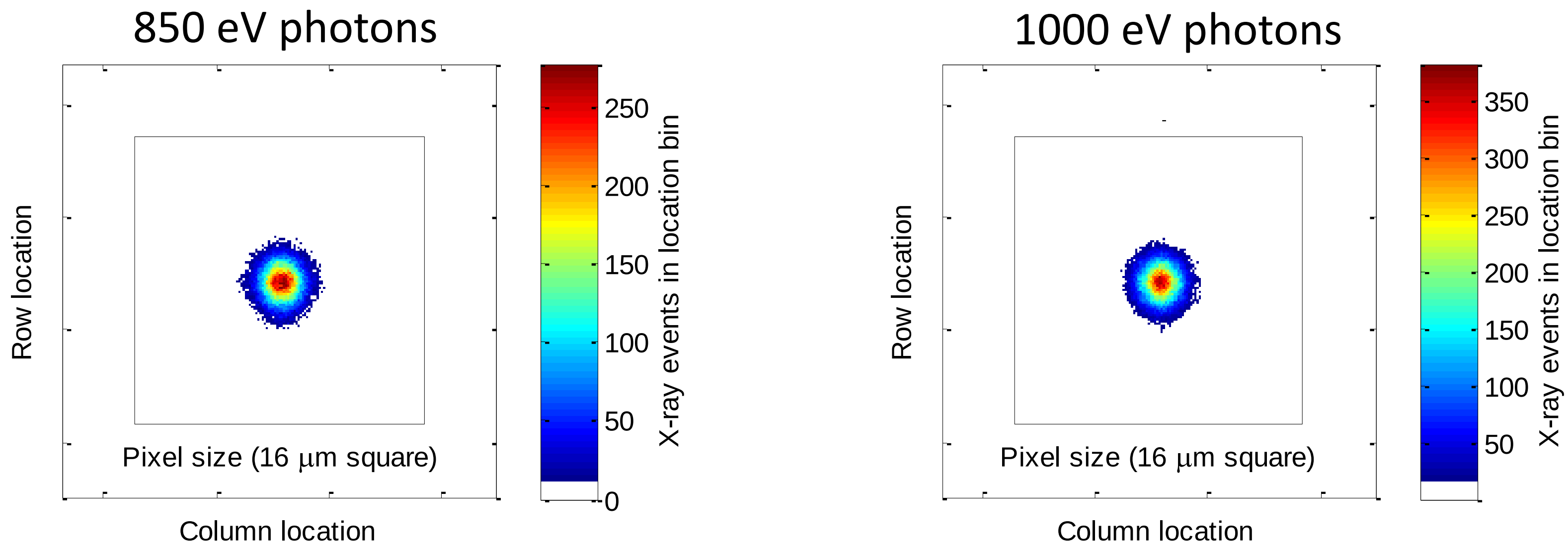
Electron Multiplying CCDs

The current CCD in the spectrometer operates in a 'pile-up' mode, unsuitable for applying centroid algorithms required to achieve sub-pixel spatial resolution.

Reducing the integration time of the current CCD to operate in a 'photon counting' mode requires increasing the readout rate to maintain the spectrometer throughput but then the readout noise is too high.

An additional register in Electron Multiplying CCDs apply a gain to the signal before readout noise is added. They are capable of operating at readout rates that will maintain the throughput of the spectrometer whilst having a low effective readout noise.

Spatial resolution at 850 and 1000 eV



Width of the distribution of locations determined using a 3×3 Centre of Mass algorithm gives worst case spatial resolution results of less than 2 μm (FWHM) for 850 eV and 1000 eV photons.

This measurement includes a contribution from the focussed X-ray beam of at least 0.02 μm

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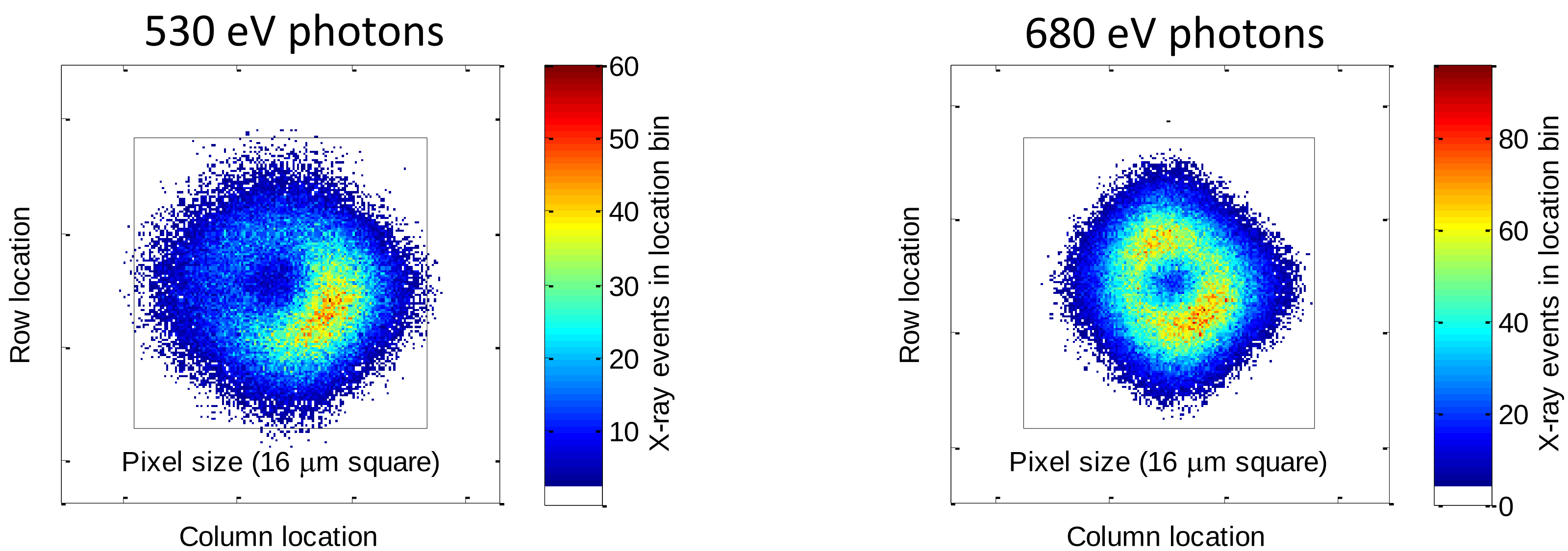
Defocussed ‘spot’ at 530 and 680 eV



