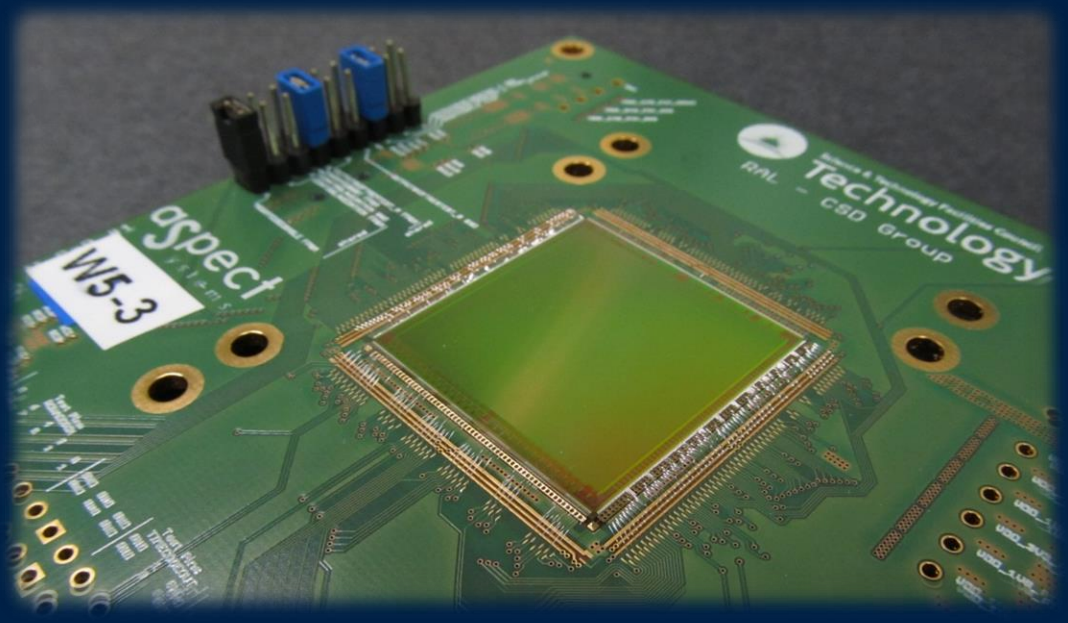
PImMS

Pixel Imaging Mass Spectrometry sensor



Jaya John John, on behalf of the PImMS Collaboration

11 September 2014, PSD10, University of Surrey

UNIVERSITY OF OXFORD
DEPARTMENT OF PHYSICS
DEPARTMENT OF CHEMISTRY
Science & Technology Facilities Council
Rutherford Appleton Laboratory

Outline

- Context and requirements for PImMS sensors
- PImMS1 and PImMS2 sensors
  - Specifications, design and operation
  - PImMS1 application results
  - PImMS2 application results
- Summary and future work

PImMS 1 ***PImMS 2***

Context – Imaging Mass Spectrometry

Combines time-of-flight mass spectrometry with 2D ion imaging – measuring time and x-y position

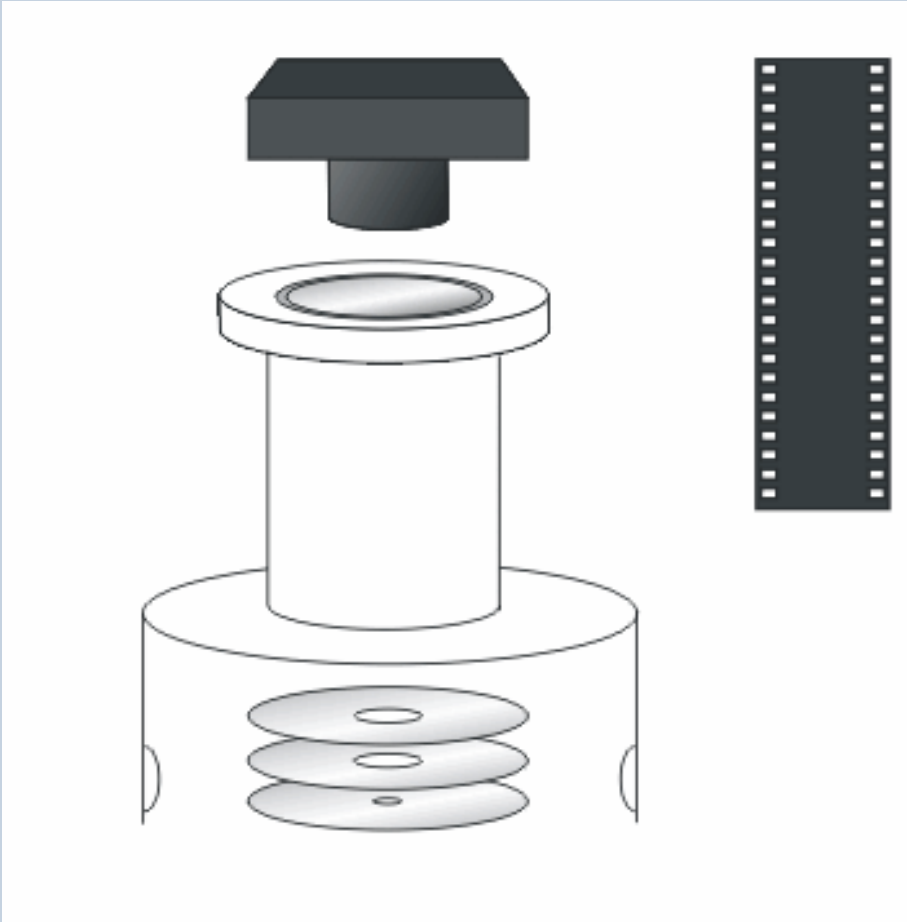
Basics of time-of-flight MS:

1) Molecules are dissociated and ionised – often with lasers

2) The ions are accelerated in an electric field created with charged plates = “ion optics”

3) Their time of arrival is proportional to their mass-to-charge ratio (m/z)

4) Ions arrive at a micro-channel plate (MCP), generating electron showers. Often these are converted to photons with a phosphor screen.



A time-of-flight mass spectrometer

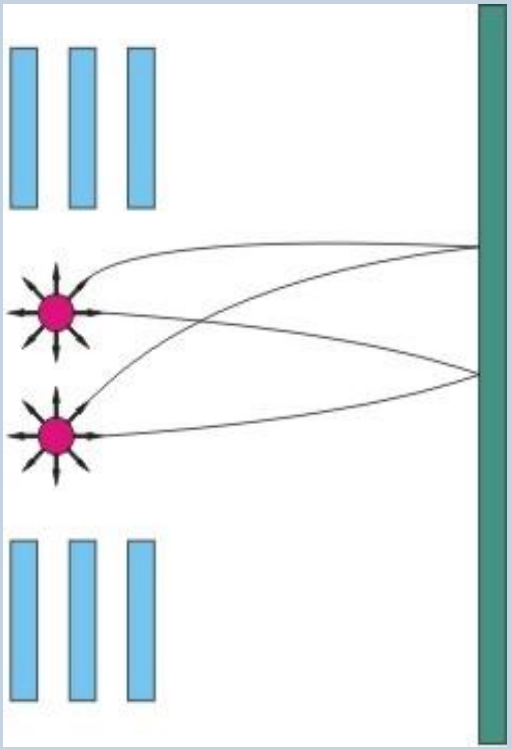
Context – Imaging Mass Spectrometry

Depending on how the ion optics are biased, we can image:

The velocities of the ions

= “velocity map imaging”

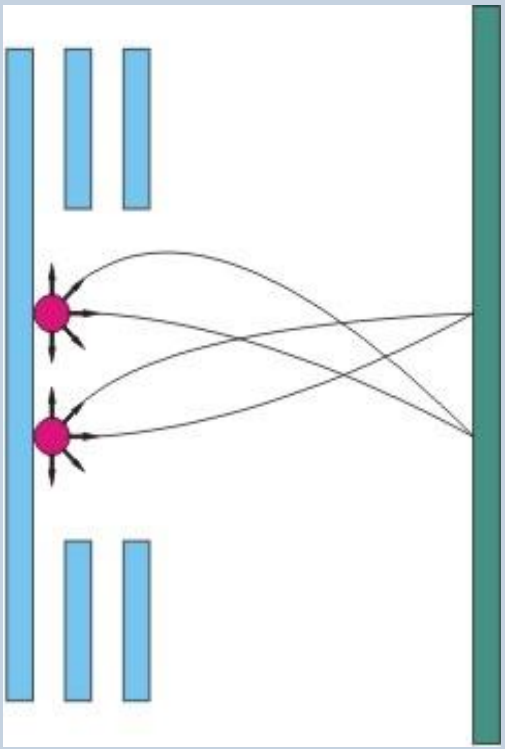
Learn about reaction dynamics



The positions of the ions

= “spatial imaging”

