Improving the spatial resolution of soft X-ray detection using an Electron Multiplying Charge Coupled Device

Matthew Soman

A brief outline

- What is Resonant Inelastic X-ray Scattering (RIXS), how is it performed and why is it useful?
- How can the performance of a RIXS spectrometer be improved by applying centroiding techniques to X-ray events?
- Example results from experimental and simulation work investigating linear and non-linear centroiding algorithms

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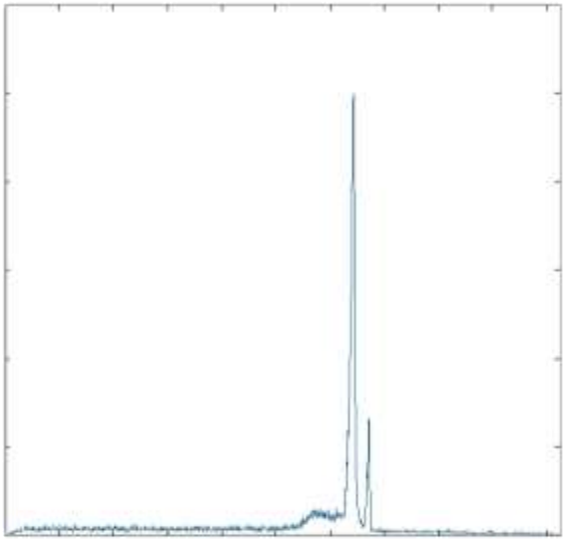
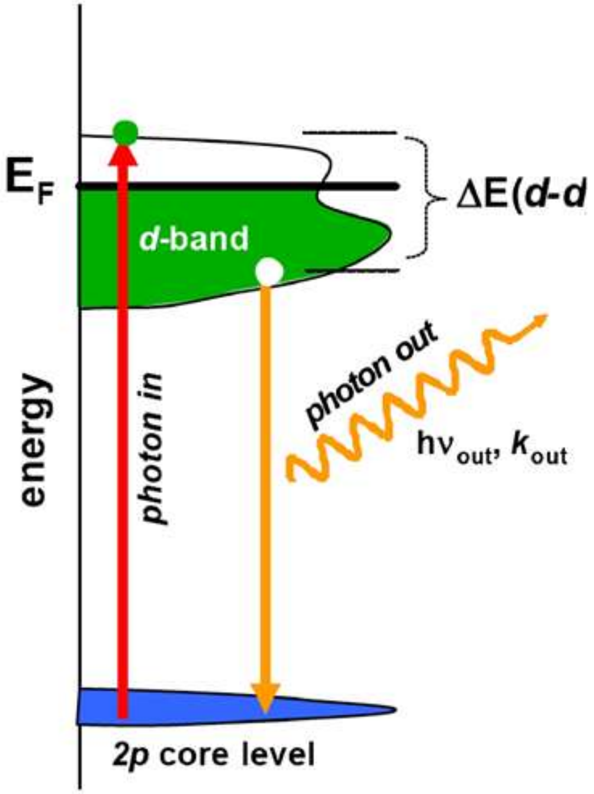
Resonant Inelastic X-ray Scattering

Target sample with photons of energy **$h\nu_{in}$** and **measure spectrum of photons scattered out** with energies **$h\nu_{out}$** and momentum change **k_{out}**



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



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

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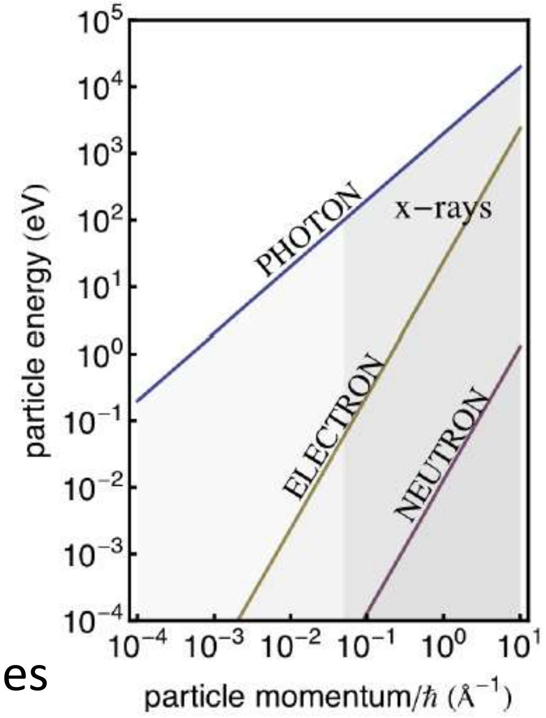
Why is RIXS useful?

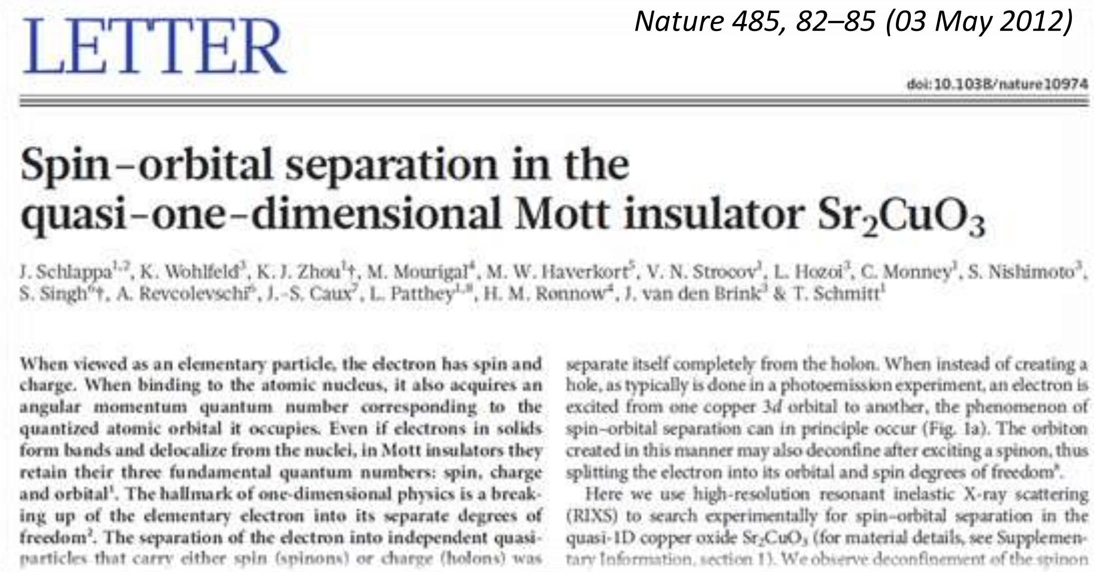
- Energy and momentum sensitive:
  - X-rays have a greater scattering phase-space than neutron or electron probes, whilst having the advantage over lower energy photons of being able to probe the full dispersion of low energy excitations in solids.
- Polarisation sensitive
  - The incident photon polarisation can be varied and the outgoing polarisation can be measured
- Element and orbital specific:
  - The incident photon energy can be tuned to element absorption edges
- Bulk sensitive, and only needs small sample volumes



Scattering phase space comparison, L.P. Ament et. al. (2010)

Why is RIXS useful?