Centroided locations of single photon events in the 1st order diffraction ‘spot’ show features of the defocussed diffraction ring

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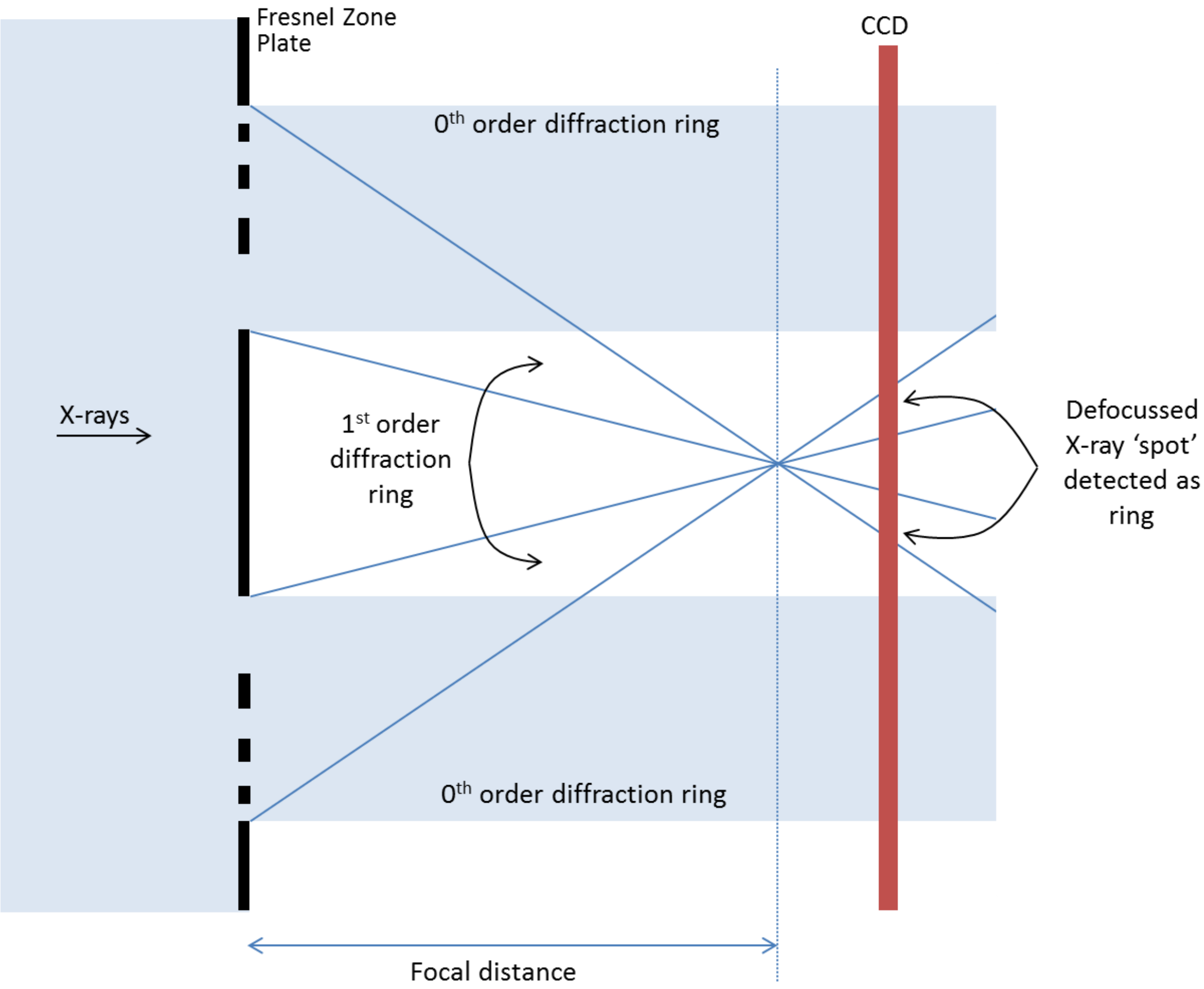
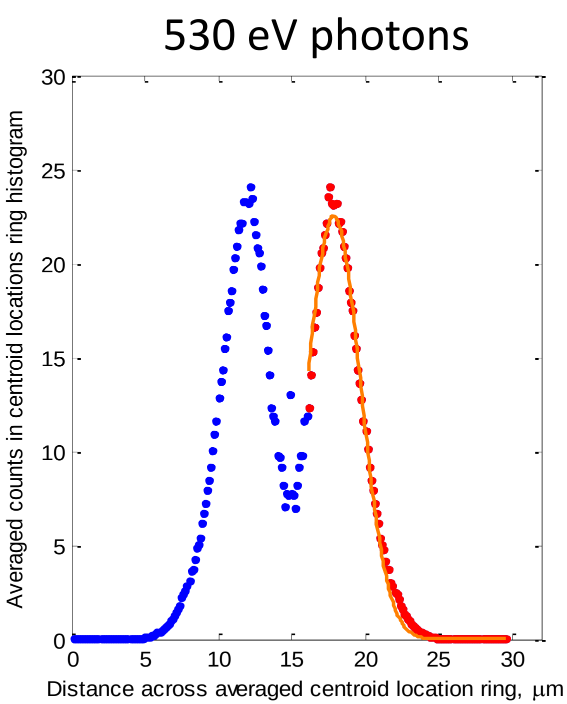
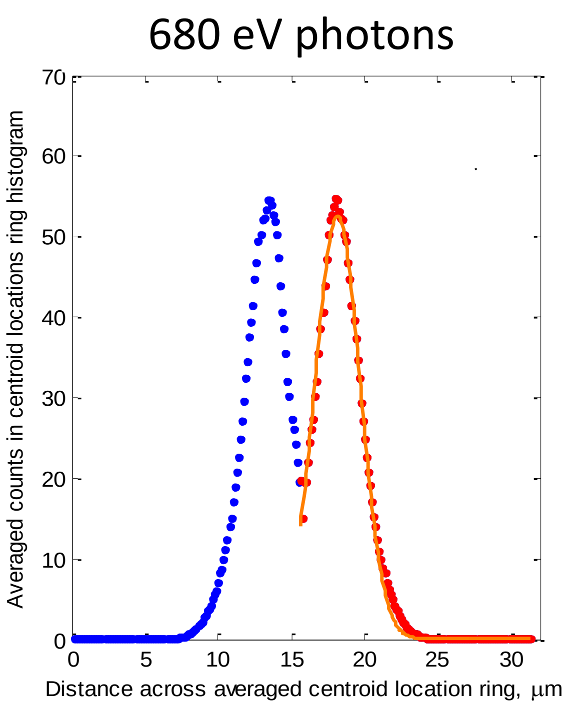
Defocussed X-ray 'spot'