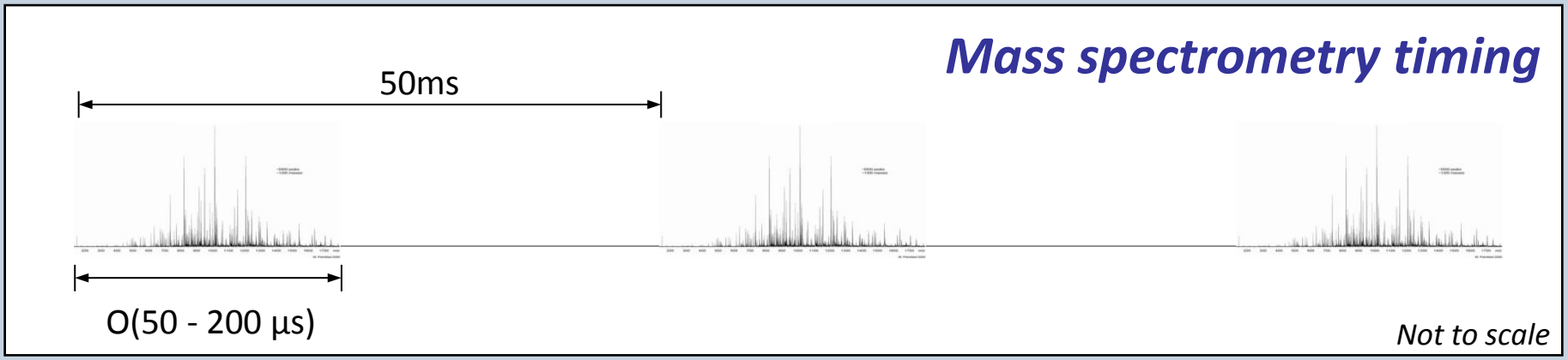
Can study tissue samples

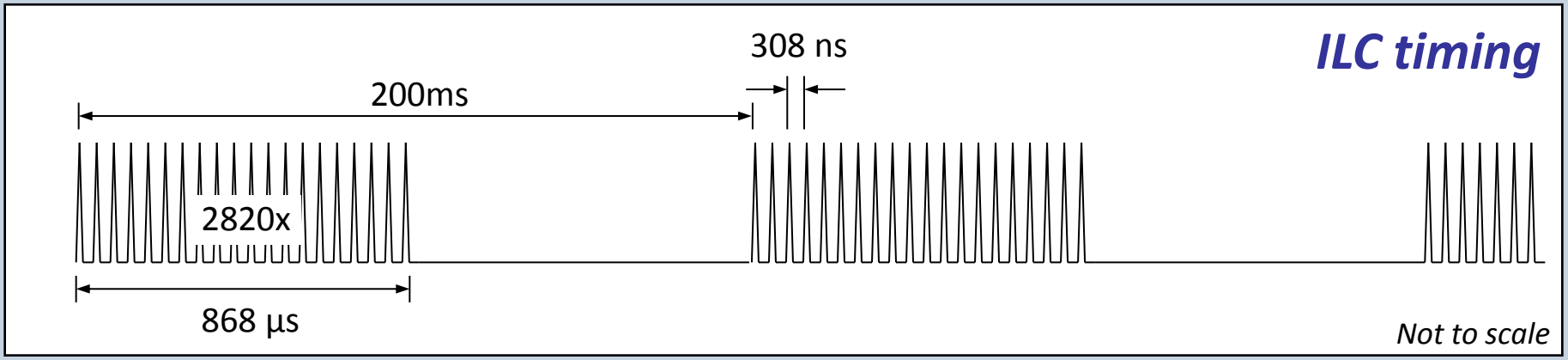


Context – timing structure of data

Mass spectrometry and the International Linear Collider have a similar time structure of data:

- MS: O(50 - 200 µs) duration @ 20 Hz
- ILC: 868 µs duration @ 5 Hz





A. Nomerotski

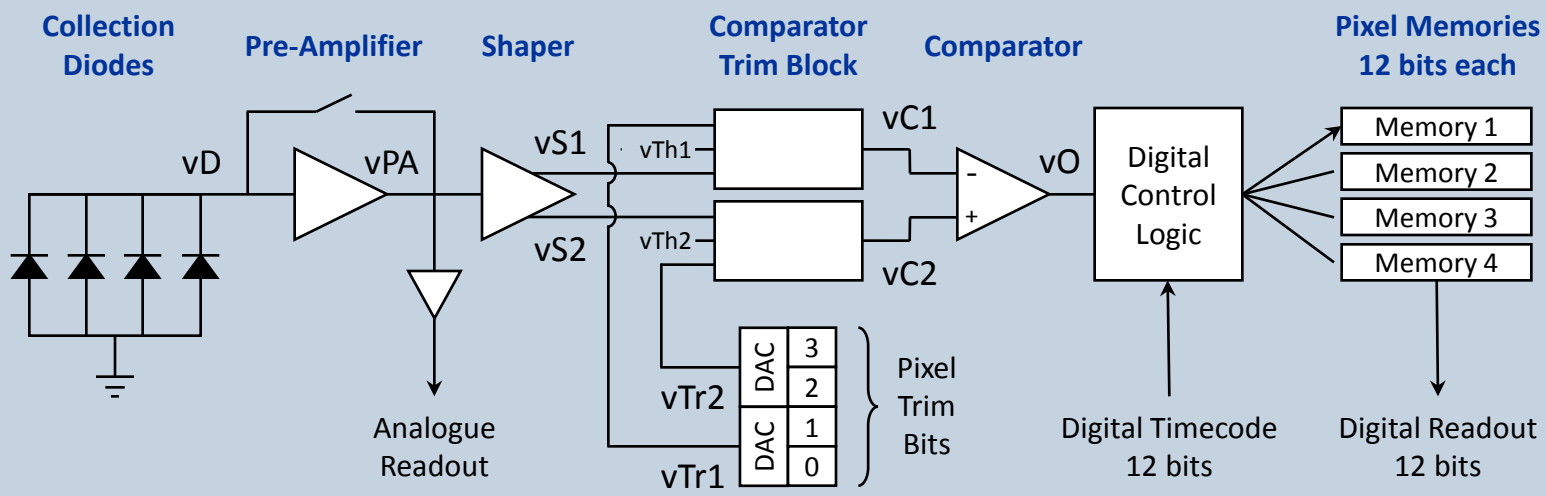
Requirements

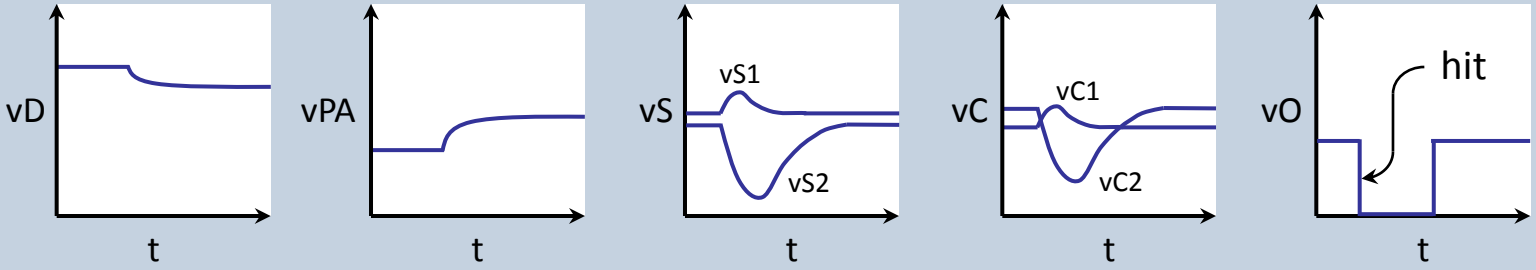
Requirement	Details
Self-triggering	Avoid needing prior knowledge of time of arrival of ions
Time-stamping and thresholding	Record the time of arrival of significant pulses of light (or electrons) as a digital timestamp
Storage of multiple timestamps	Avoid the 'loss' of a pixel after being hit once Optimised science versus pixel size constraints to arrive at 4 timestamps per pixel
Time resolution	Initial spec: 50ns time bins to gain sufficient mass resolution Updated spec after improvements to mass spectrometers: 12.5ns time bins
Length of experimental cycle	The period when ion data should be recorded is generally 50 - 200µs long
Readout frame rate	10 Hz minimum, higher desirable Based on repetition rate of commonly-used lasers

PImMS sensors: specifications

Spec	PImMS1	PImMS2
Array size	72 x 72 pixels	324 x 324 pixels
Active area	5mm x 5mm	22.7mm x 22.7mm
Sensor size	7mm x 7mm	25.4mm x 26.1mm
Pixel size	70µm x 70µm	
Pixel threshold trim	4 trim bits + 1 masking bit per pixel	
Timestamp storage	Four 12-bit registers per pixel	
Test pixel	1 test pixel with access to inner analogue nodes	
Time resolution (timecode period)	Initial spec: 50ns Simulation target: 25ns	
Current performance	12.5ns timecode period	
Substrate	5µm epi	5µm epi 18µm high-resistivity epi

PImMS pixel


Collection Diodes
Pre-Amplifier
Shaper
Comparator Trim Block
Comparator
Pixel Memories 12 bits each
vD
vPA
vS1
vS2
vTh1
vTh2
vC1
vC2
vO
Digital Control Logic
Memory 1
Memory 2
Memory 3
Memory 4
DAC
DAC
3
2
1
0
vTr2
vTr1
Pixel Trim Bits
Analogue Readout
Digital Timecode 12 bits
Digital Readout 12 bits