Nature 485, 82–85 (03 May 2012)



LETTER

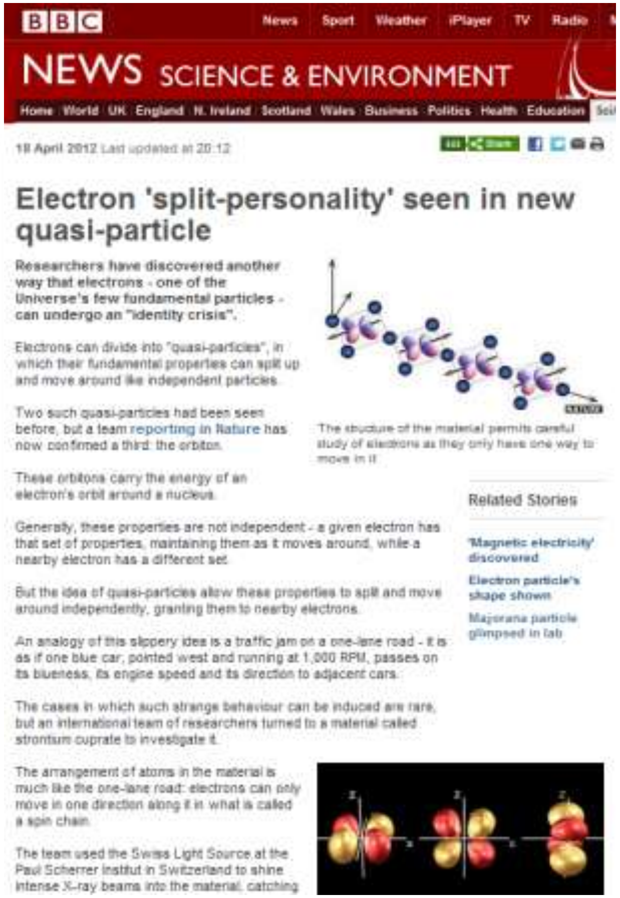
doi:10.1038/nature10974

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[3].

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



BBC NEWS SCIENCE & ENVIRONMENT

18 April 2012 Last updated at 20:12

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".

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.

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

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

Related Stories

'Magnetic electricity' discovered

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Majorana particle glimpsed in lab

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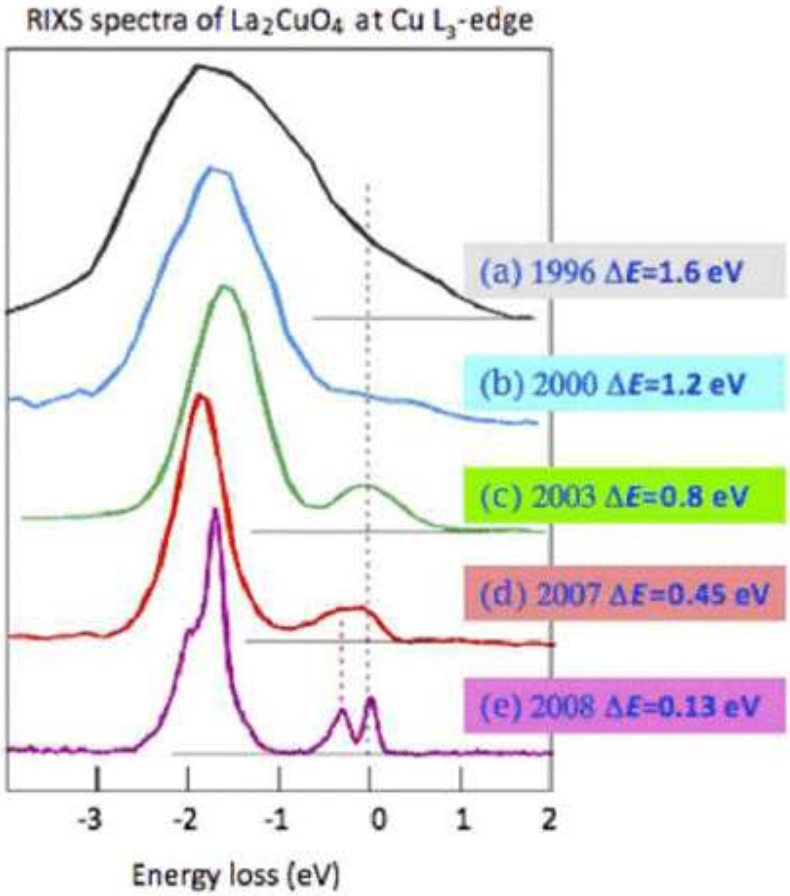
Past energy resolution improvement



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

Improvements in the resolution of spectrometers used for Resonant Inelastic X-ray Scattering (like SAXES) have allowed smaller spectral features to be resolved in the past 15 years.

The experimental results included in the most recent nature publication used an energy resolution of 0.14 eV

SAXES: a RIXS spectrometer

At the Swiss Light Source at the Paul Scherrer Institute near Zurich, Switzerland (venue of iWoRID 2011)

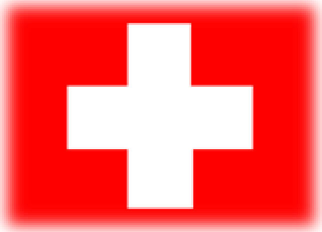


Image courtesy of PSI, www.psi.ch

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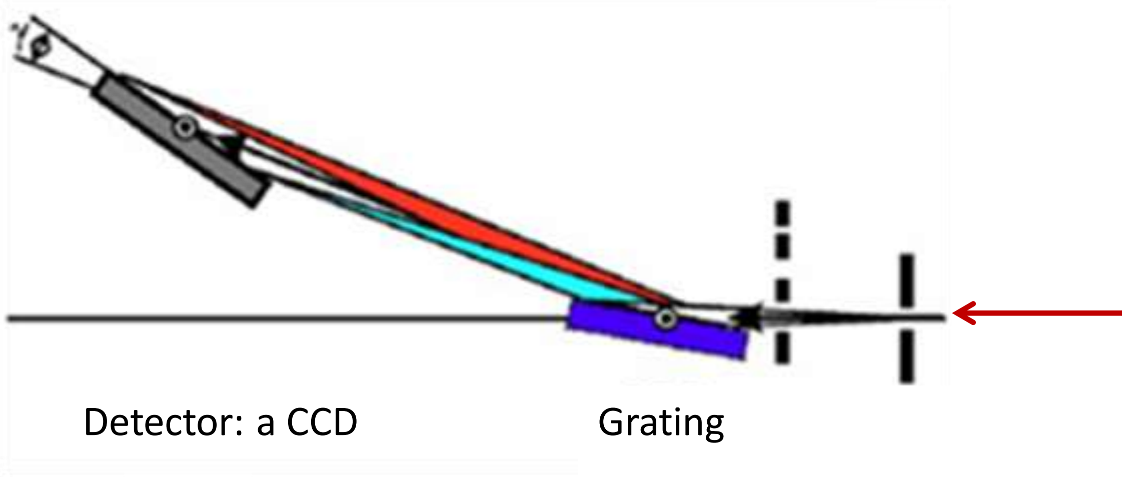
SAXES: a RIXS spectrometer

SAXES is a high resolution soft X-ray grating spectrometer operating at energies between 400 and 1600 eV

http://www.psi.ch/sls/adress/HomeEN/ADRESS_ESRF_Nov2006.pdf

SAXES: a RIXS spectrometer



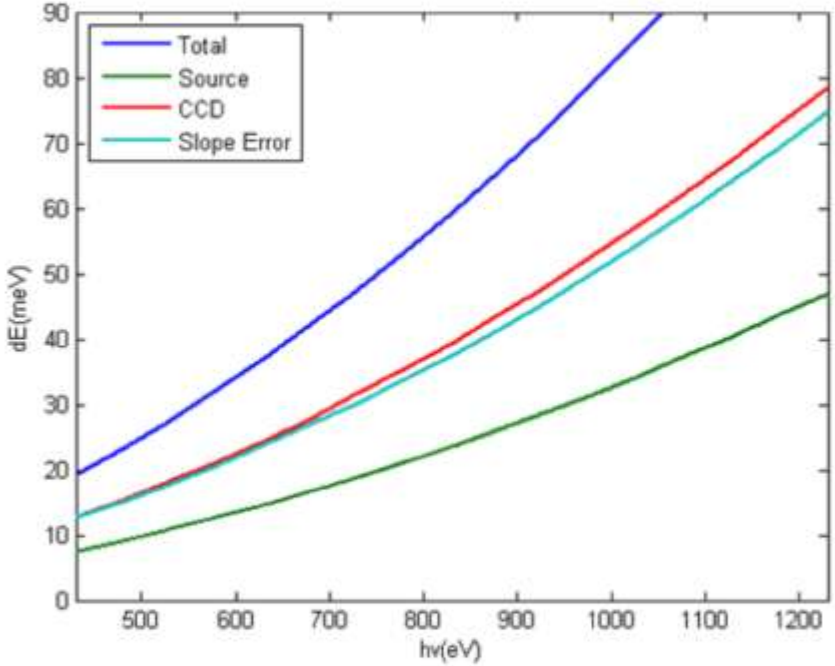
Detector: a CCD

Grating

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

G. Ghiringhelli *et al.* (2006)

SAXES: improved energy resolution



Current setup:

3200 lines/mm grating

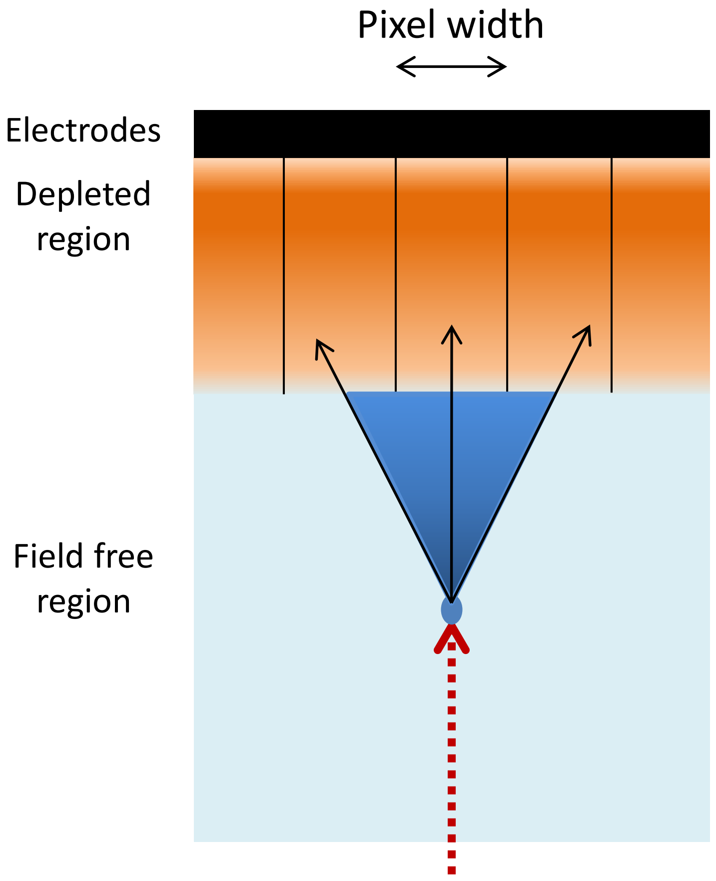
Present CCD (24 µm)

Slope error of 0.67 µrad rms

Simulation by V. Strocov

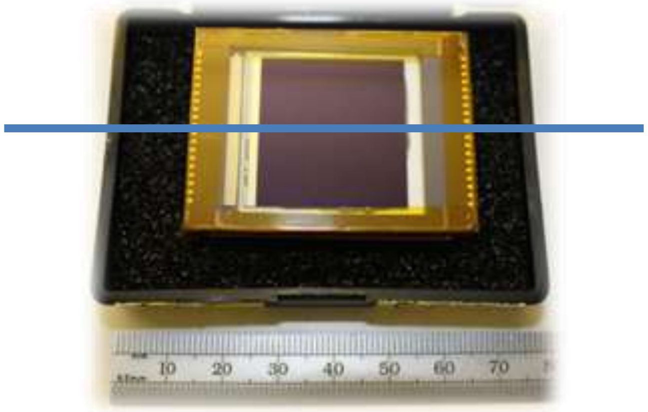
Matthew Soman

CCD soft X-ray detection



Doping in the silicon combines with voltages applied to electrodes above the silicon to form the pixel structure to store electrons

X-ray interaction excites electrons to the conduction band which diffuse until being attracted into the potential wells



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

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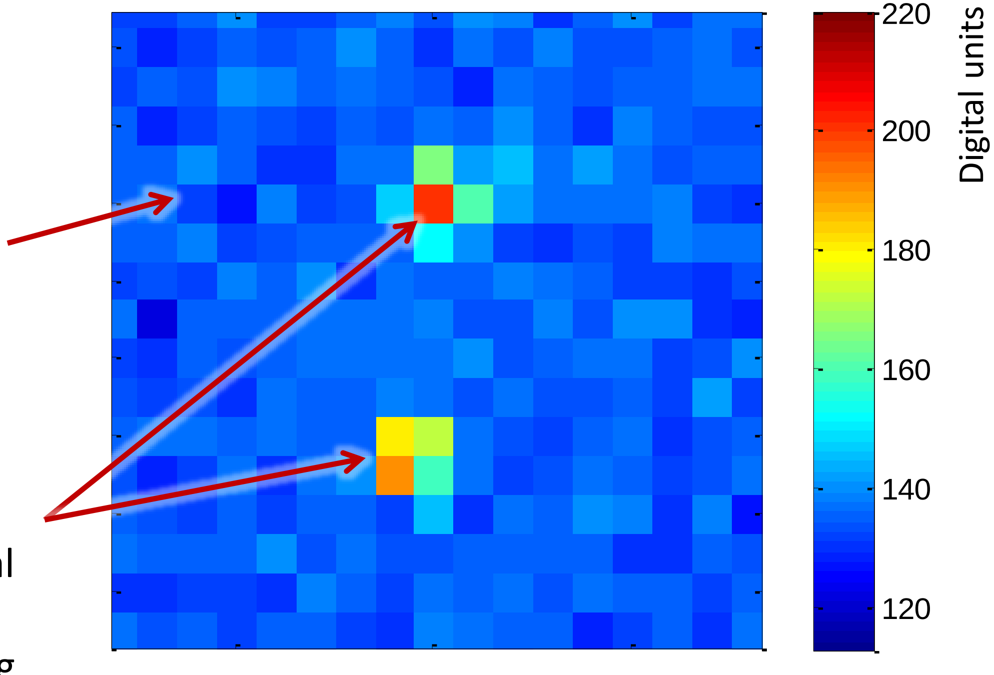
Typical X-ray events in a CCD

Signal electrons from X-ray interactions spread in a 2D Gaussian-like distribution across the plane of the detector. This distribution is sampled by the pixels.