Resolved diffraction ring features





Worst case spatial resolution limits achieved at these lower photon energies are given by the smallest features observed:
4.3 µm and 3.7 µm (FWHM) at 530 eV and 680 eV respectively.

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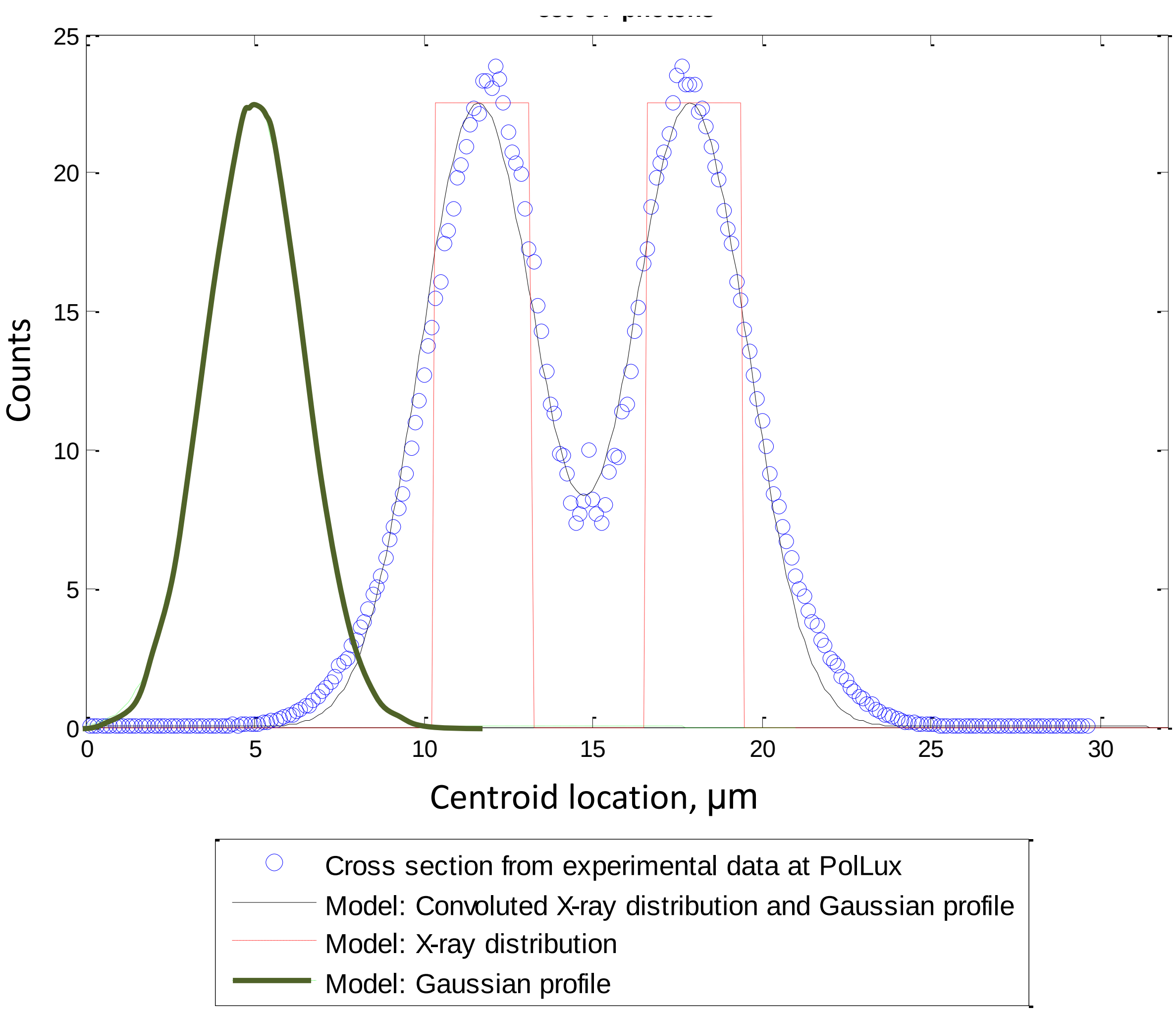
De-convolving diffraction ring size