vD
t
vPA
t
vS
vS1
vS2
t
vC
vC1
vC2
t
vO
hit
t

Pixel operation

diode

preamplifier

shaper

comparator inputs

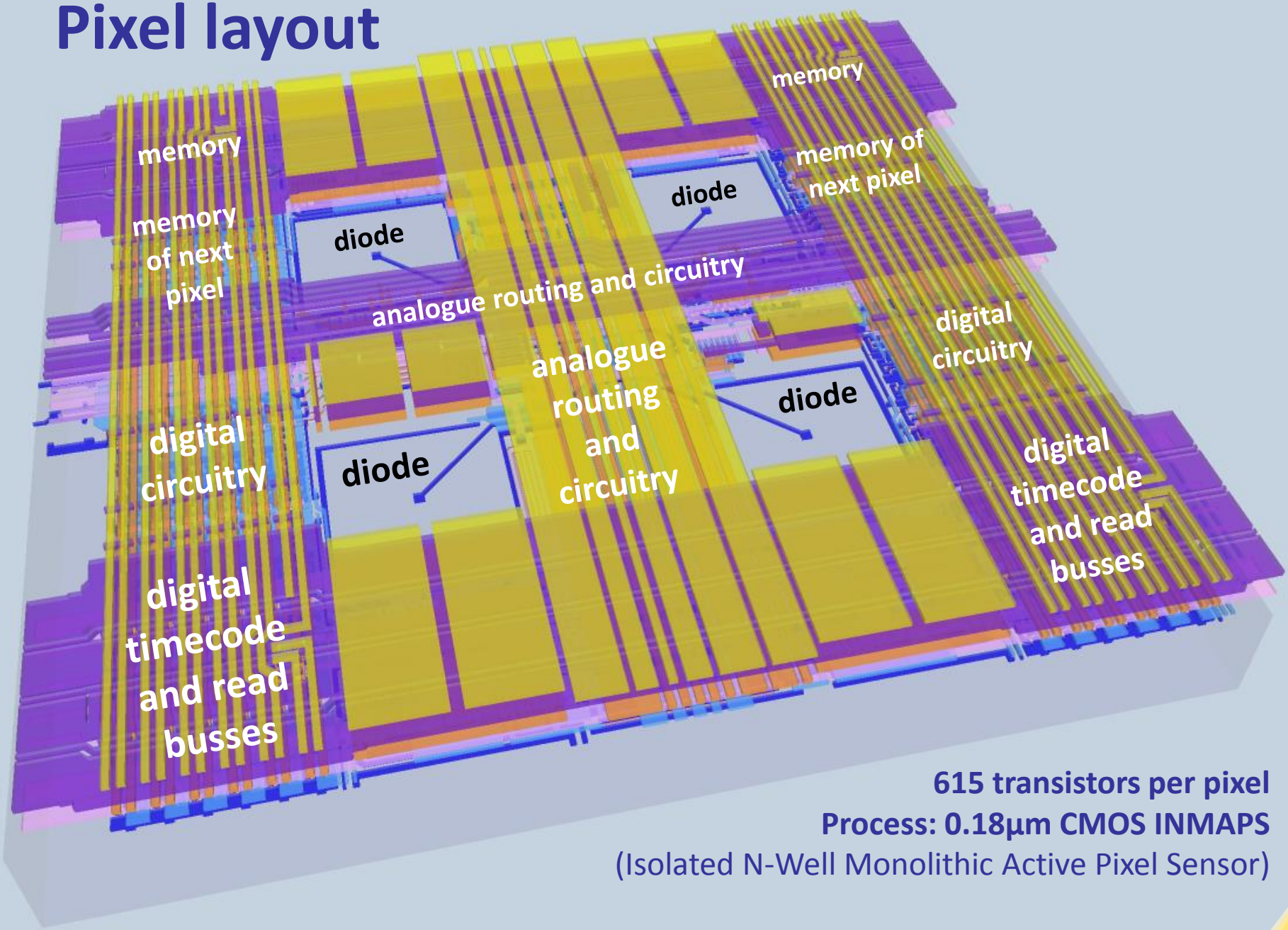
hit indicator

timecode

memory 1

memory 2

Pixel layout



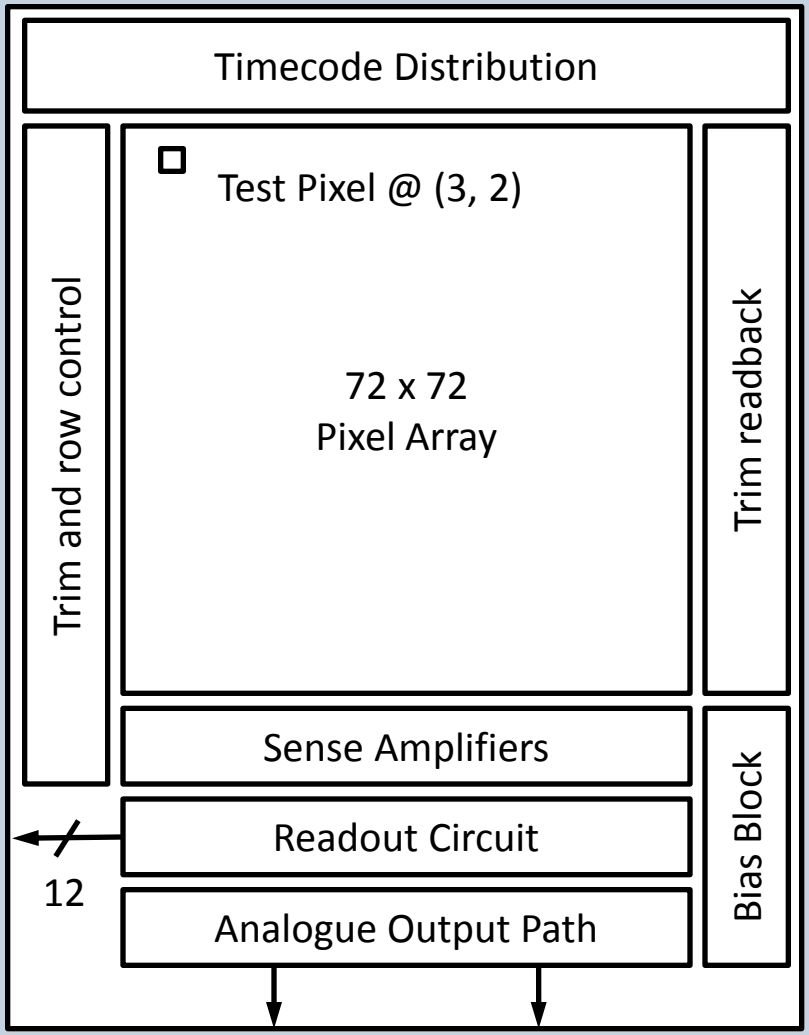
615 transistors per pixel

Process: 0.18µm CMOS INMAPS

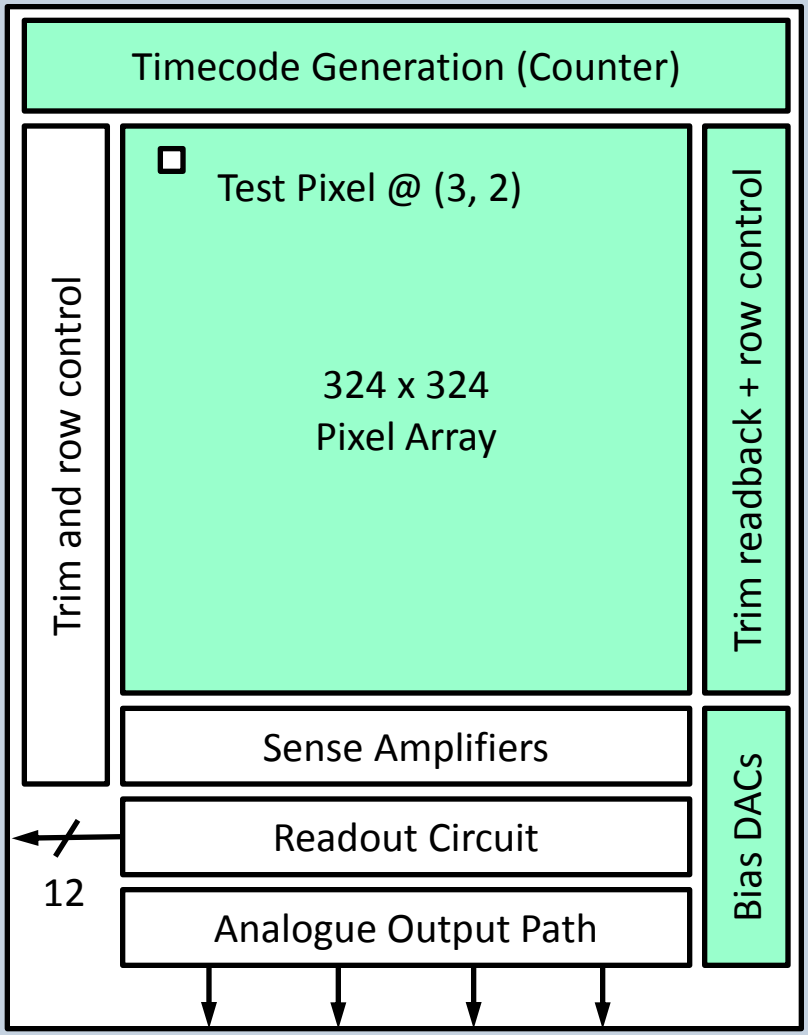
(Isolated N-Well Monolithic Active Pixel Sensor)