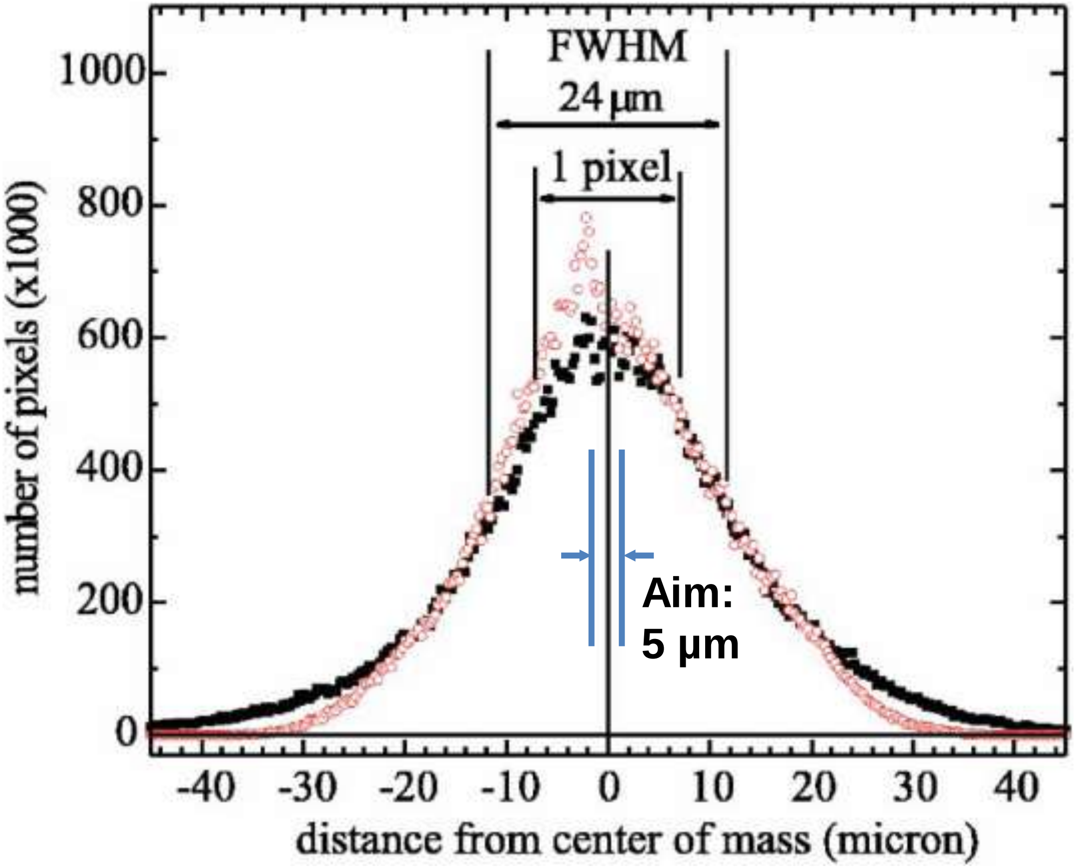


Majority of pixels have a signal at a background level (with noise)

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

SAXES data, from T. Schmitt

SAXES: detector spatial resolution



This distribution shows the size of the Guassian-like charge cloud sampled by the pixels.

The current spatial resolution of the detector is given by the width of this distribution.

The resolution goal is shown. It is much better than the intrinsic resolution of the detector, and even smaller than the pixel.

Figure from Ghiringhelli et al. (2006)

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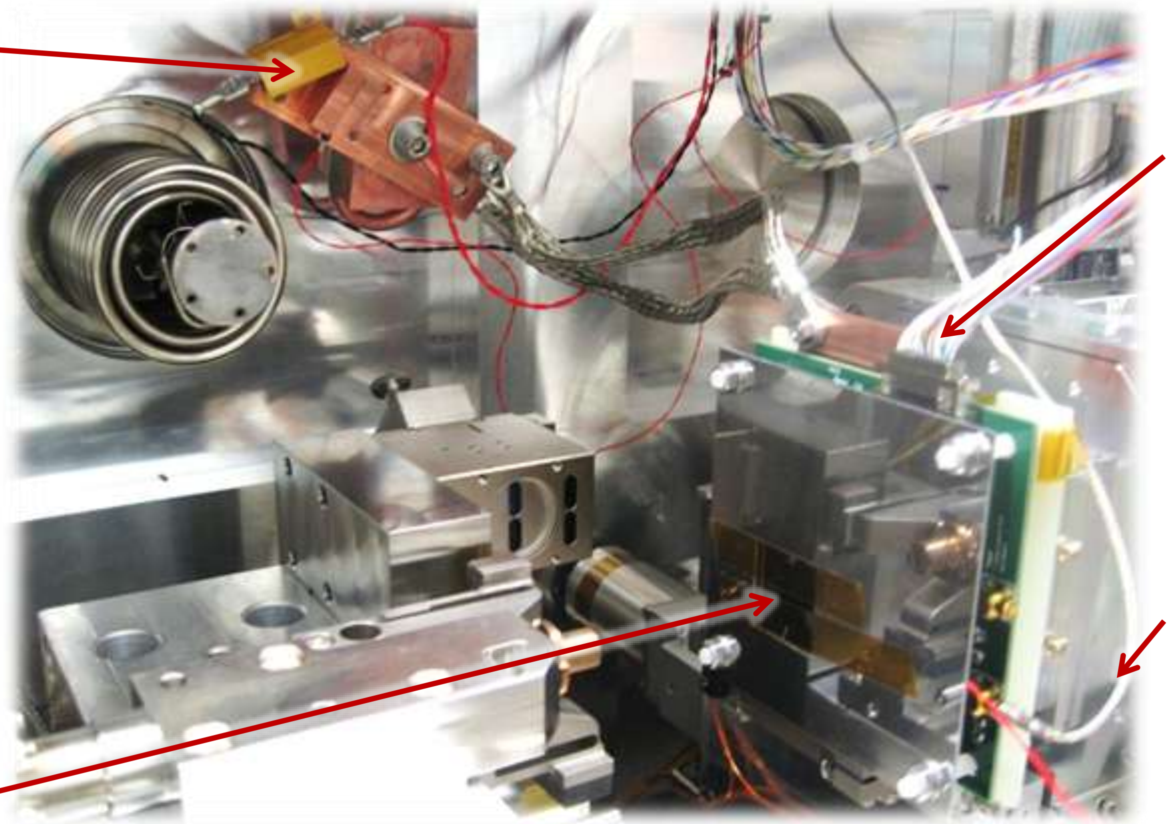
Setup in PolLux microspectroscope



Liquid nitrogen cold finger

Bias and clock inputs

Signal output

X-rays incident on device's detecting area

PolLux testing campaign progress

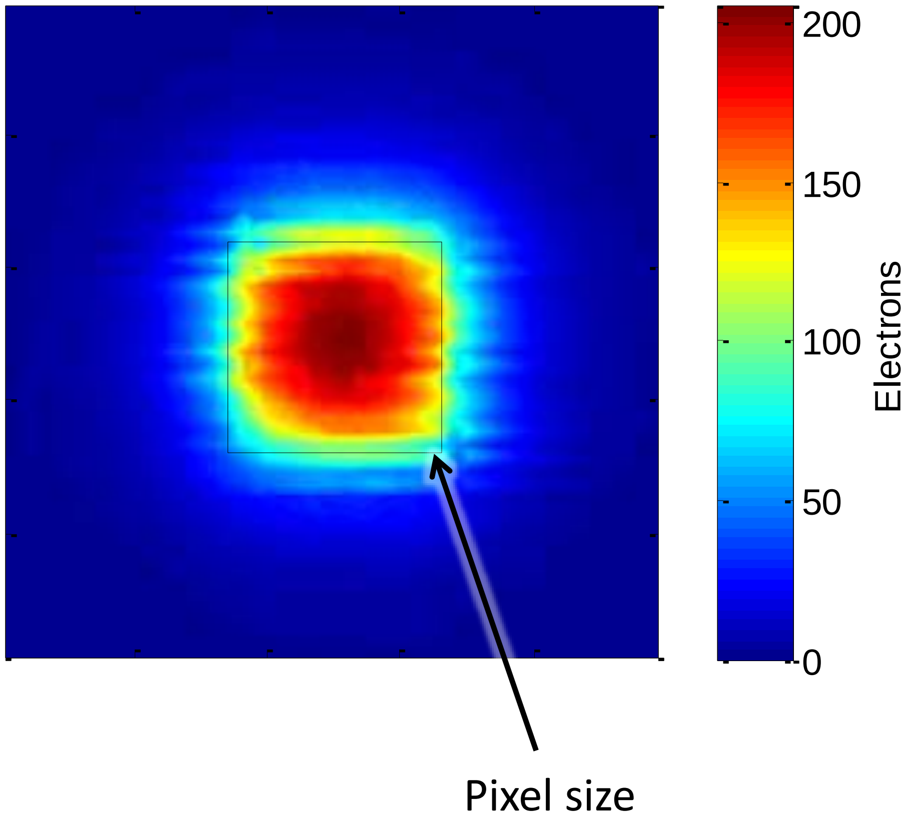
Jun 2011	Sep 2011	Dec 2011	May 2012
CCD97	CCD42	CCD97	CCD207
1D data collection across pixel centre	1D data collection	**2D rastering across a pixel** using custom automated camera and translational stage software	2D rastering across a pixel
1 energy	**4 energies**	4 energies	1 energy
Standard area electron multiplying CCD	Conventional CCD with architecture identical to the device in SAXES	Standard area electron multiplying CCD	Large area electron multiplying CCD