A simple model has been used to de-convolve the contribution of the diffraction ring sizes to the worst case spatial resolution measurements.

Spatial resolutions are estimated at 3.5 µm and 3.0 µm (FWHM) at 530 eV and 680 eV respectively.

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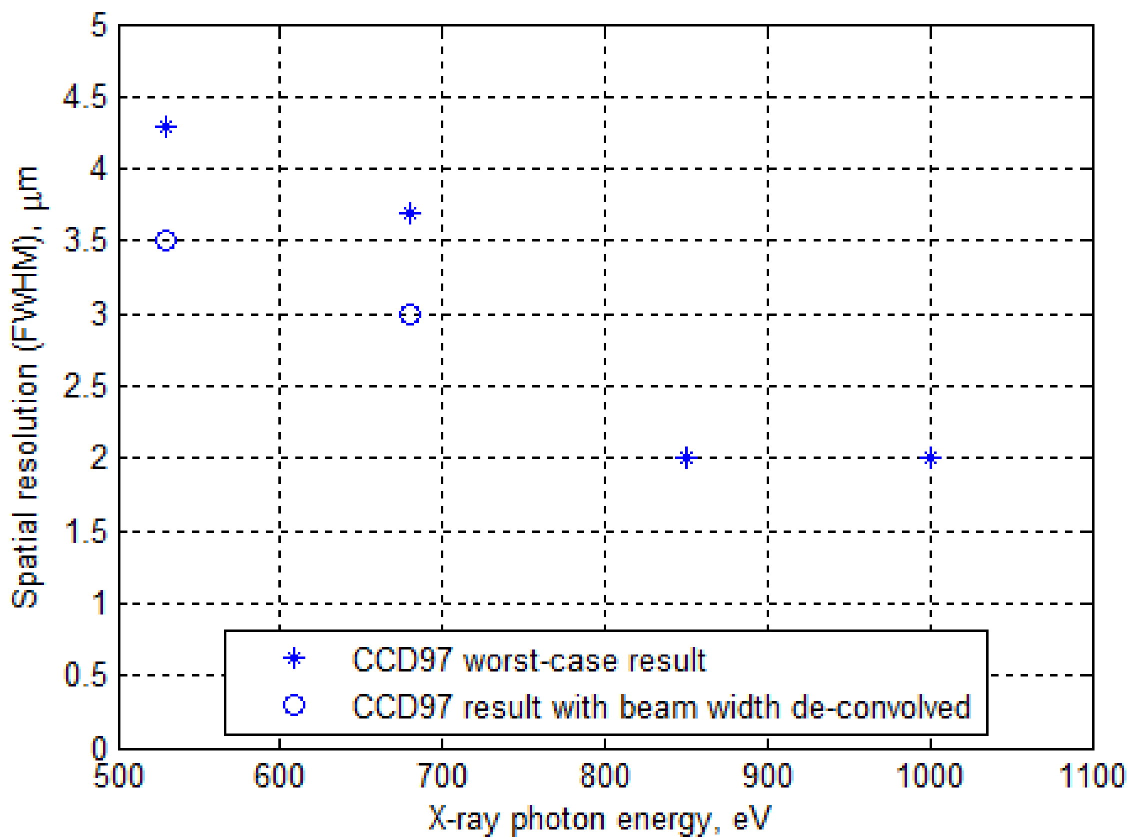
Soft X-ray spatial resolutions



Results were achieved with an e2v technologies Electron Multiplying CCD97 operated in a photon counting mode with an overall image noise of less than 1 electron rms.

A Centre of Mass algorithm across a 3×3 pixel area was applied to single photon interaction events.