PImMS sensors: overview

PImMS1

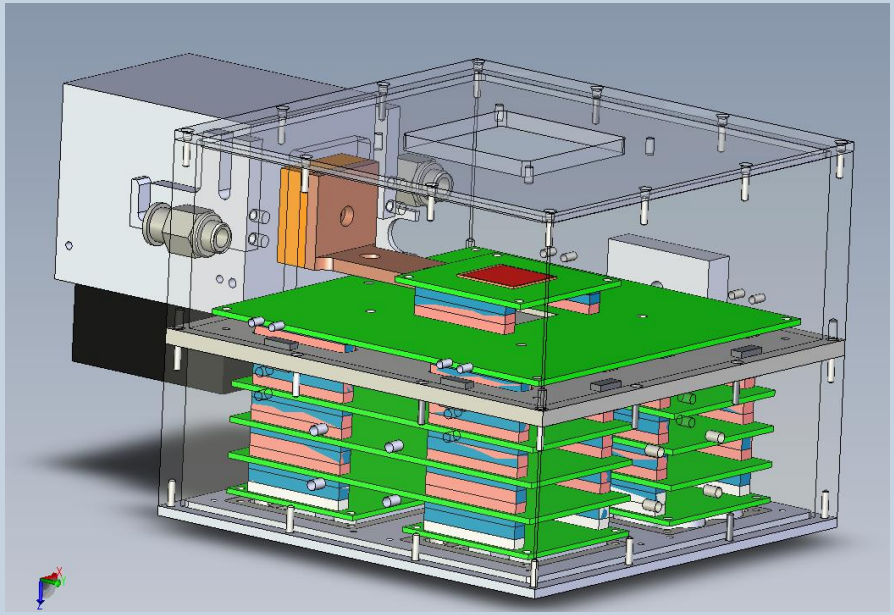


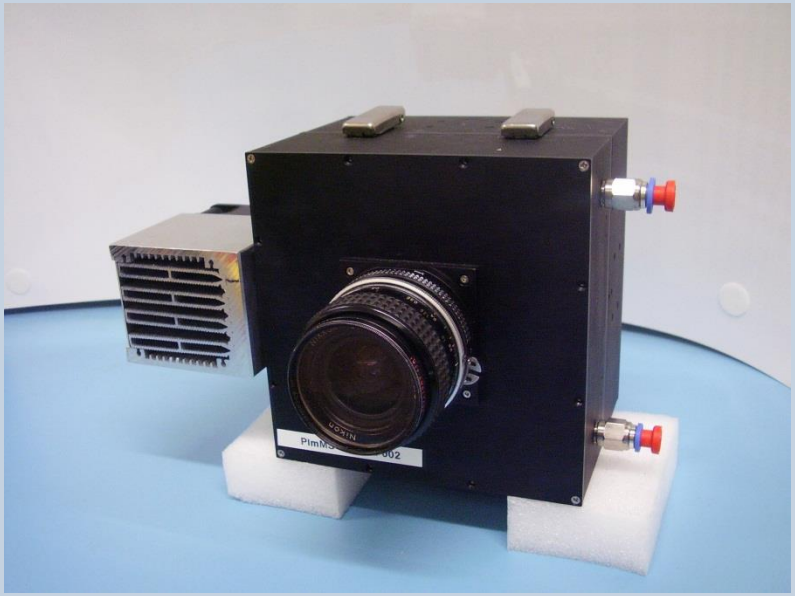
PImMS2



Readout: camera

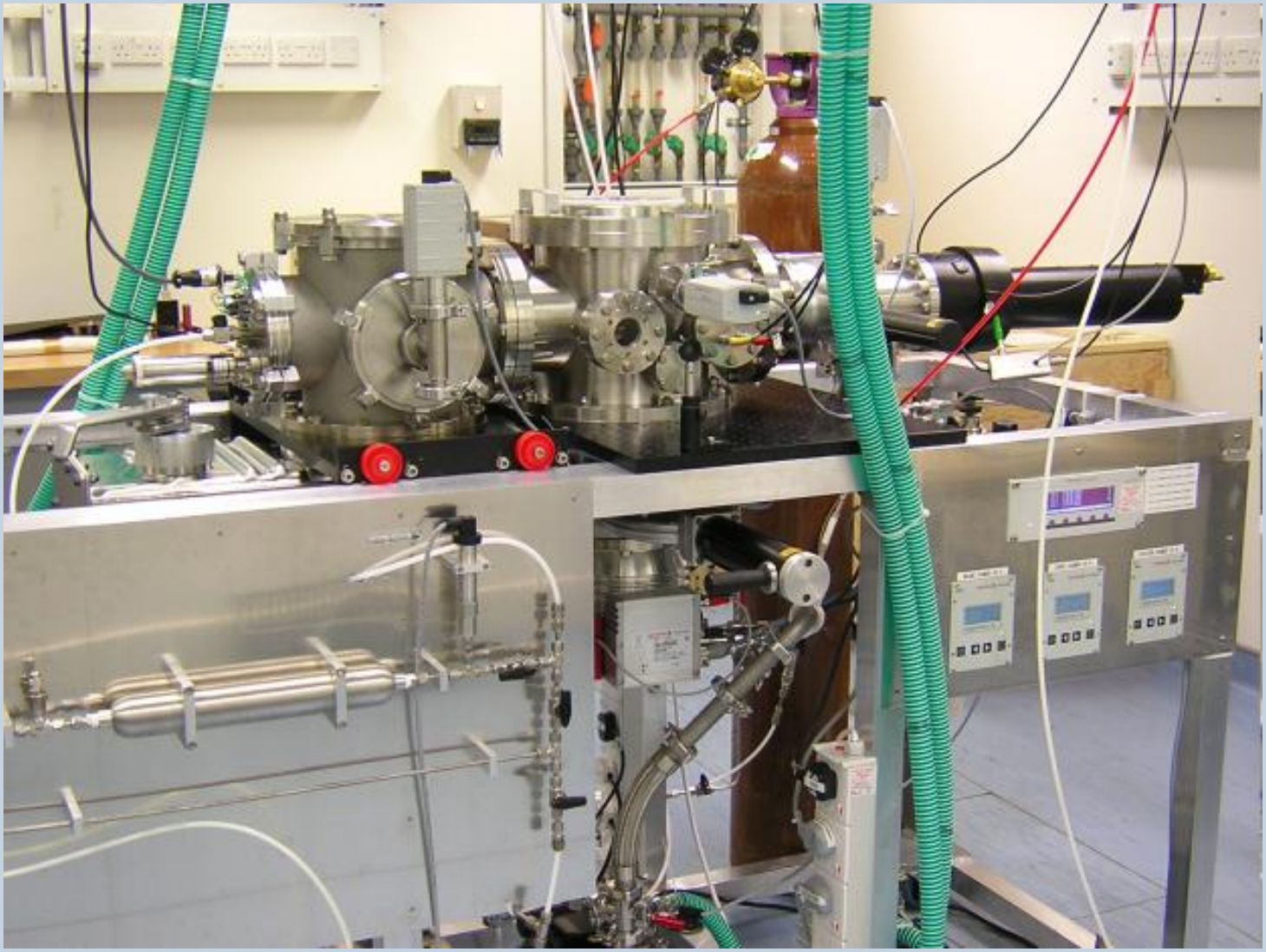
- USB control and readout
- F-mount SLR lens
- C-mount SLR lens also possible – delivers more light to sensor





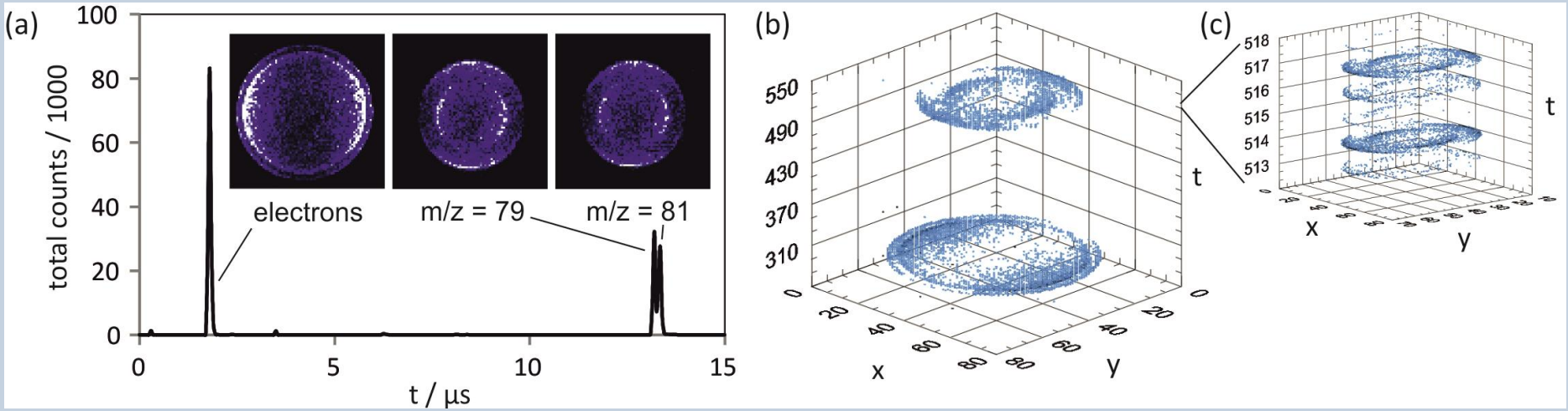
- Cooling system based on copper finger and Peltier device
- Connection for nitrogen/dry air flushing

