Non-standard configuration of SANS instruments

Charles Dewhurst

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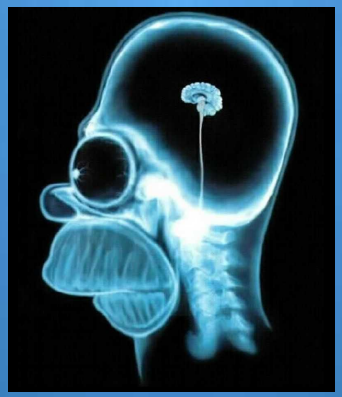
France

Neutrons

Mad Ideas



Sorry, no x-rays

'Screwing around with your SANS instrument'

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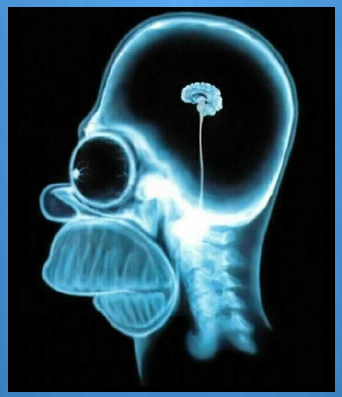


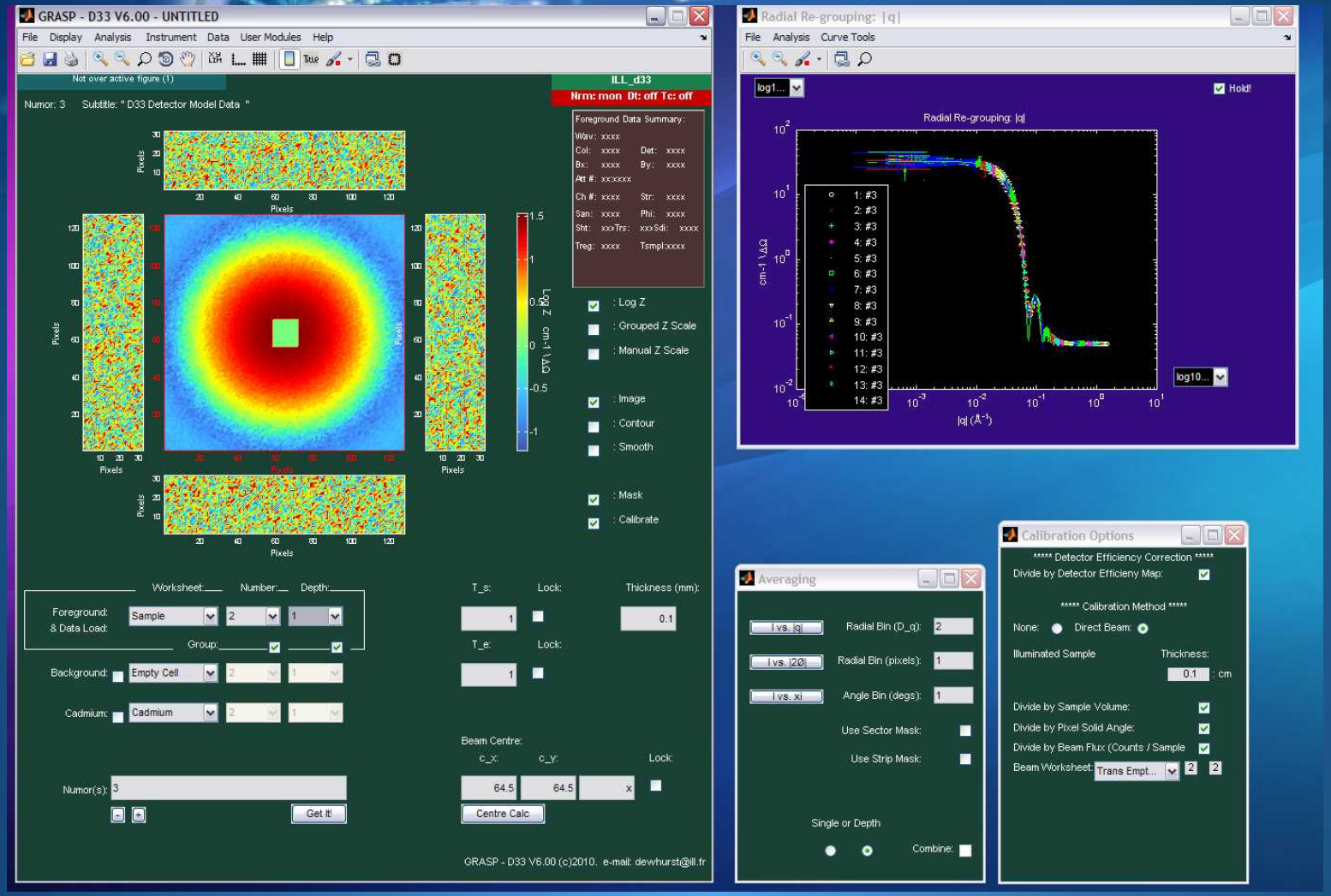
Sorry, no x-rays

'Screwing around with your SANS instrument'