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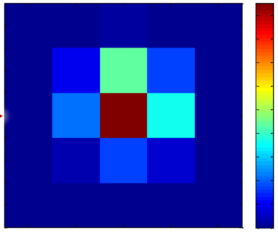
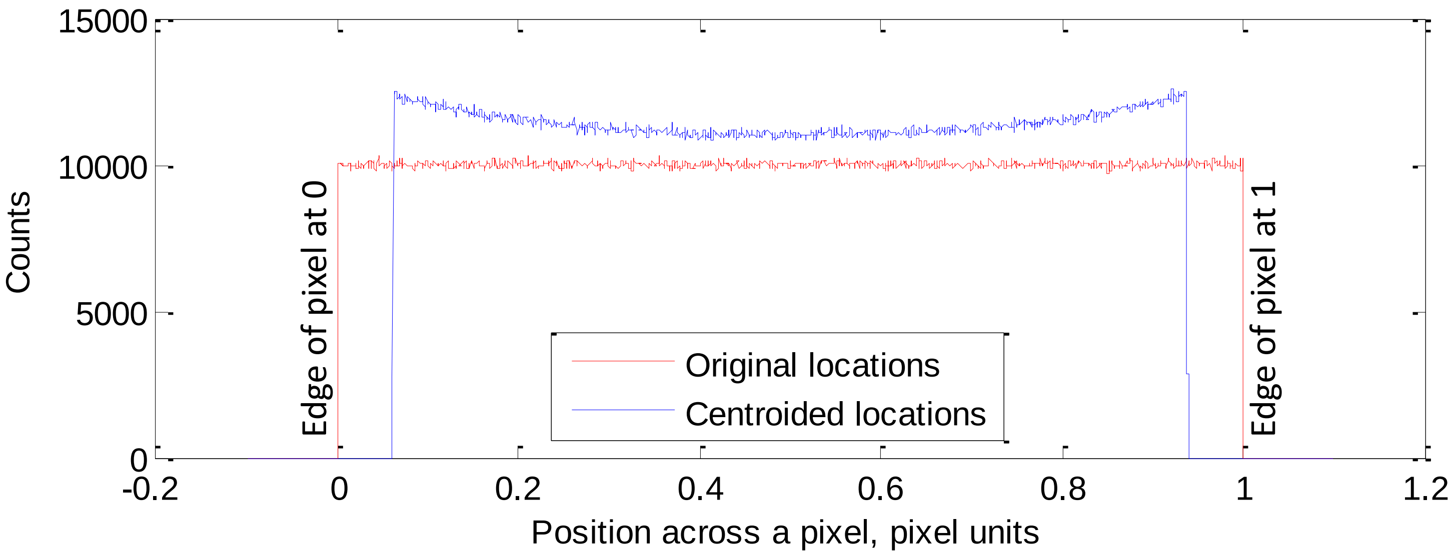
- **Initial results from investigating non-linear centroiding algorithms**

Problem with linear algorithm

Set up a Monte Carlo simulation:

- Sample a 2D Gaussian profile signal with a pixel array
- Centroid using the Centre of Mass algorithm
- Centre the next Gaussian profile in a different position of the pixel

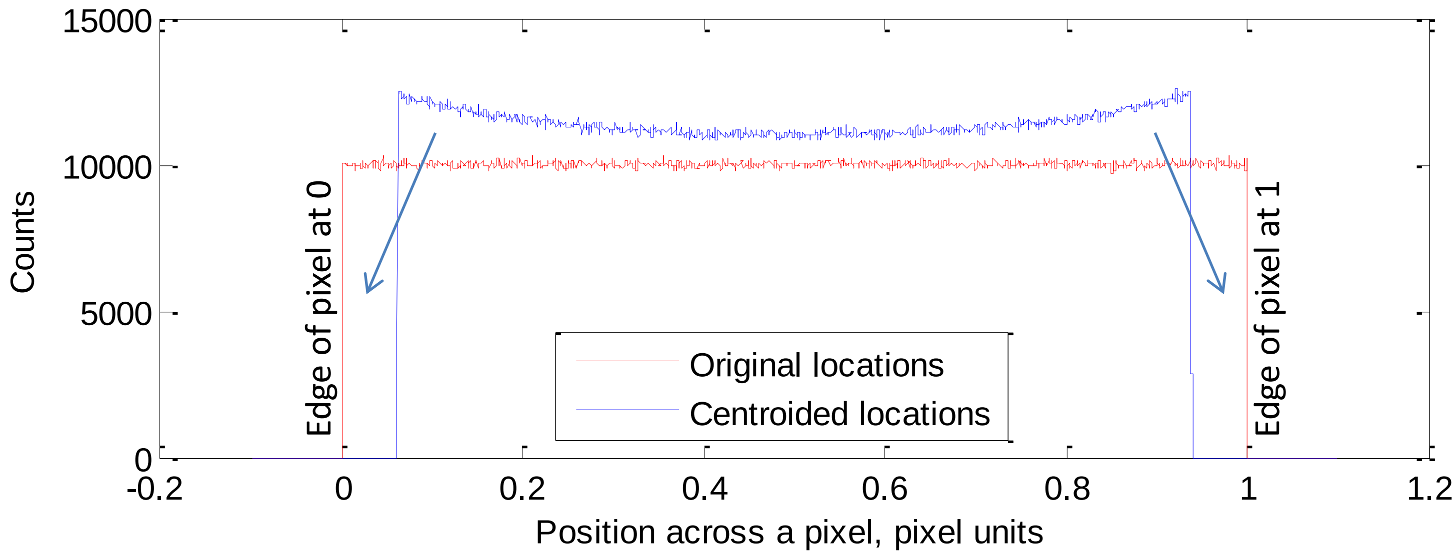




Solution: non-linear η algorithm

η

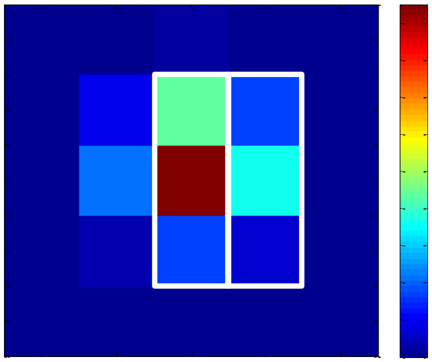
- Like the simulation, use a flat field of X-rays.
- Correct the linear centroided algorithm by knowing that the distribution of interaction positions should be a flat field