Application results



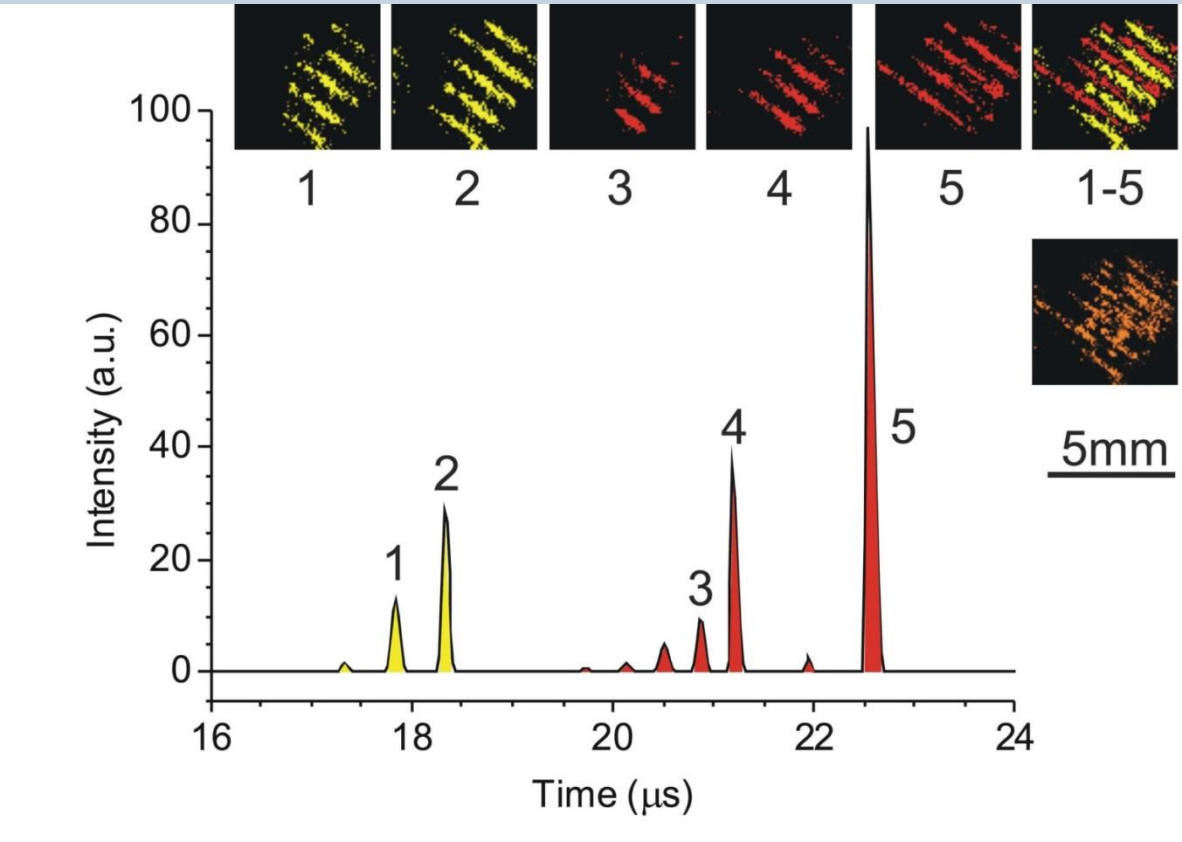
Coincidence imaging

- Here bromine gas (Br_2) is dissociated. By switching the polarity of the ion optics, first the electrons are imaged, then the ions.
- (a) shows the mass spectrum including $^{79}Br^+$ and $^{81}Br^+$
- (b) shows the mass intersections for the electrons and Br ions
- (c) zooms in on the two isotopes, $^{79}Br^+$ and $^{81}Br^+$



A.T. Clark *et al.*, *J. Phys. Chem. A* **116**, 10897, (2012).

Spatial imaging

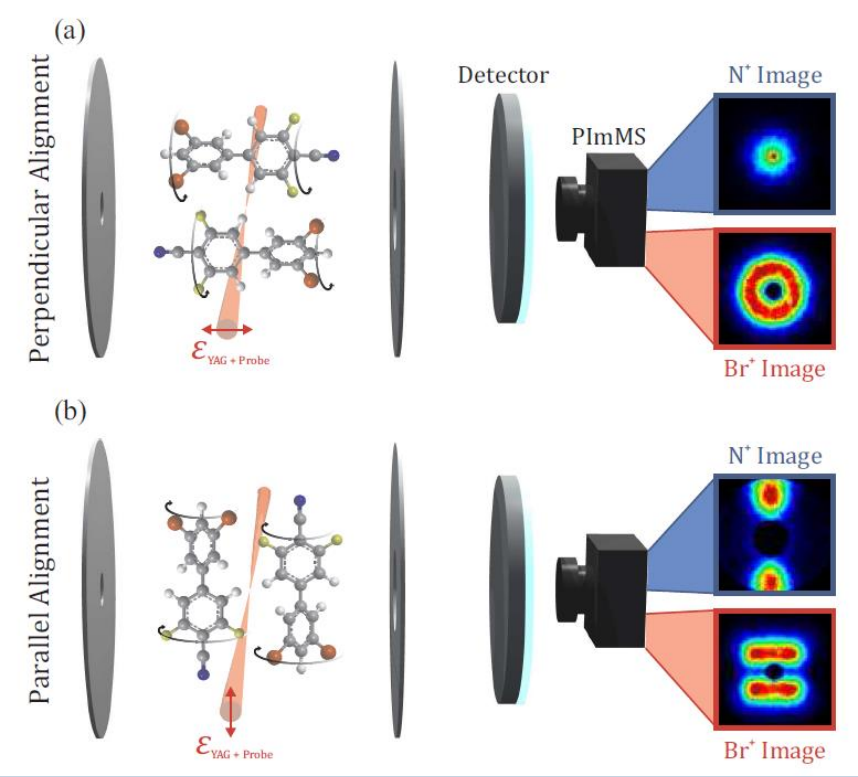


M. Brouard *et al.*, *Rev. Sci. Instrum.* **83**, 114101, (2012)

- This is imaging the mass spectrum over a 2D surface.
- Materials used: lines of Auramine O (yellow) and Rhodamine 590 (red)
- The samples produced 10 mass peaks in all. 5 are highlighted here.
- Data taken at 25ns time resolution
- Demonstrates multi-mass imaging

Coulomb Explosion Imaging

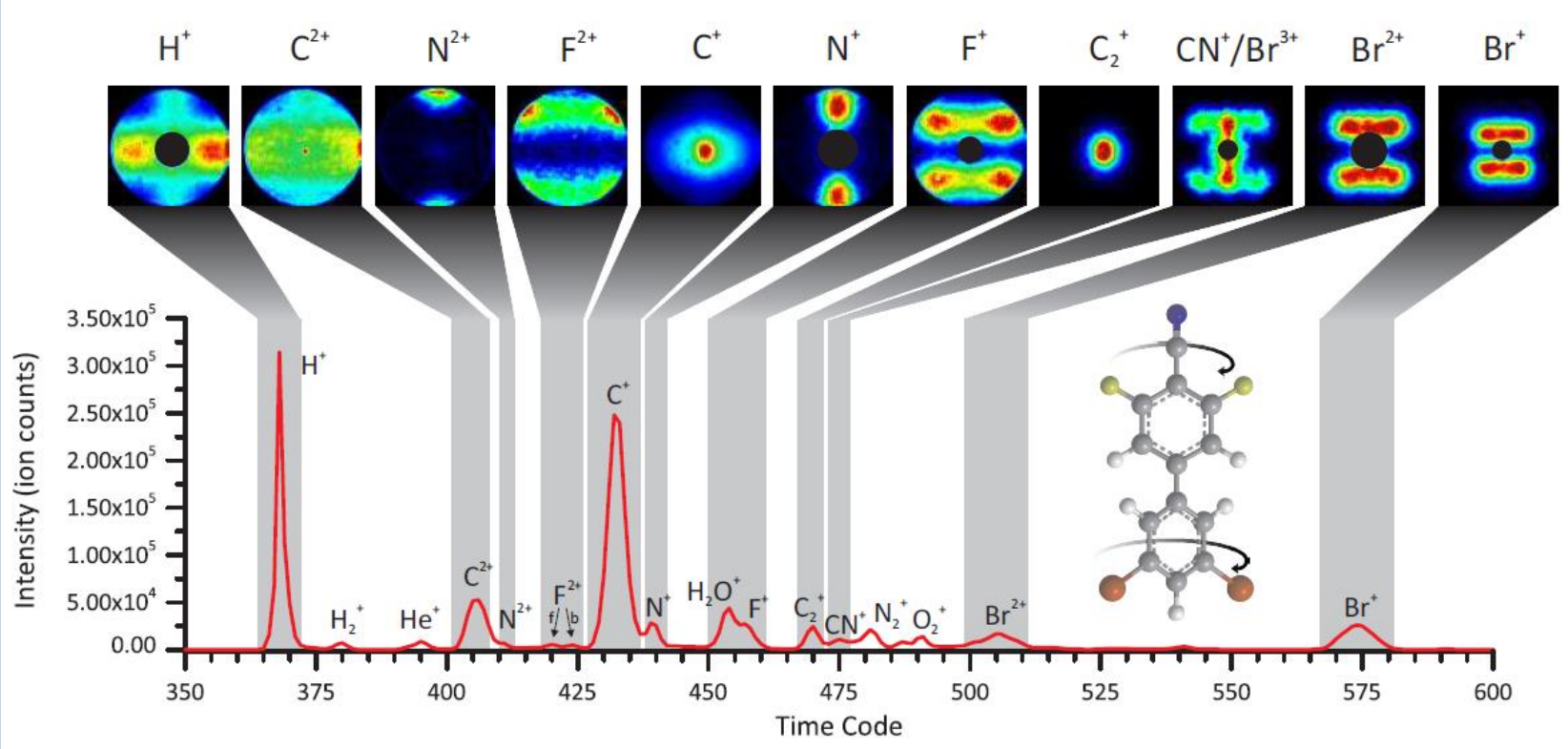
- Using PImMS to record images on Henrik Stapelfeldt's coulomb explosion rig
- Acknowledgements: Aarhus: Henrik Stapelfeldt, Lauge Christensen, Jens Nielsen
- Oxford: Craig Slater, Alexandra Lauer, Sophie Blake



C.S. Slater *et al.*, *Phys. Rev. A* **89**, 011401(R), (2014).