Back illuminated CCDs investigated

	CCD97	CCD42-10	CCD207-40
Pixel size (square)	16 µm	13.5 µm	16 µm
Image area (pixels)	512x512	2048x512	1632x1608
Effective overall noise (electrons rms)	<1	5	<1

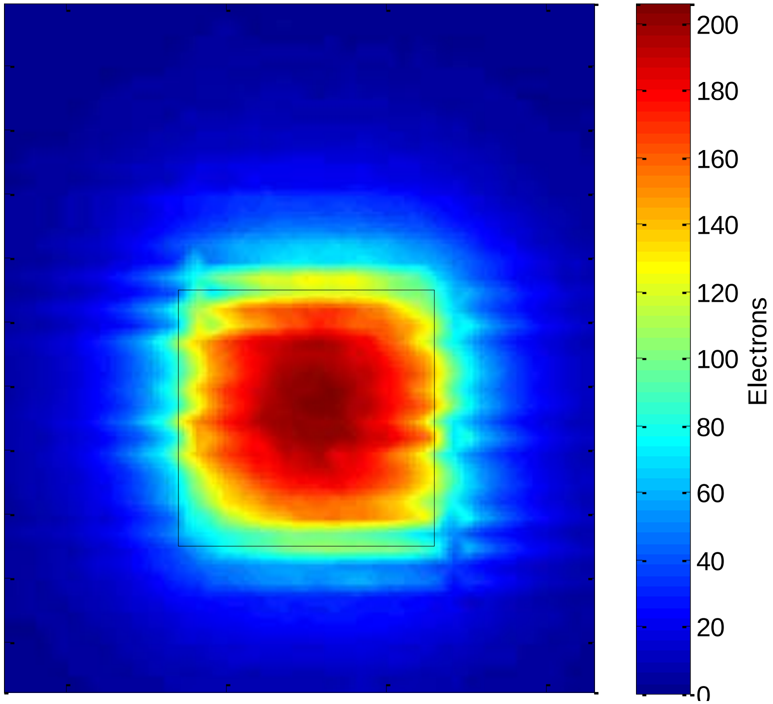
Sampling the electron charge cloud

Oversampled electron charge cloud



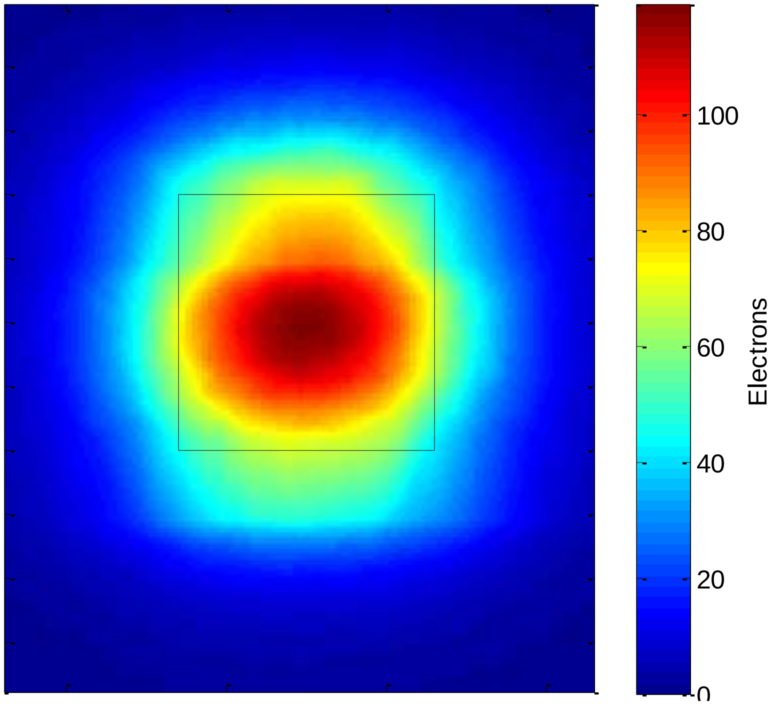
By taking the mean signals from pixels surrounding single 1000 eV photon interaction events and oversampling from each of the 2D stage positions, the average electron charge cloud is determined