Practical application of η algorithm

- Interactions in 0th order ring used as an approximate flat field
- As an initial investigation, compare the total signal in two 3×1 pixel areas (S_L and S_R) around single photon events

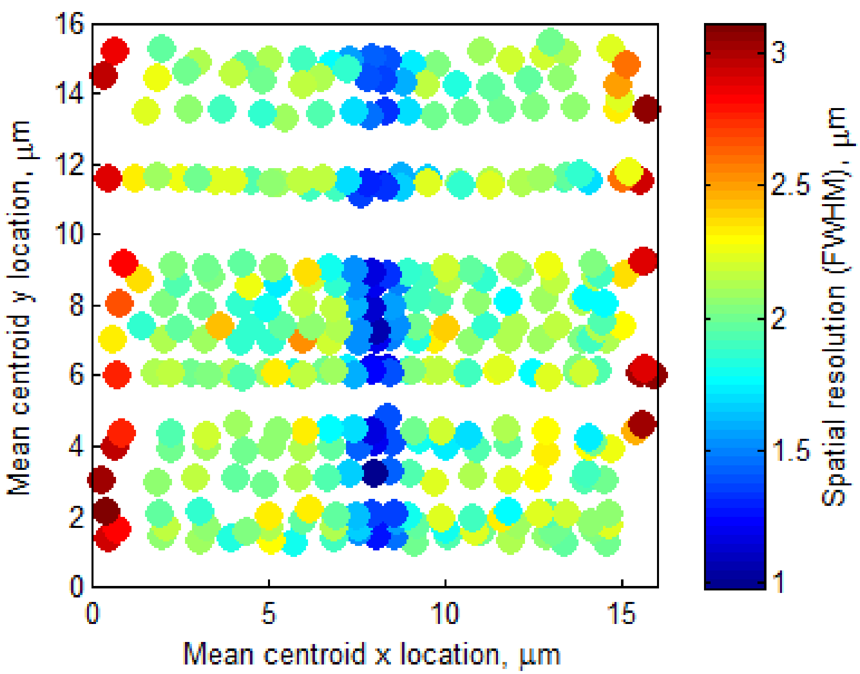
Adjacent 3×1 pixel areas



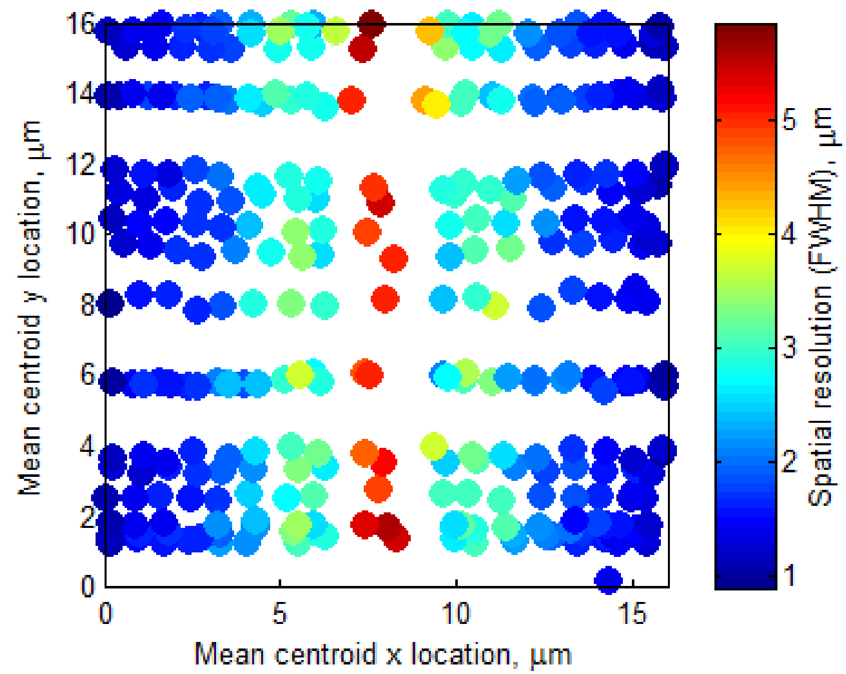
$$\eta = \frac{S_R}{S_L + S_R}$$

η algorithm results

1D spatial resolution of applying centroiding algorithms to 1000 eV photon events as a function of position of interaction in pixel (16 μm square)



Centre of Mass: 3×3 pixel area



η: adjacent 3×1 pixel areas

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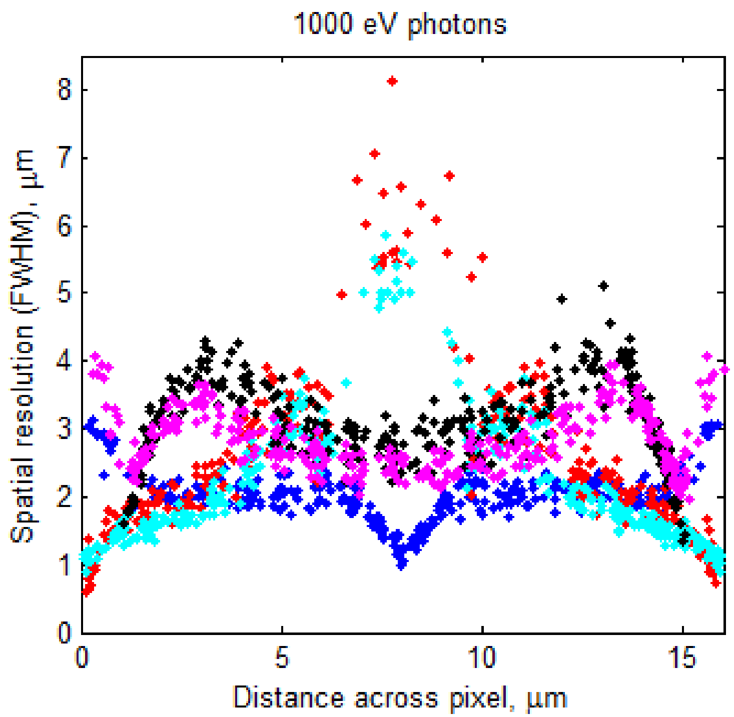
Spatial resolution of other η algorithms