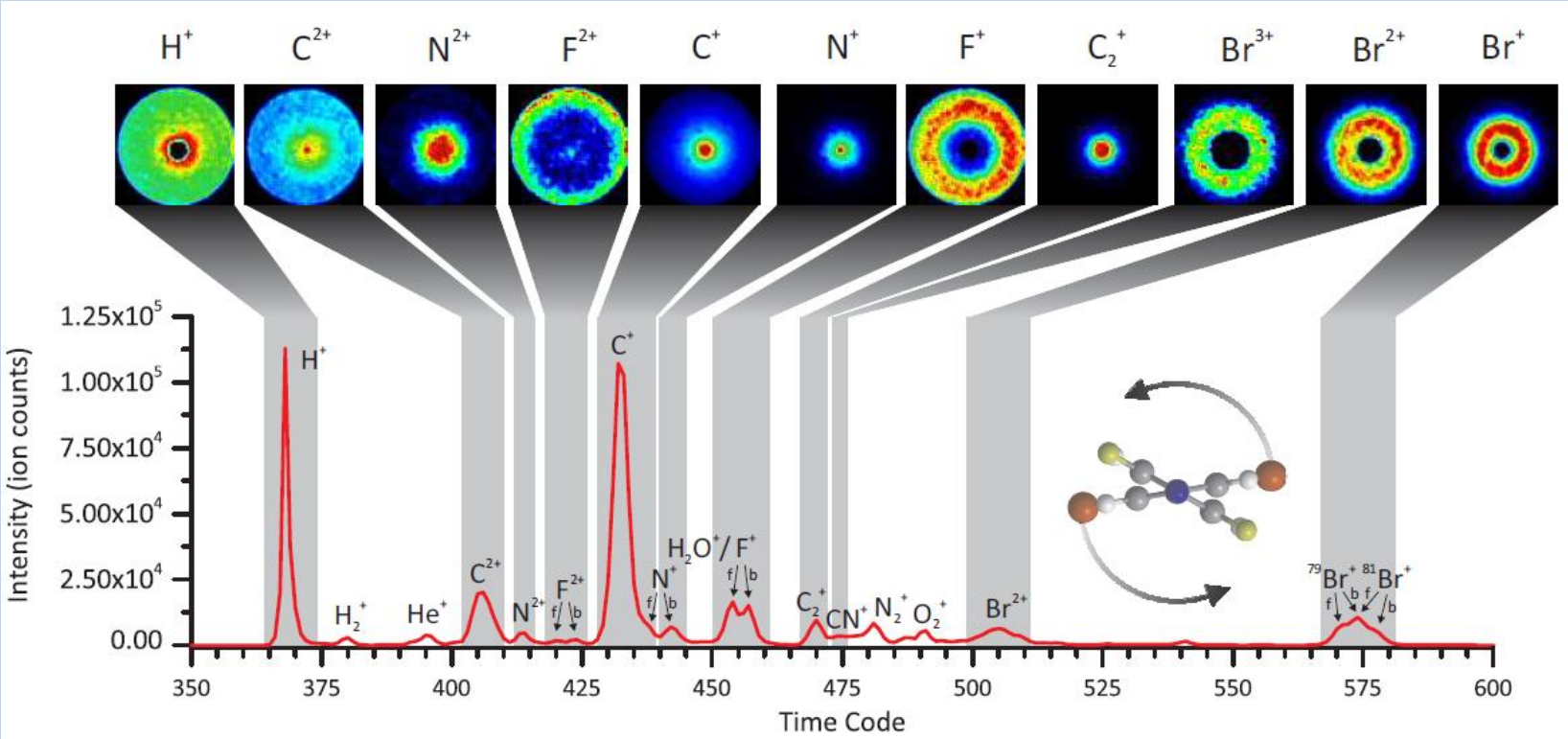
- A biphenyl molecule is aligned using a 1064 nm, 10 ns pulse, linearly polarised (from a Nd:YAG laser, 20 Hz)
- It is then ionised using an 800 nm, ~ 30 fs probe pulse (amplified Ti:Sapphire laser)
- Stripped of valence electrons, the molecule breaks up due to electrostatic repulsion, termed a coulomb explosion

Coulomb Explosion Imaging 2



Parallel 1D alignment and Coulomb explosion imaging

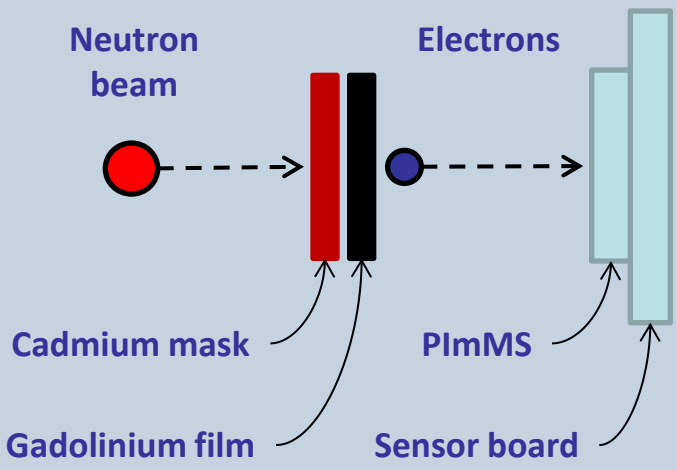
Coulomb Explosion Imaging 3



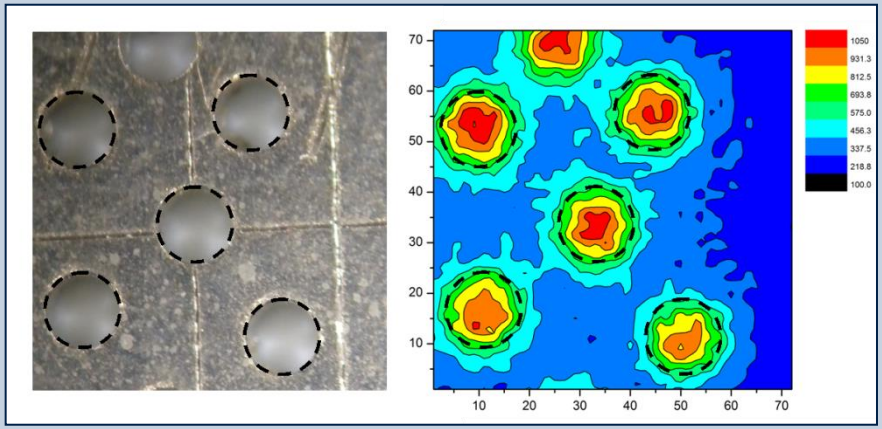
Perpendicular 1D alignment and Coulomb explosion imaging

Neutron detection

- Daniel Pooley of ISIS' Neutron Detectors Group is developing a neutron detector based on PImMS, working with Jason Lee (Oxford Chemistry)
- Gadolinium is thinly sputtered onto the surface of PImMS (4µm) which creates showers of electrons immediately above the pixel array
- Here are early results using a cadmium mask to demonstrate neutron sensitivity:

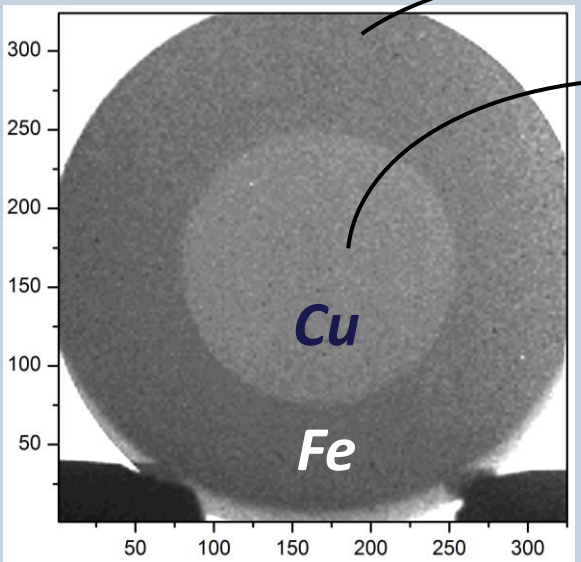


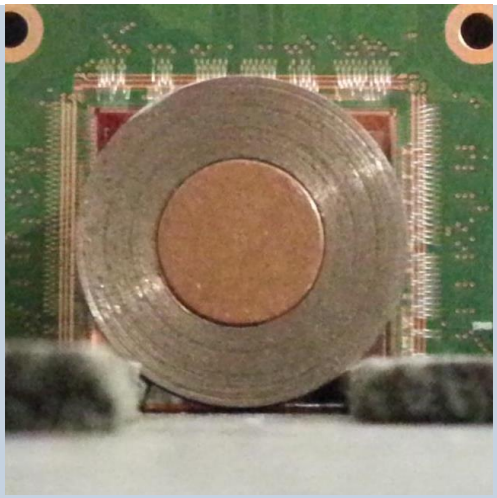
Not to scale

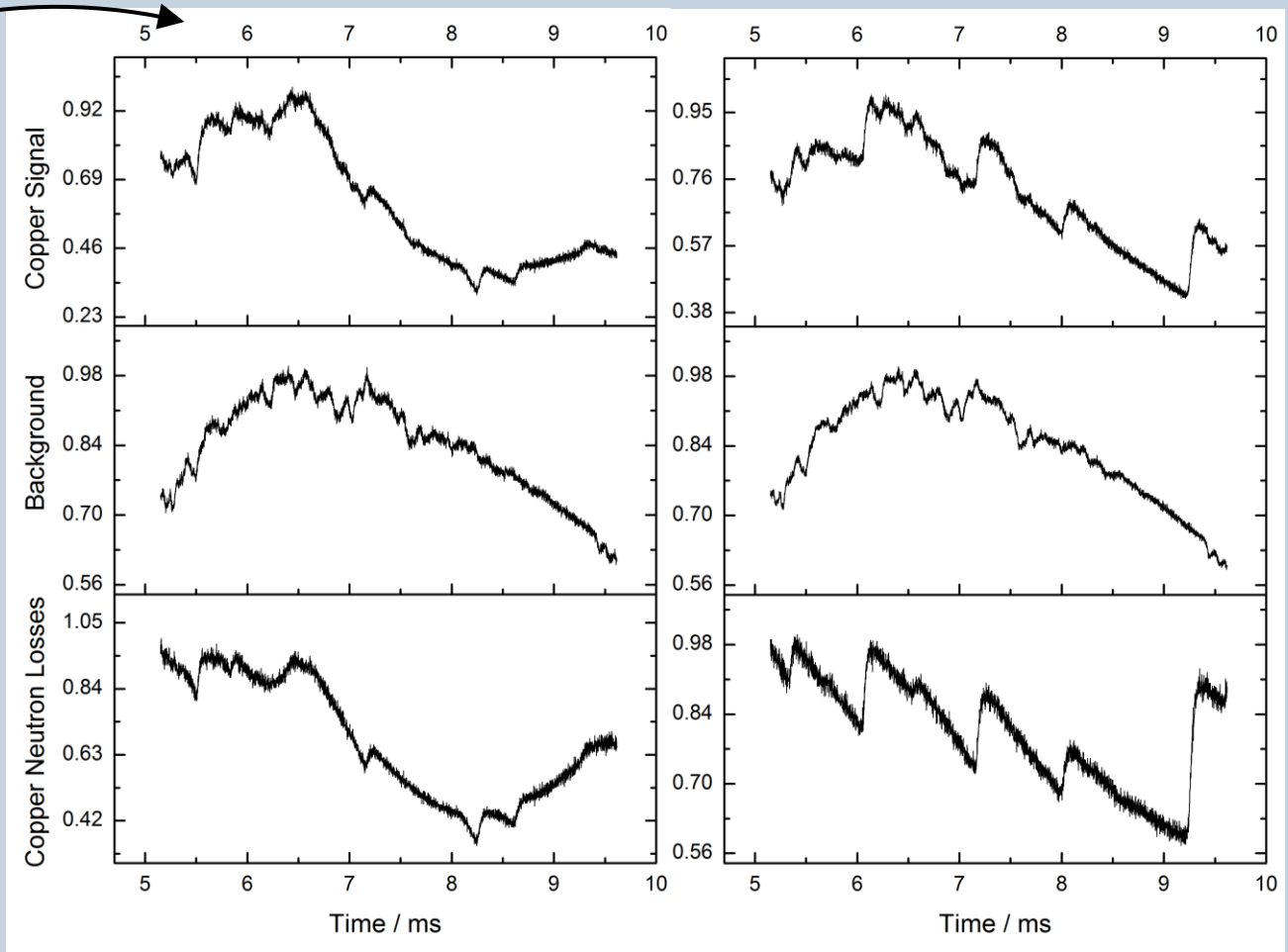


DE Pooley, JWL Lee

Imaging two materials with PImMS2 (GP2)

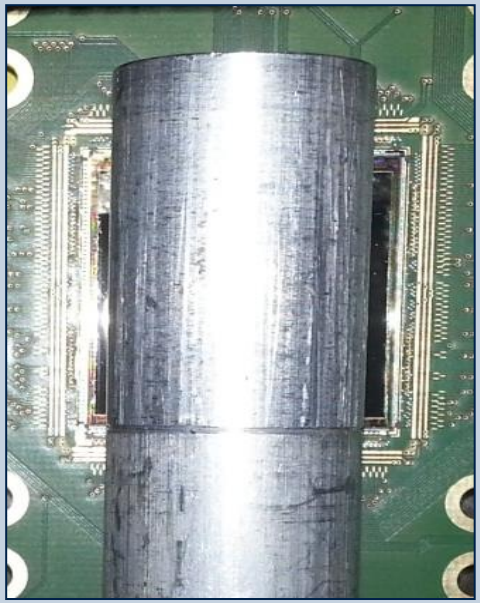


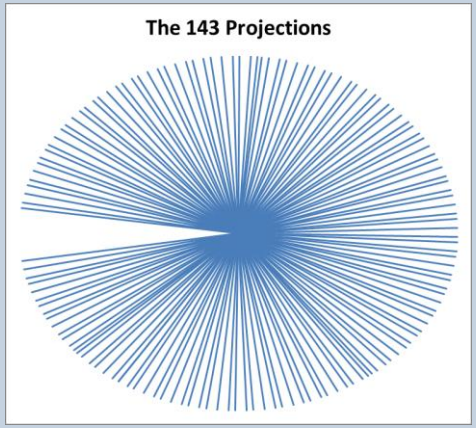


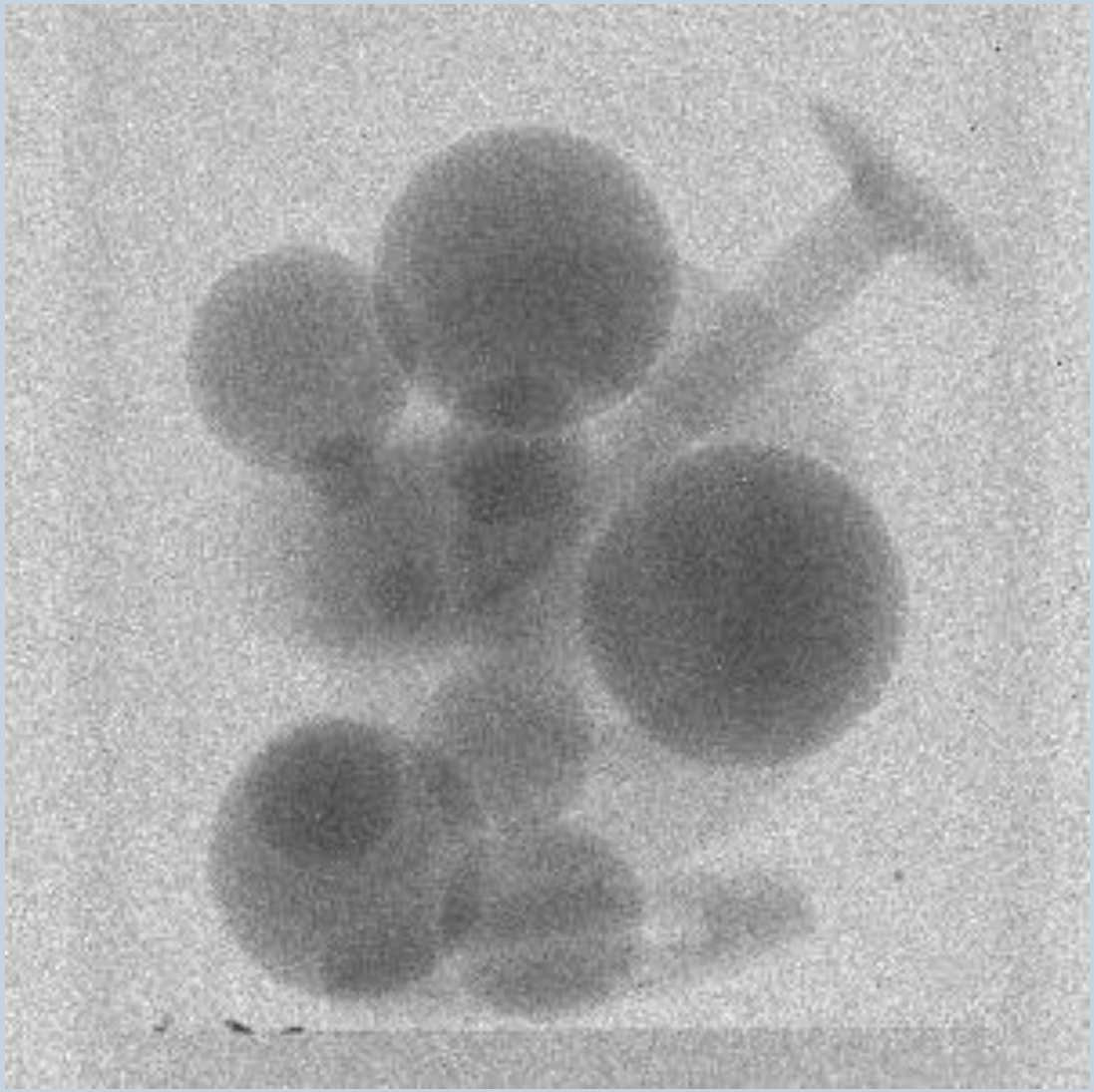


DE Pooley, JWL Lee

Neutron tomography – assorted metal

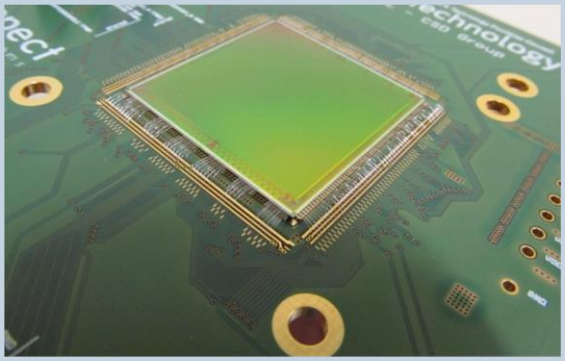






Summary and future work

- PImMS is a self-triggered time-stamping sensor.
- Initially designed for imaging mass spectrometry, it has also been successfully applied to neutron imaging.
- PImMS1 is producing science in a variety of chemistry applications.
- PImMS2 is under development as a neutron imaging sensor.



PImMS 2

- PImMS2 is currently being commissioned for chemistry work – calibration is under development.
- Once PImMS2 calibration is established, much interesting sensor characterisation becomes possible.

Thank you for your attention. Questions?