Oversampled electron charge cloud



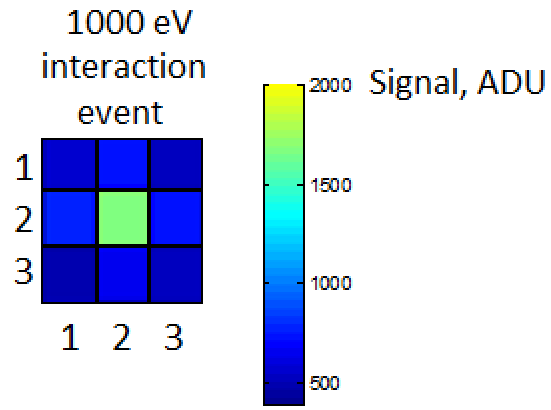
1000 eV

680 eV

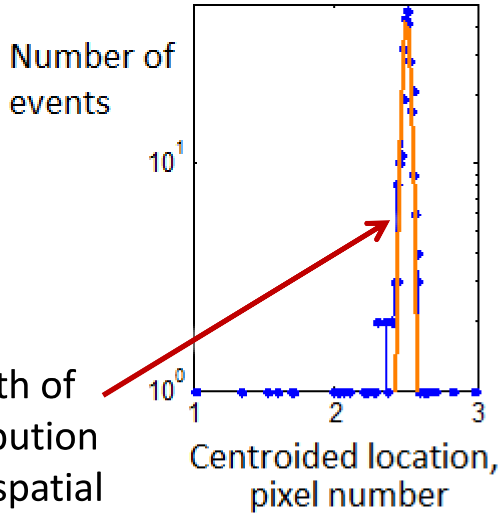


Investigating centroiding

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

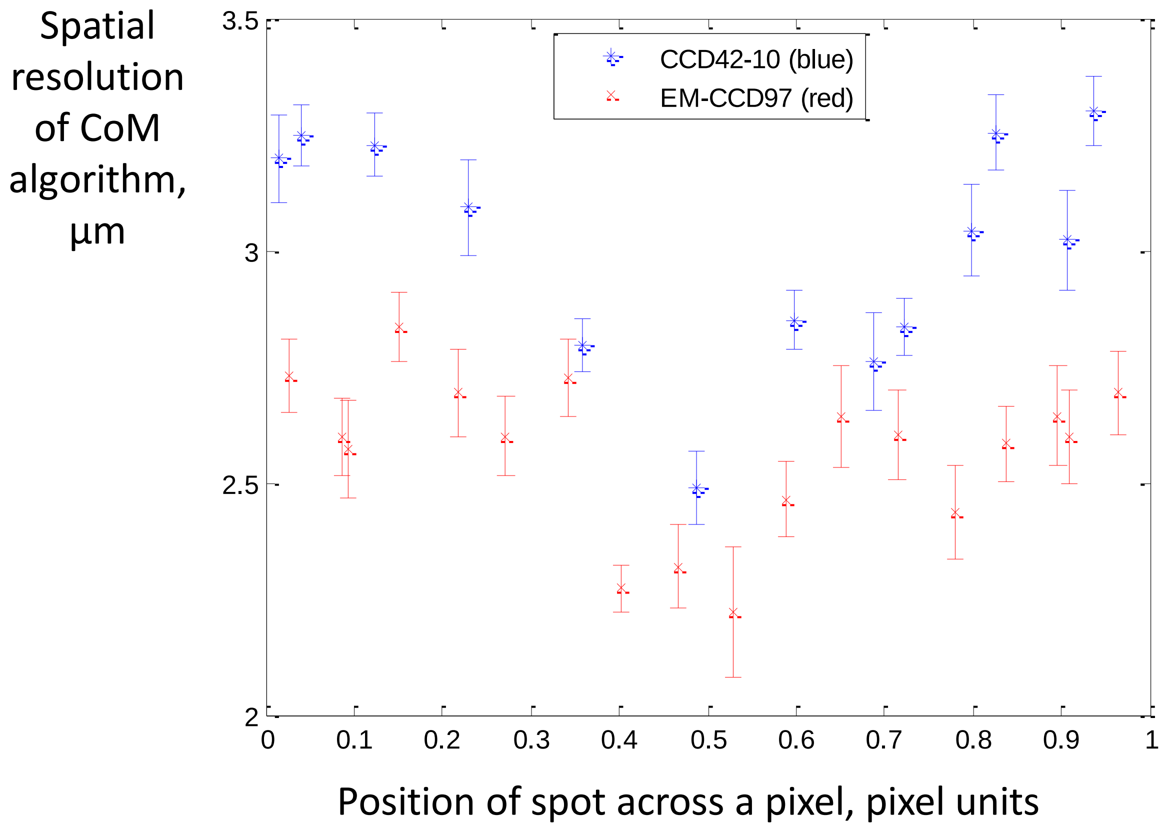


Applying centroiding algorithms to the interaction events allows the distribution of centroided positions to be determined.

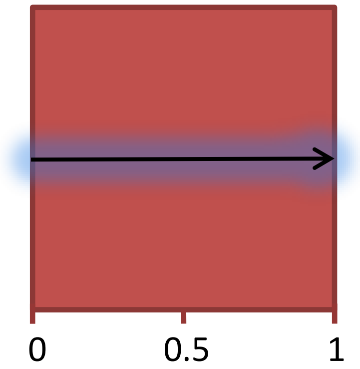


Width of distribution gives spatial resolution

Centroiding algorithm: CoM



Scan across the centre of a square pixel

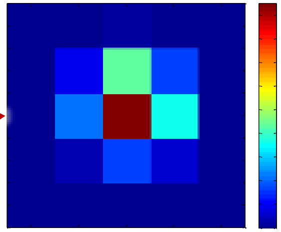


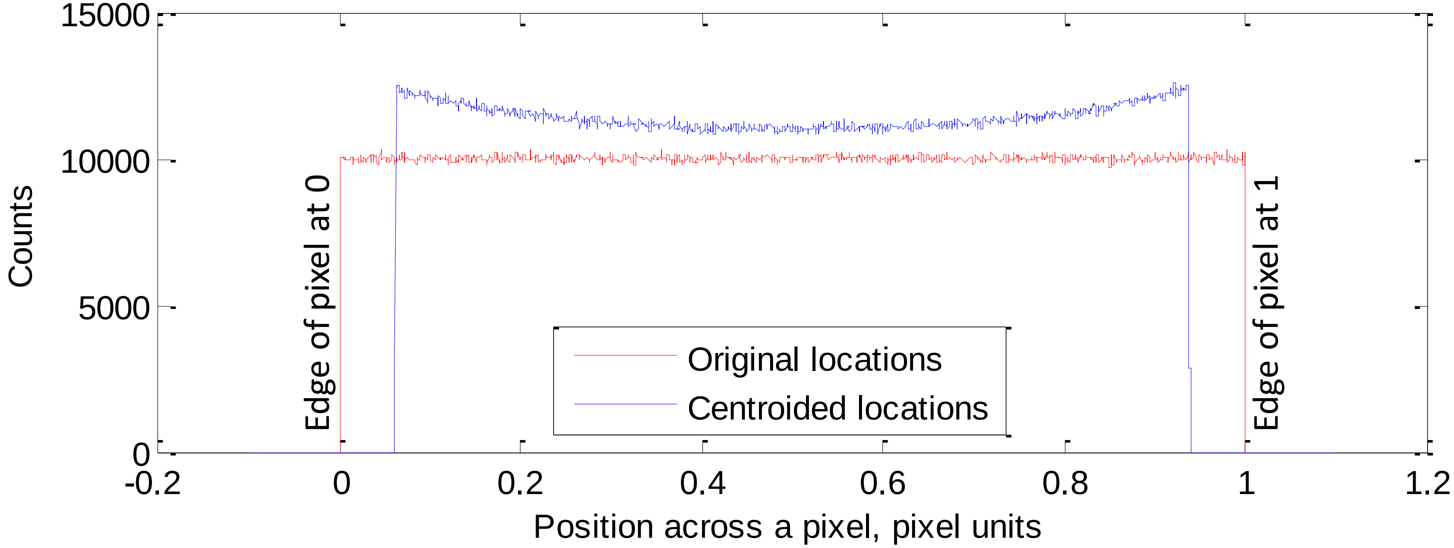
CoM is an algorithm that finds the centre of the signal distribution using a 'Centre of Mass' style calculation

Problem with CoM algorithm

Set up a Monte Carlo simulation:

- Sample a 2D Gaussian profile signal with a pixel array
- Centroid using the Centre of Mass (CoM) algorithm
- Vary the location of the centre of the Gaussian across a pixel
- Compare the distributions of the initial and centroided locations





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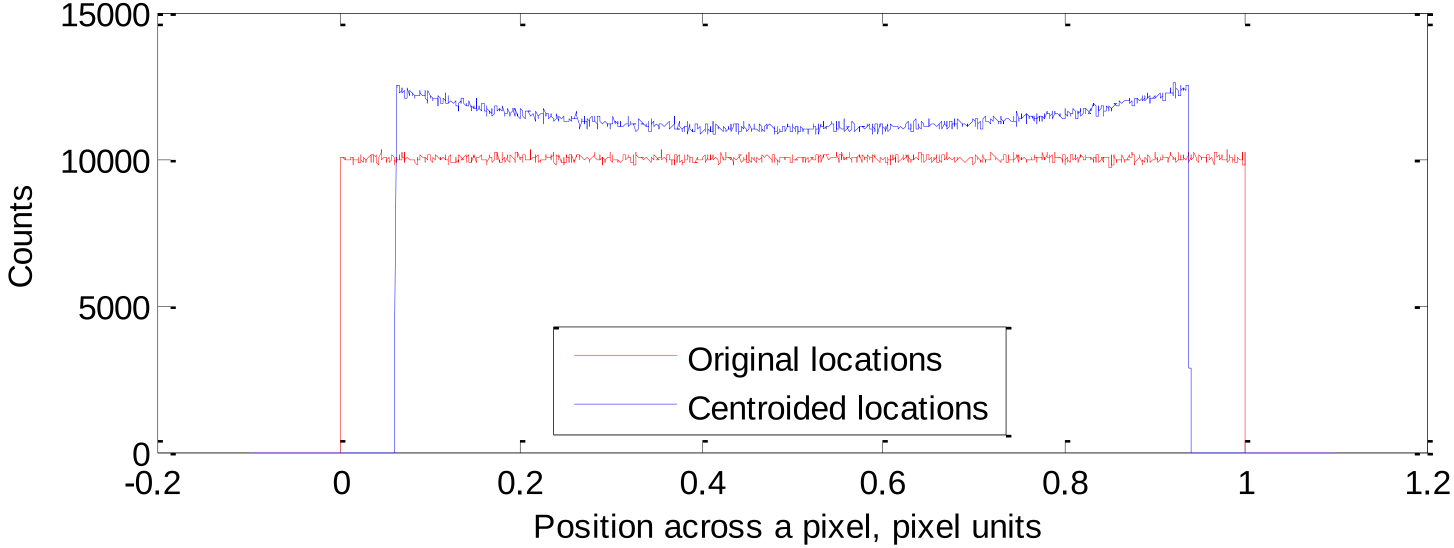
Solution: non-linear η algorithm