The ratio of signal summed from other pixel areas may be compared in non-linear algorithms:



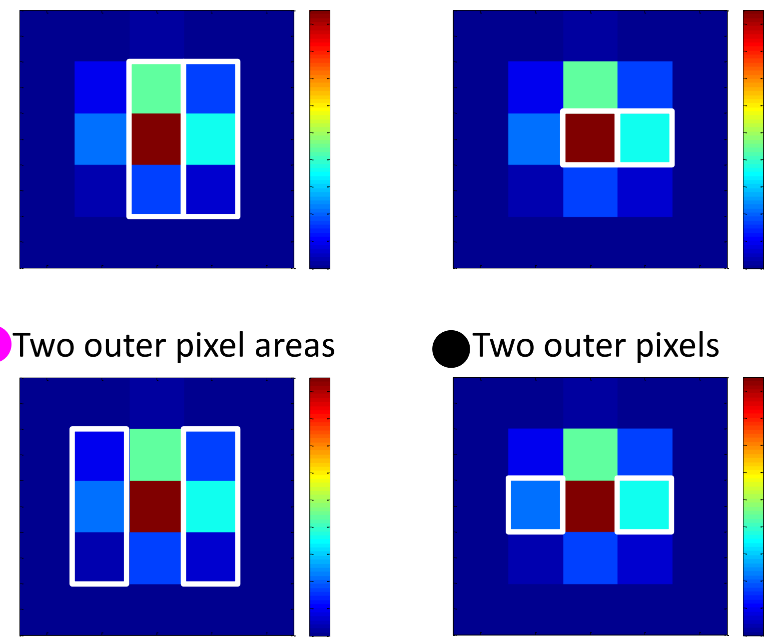
Centre of Mass: 3×3 pixel area

Two adjacent pixel areas

Two adjacent pixels

Two outer pixel areas

Two outer pixels



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5 µm goal is achievable

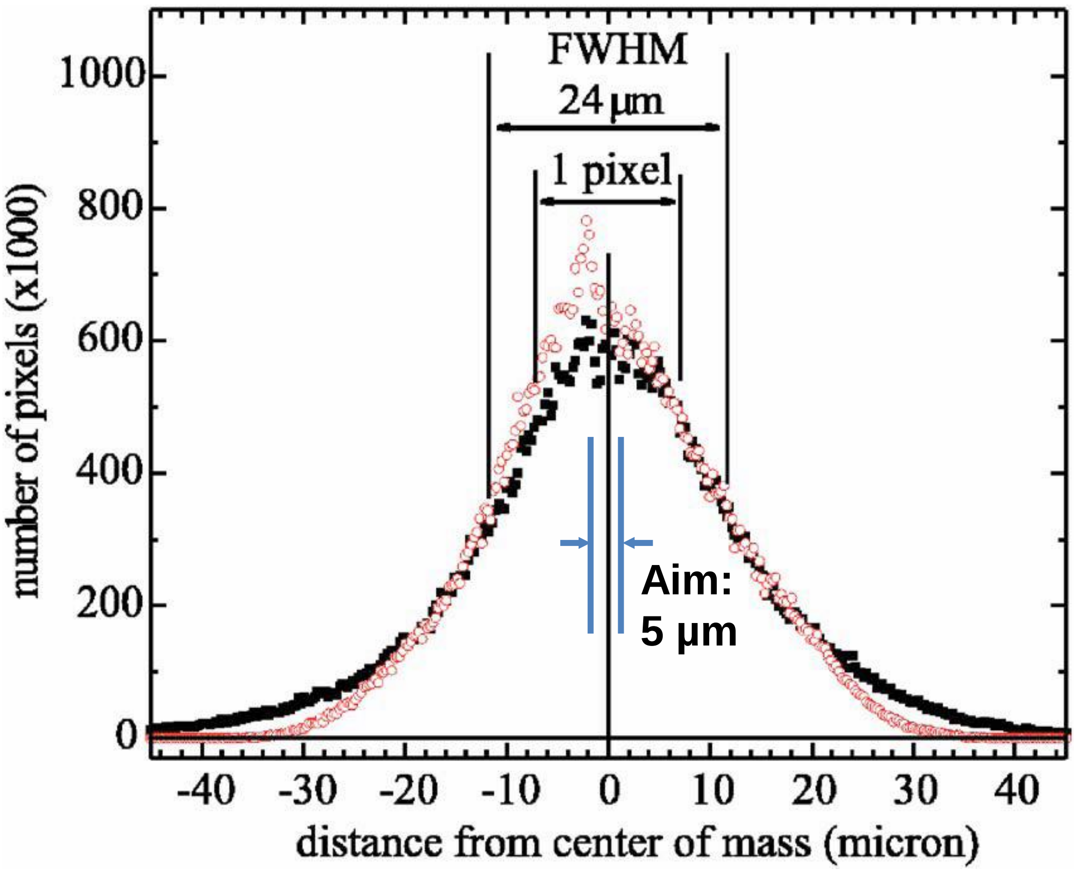
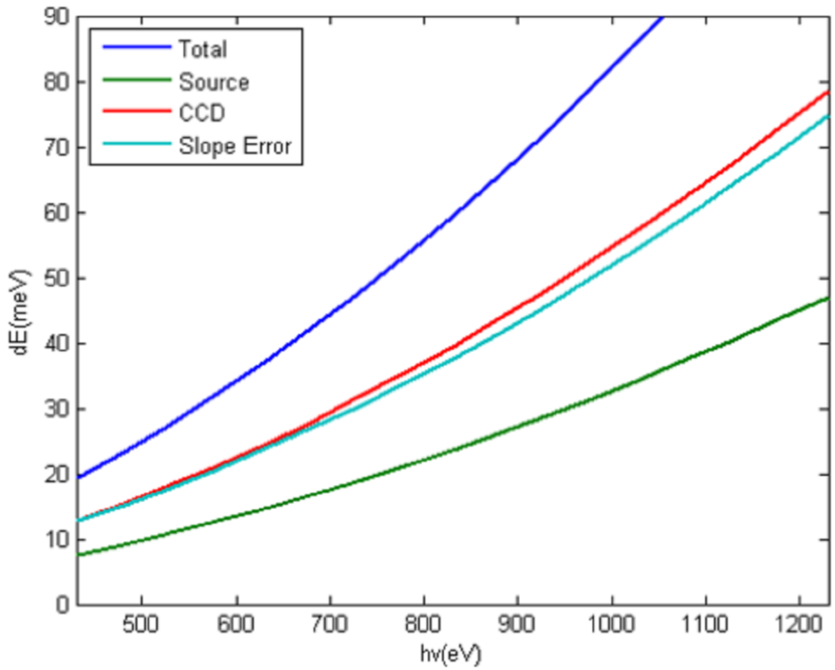