The PImMS Collaboration

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Andrei Nomerotski, **Richard Nickerson**, Todd Huffman, Jaya John John, Richard Makin
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Renato Turchetta, Iain Sedgwick, Jamie Crooks (Andy Clark)
STFC Rutherford Appleton Laboratory

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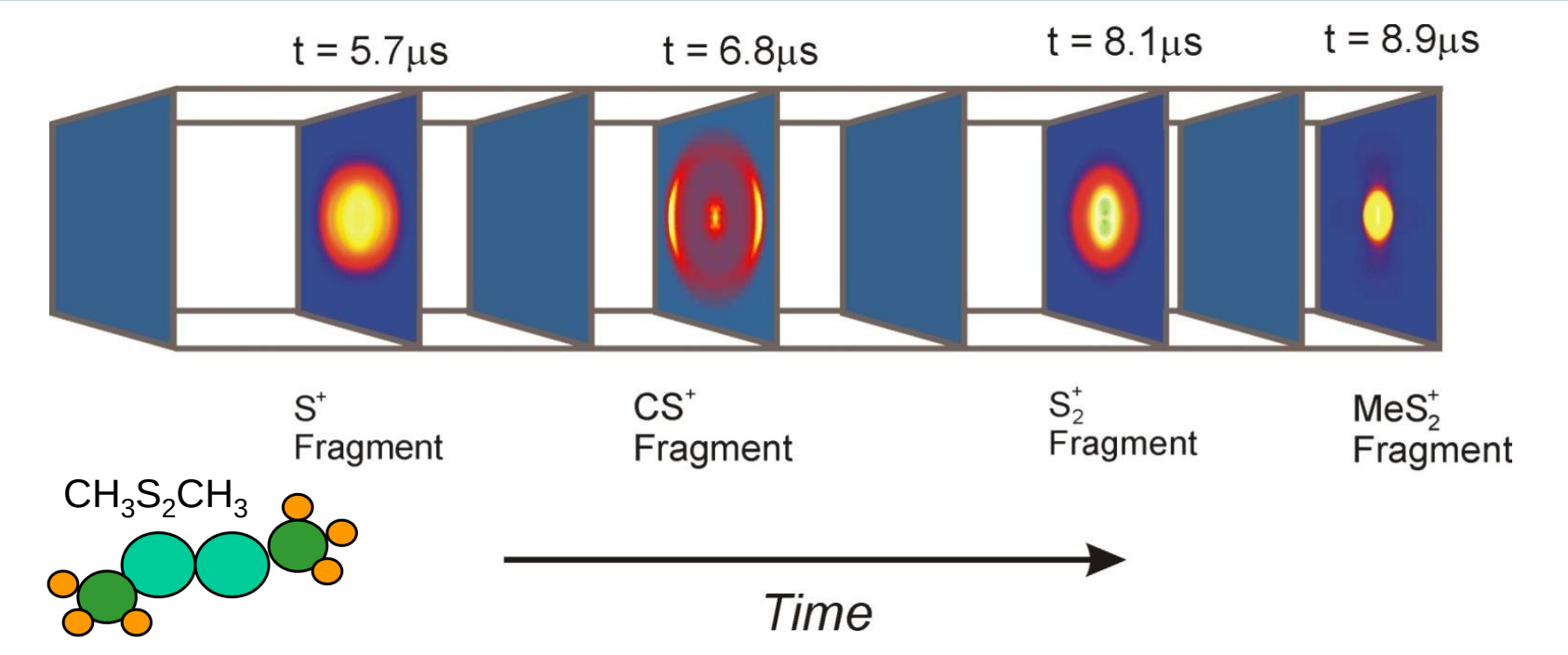
Backup material

Requirements: self-triggering

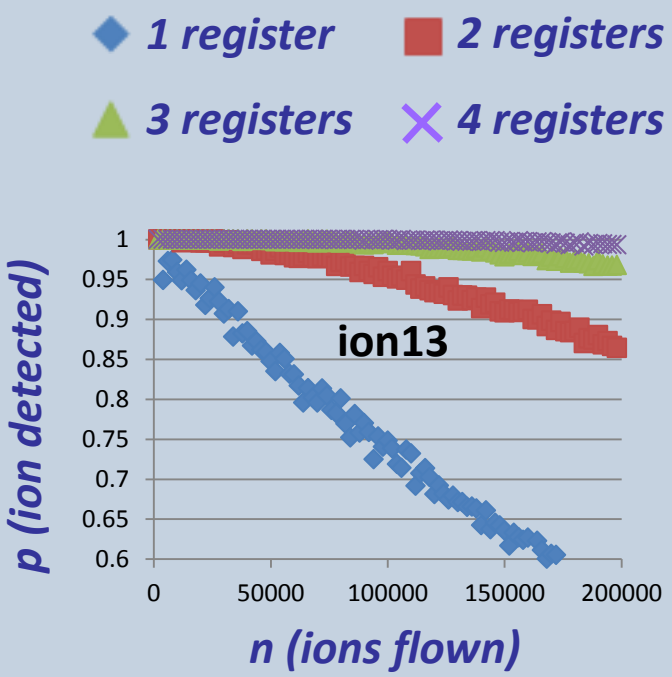
- Proof of concept experiments with a fast-framing camera: multiphoton fragmentation of dimethyldisulfide (images recorded in 2008 using a Dalsa Zenith CCD camera).
- Required prior knowledge of timing of mass peaks, programming the framing for the known time of arrival of each peak.

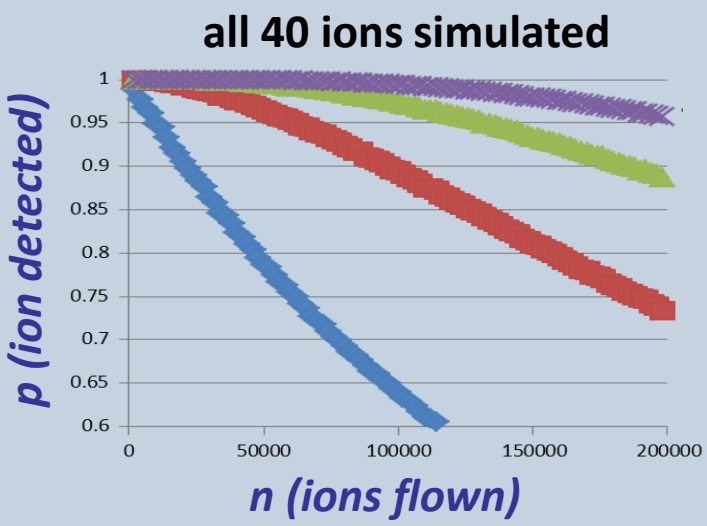


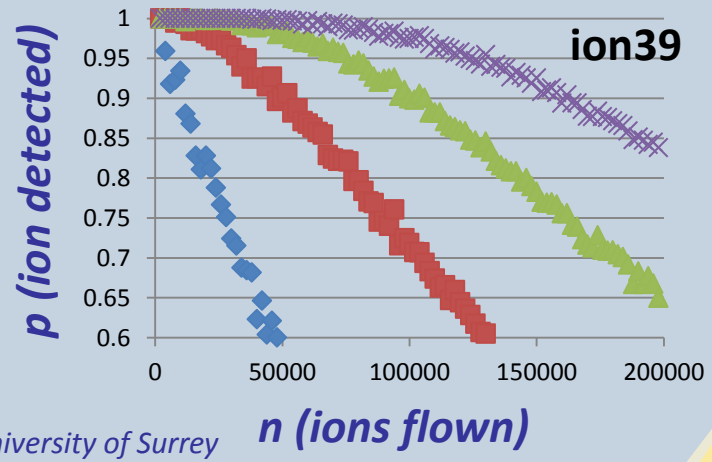
M. Brouard, E.K. Campbell, A.J. Johnsen, C. Vallance, W.H. Yuen, and A. Nomerotski, Rev. Sci. Instrum. 79, 123115, (2008)

Requirements: multiple timestamps

- Want a fast sensor, flexible to analyse any mass spectrum
- Sparse events → consider time-stamping approach
- To record both early and late ions, need multiple memories. How many? Simulate:

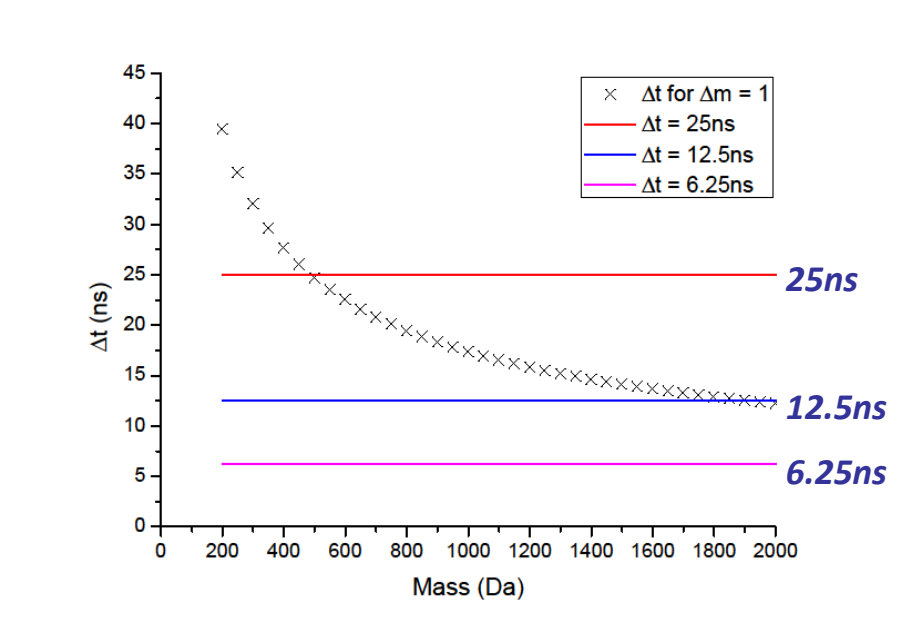






Requirements: timing resolution

- Initial spec for time resolution: 50ns
- Updated spec, based on our significant progress in mass spectrometer timing, is to distinguish ions with a mass difference of 1 Dalton over a wide range of masses.
- This gives an updated target spec of 12.5ns



Time Resolution for Δm = 1

If we want Δm = 1:

- $m/\Delta m \approx t/2\Delta t$
- $\Delta t = t/2m$