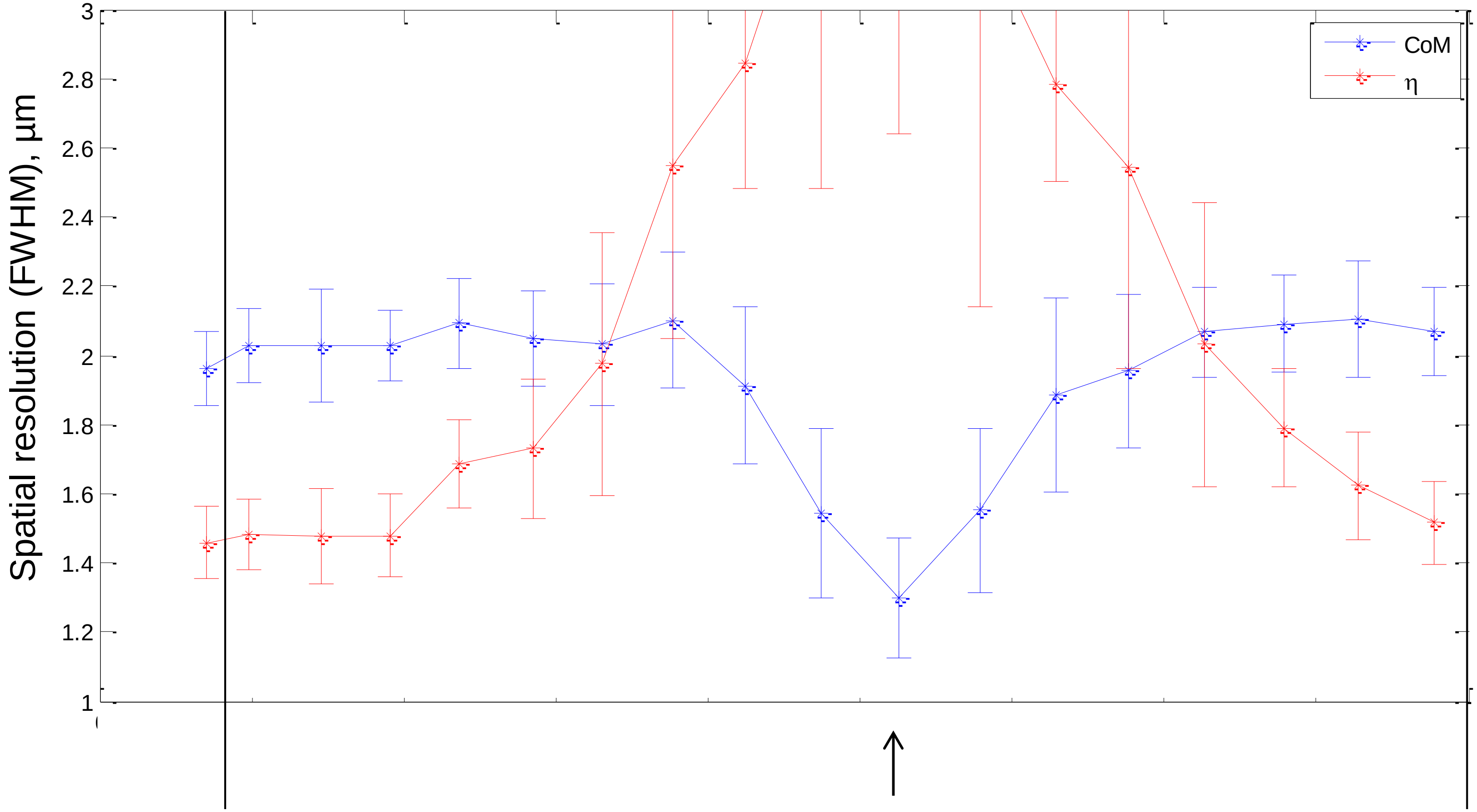
η

1) Like the simulation, use a flat field of X-rays.

2) Correct the linear centroided algorithm by knowing that the distribution of interaction positions should be a flat field