Figure from Ghiringhelli et al. (2006)

SAXES: improved energy resolution

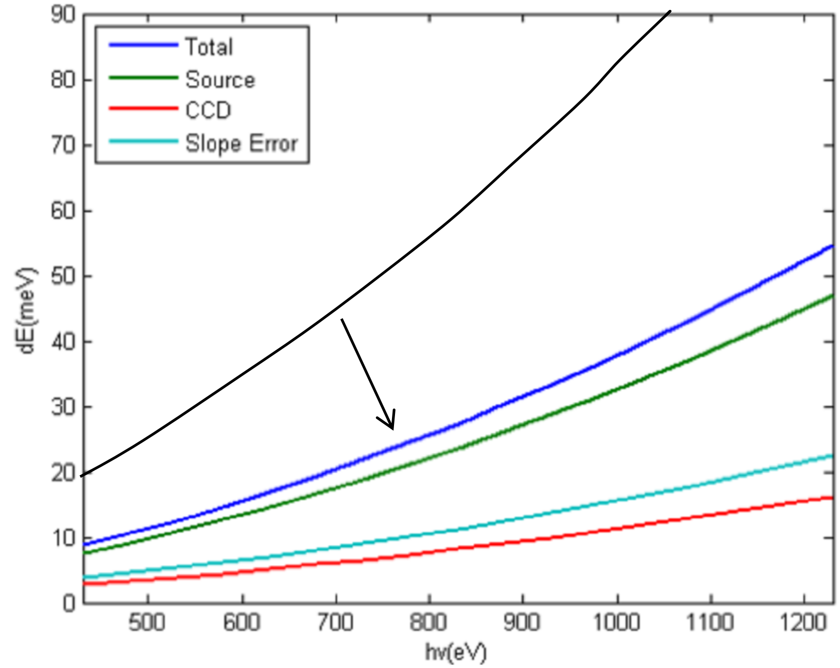


Current setup:

3200 lines/mm grating

Present CCD (24 μm)

Slope error of 0.67 μrad rms



Predicted response from upgraded setup:

Improved 3200 lines/mm grating

Improved detector (5 μm)

Slope error of 0.2 μrad rms

Simulation by V. Strocov

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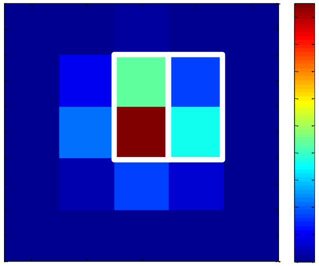
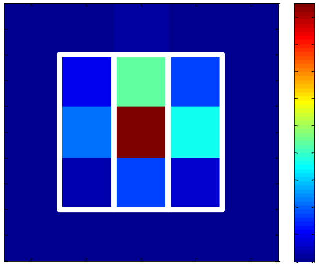
Future work

- Investigate non-linear correction for signal ratios in other pixels areas (e.g. two 2×1 areas)



- Investigate eta algorithm applied to other linear functions of the pixel signals (e.g. non-linear correction of 3×3 ‘centre of mass’ style algorithm)



- Further analysis of data collected during past experimental campaigns

e2v centre for electronic imaging

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e2v centre for electronic imaging, The Open University, MK7 6AA, UK.

T. Schmitt, J. Raabe and B. Schmitt
Paul Scherrer Institut, 5232-Villigen Switzerland.

The SAXES instrument was jointly built by the Paul Scherrer Institut
and Politecnico di Milano, Italy.
The experimental work was performed at the PolLux facility at the Swiss Light Source, Switzerland.
CCDs used in this work were provided by e2v technologies plc.

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