Spatial resolution – preliminary results

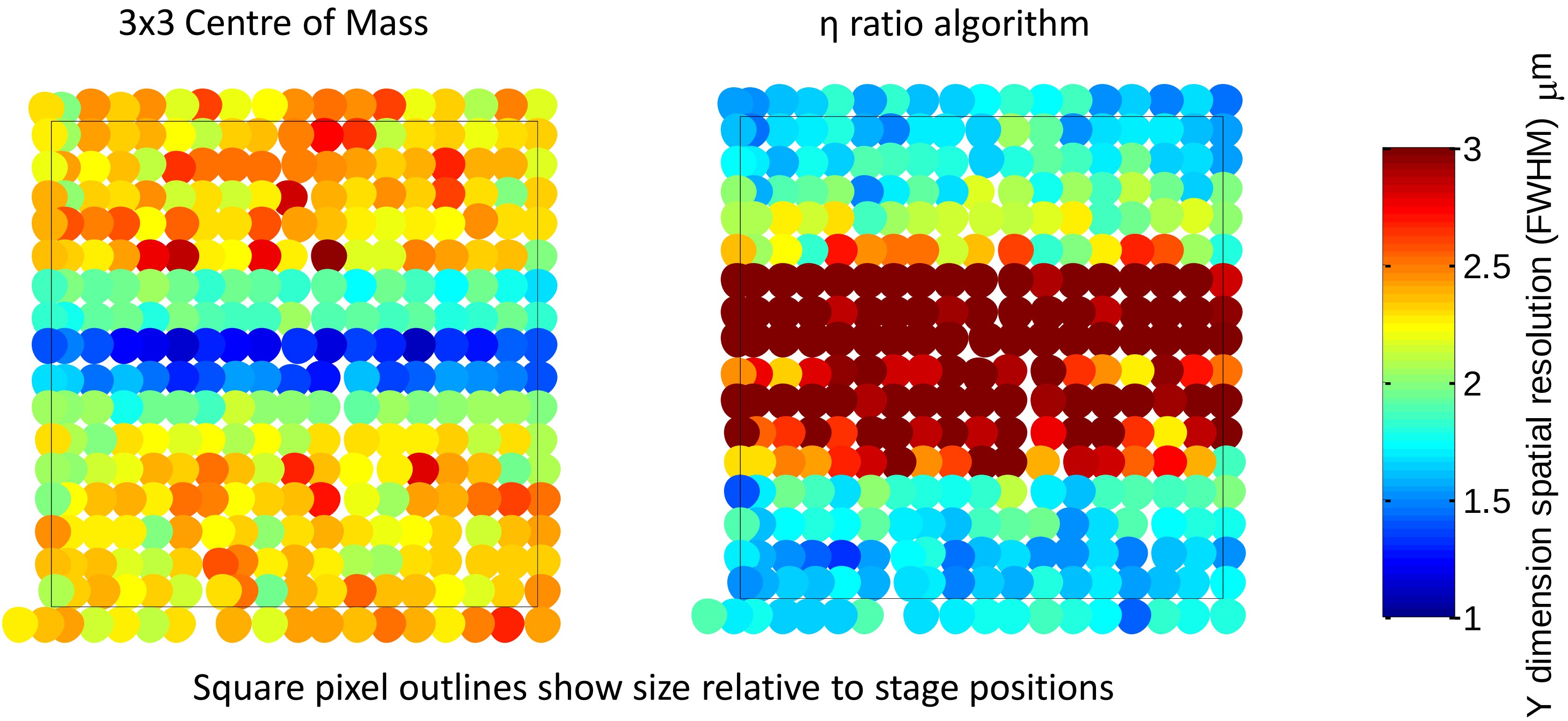


Edge of pixel

Centre of pixel

Edge of pixel

Spatial resolution – preliminary results



Square pixel outlines show size relative to stage positions

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5 µm goal is achievable

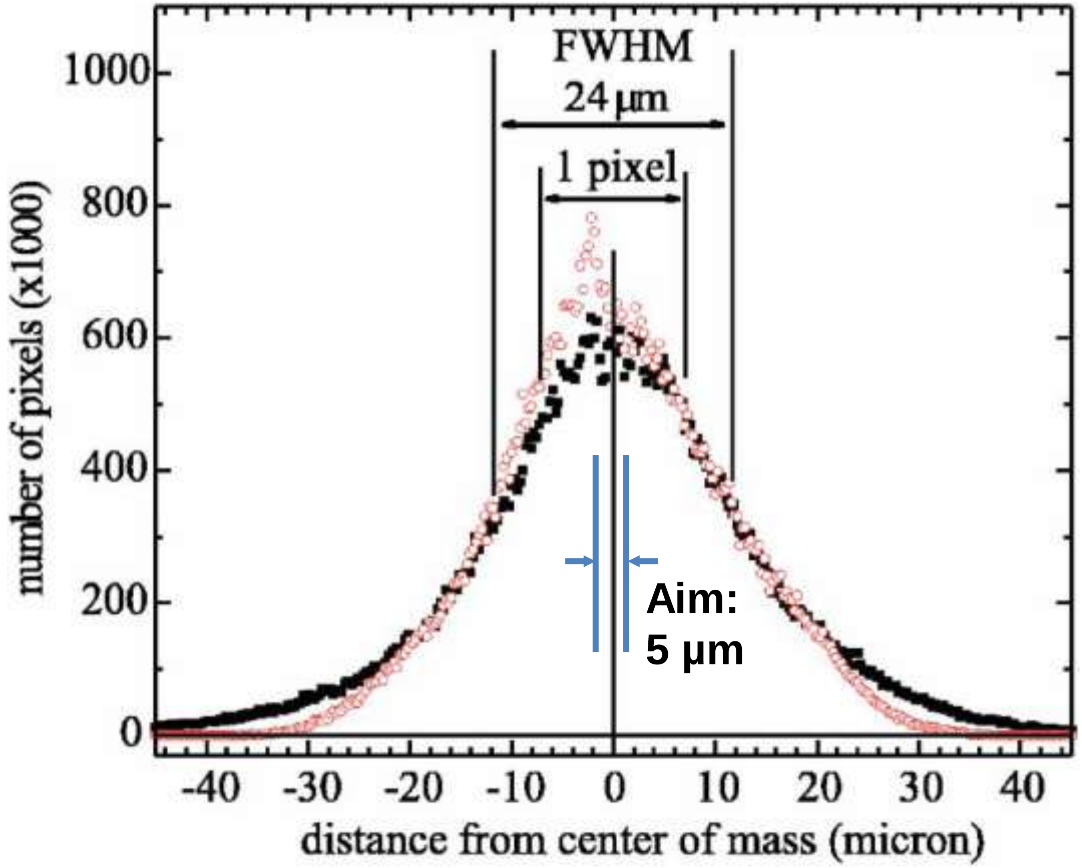

Figure from Ghiringhelli et al. (2006)

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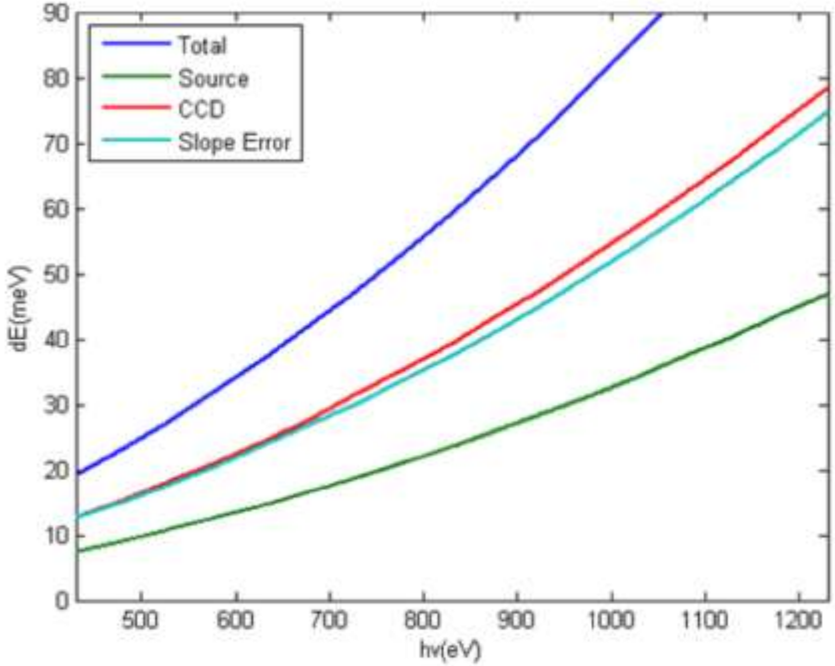
SAXES: improved energy resolution

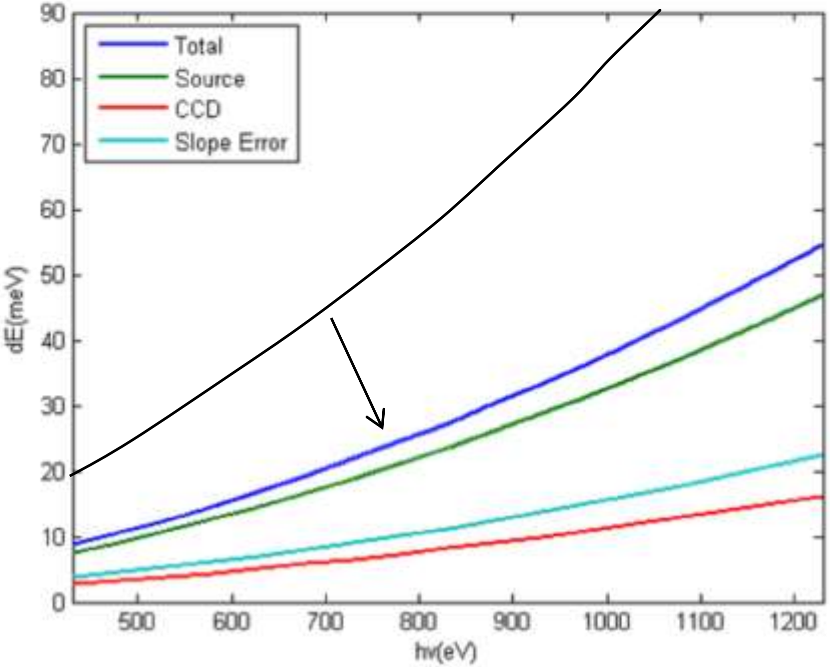


Current setup:

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

- In-depth investigation into applying eta non-linearity fix to further centroiding algorithms
- Further analysis of data collected during past experimental campaigns
- Supporting proposals to develop a new camera using this work

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Paul Scherrer Institut, 5232-Villigen Switzerland.

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The SAXES instrument was jointly built by the Paul Scherrer Institut and Politecnico di Milano, Italy.
The measurements have been performed at the PolLux facility at the Swiss Light Source, Switzerland.