- Very important for your sanity
- Relieves 'local-contact boredom'
- Great fun
- Often gets you in trouble with radio protection
- Get to know every nut & bolt of your instrument

- Leads to new developments and ideas

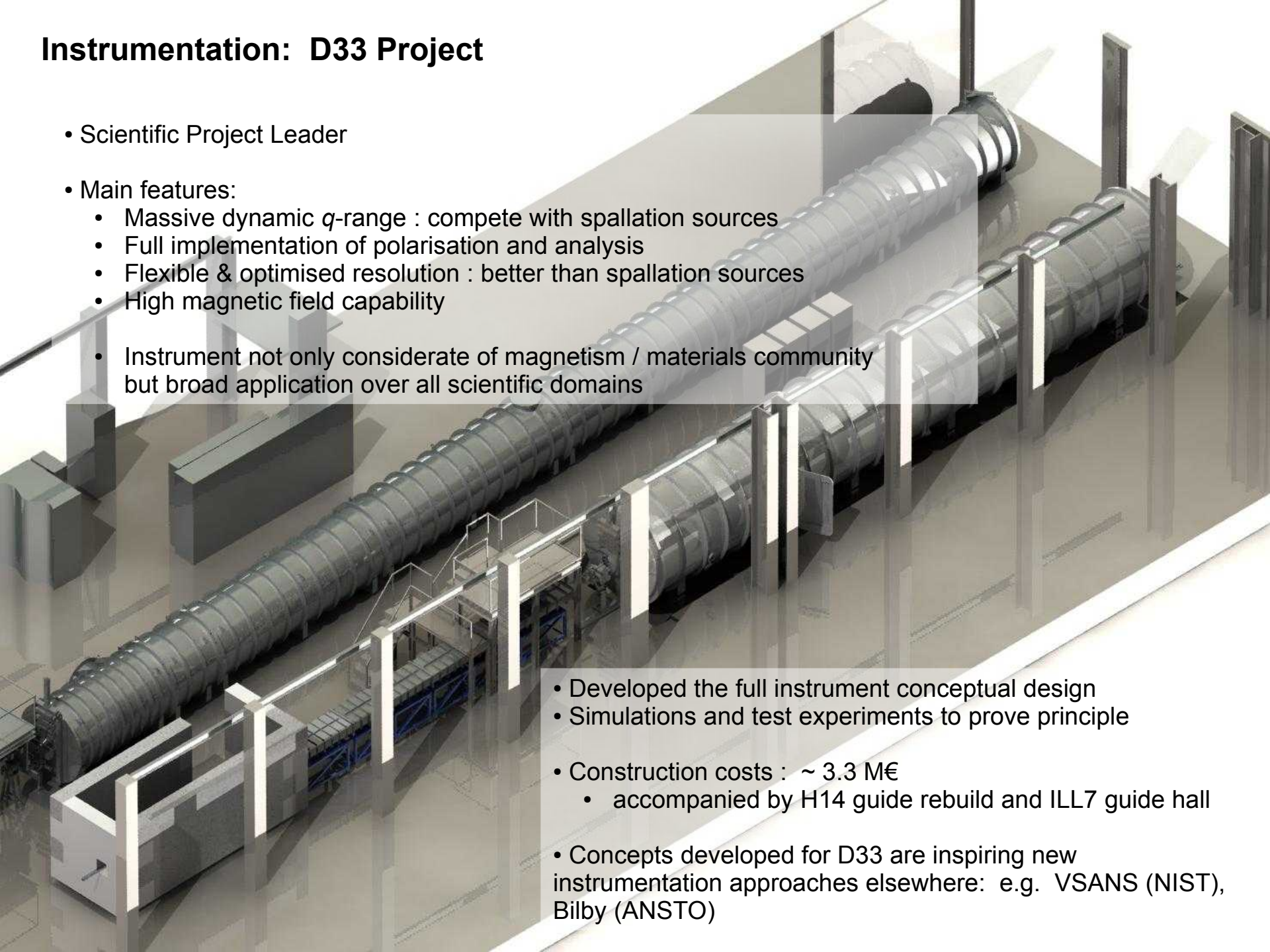
Grasp: SANS data reduction and analysis tool



Having the right software tools and ability to modify is crucial for:

- Rapid instrument commissioning
- Development of new techniques (software & instrumentation)

Instrumentation: D33 Project



- Scientific Project Leader

- Main features:
  - Massive dynamic *q*-range : compete with spallation sources
  - Full implementation of polarisation and analysis
  - Flexible & optimised resolution : better than spallation sources
  - High magnetic field capability

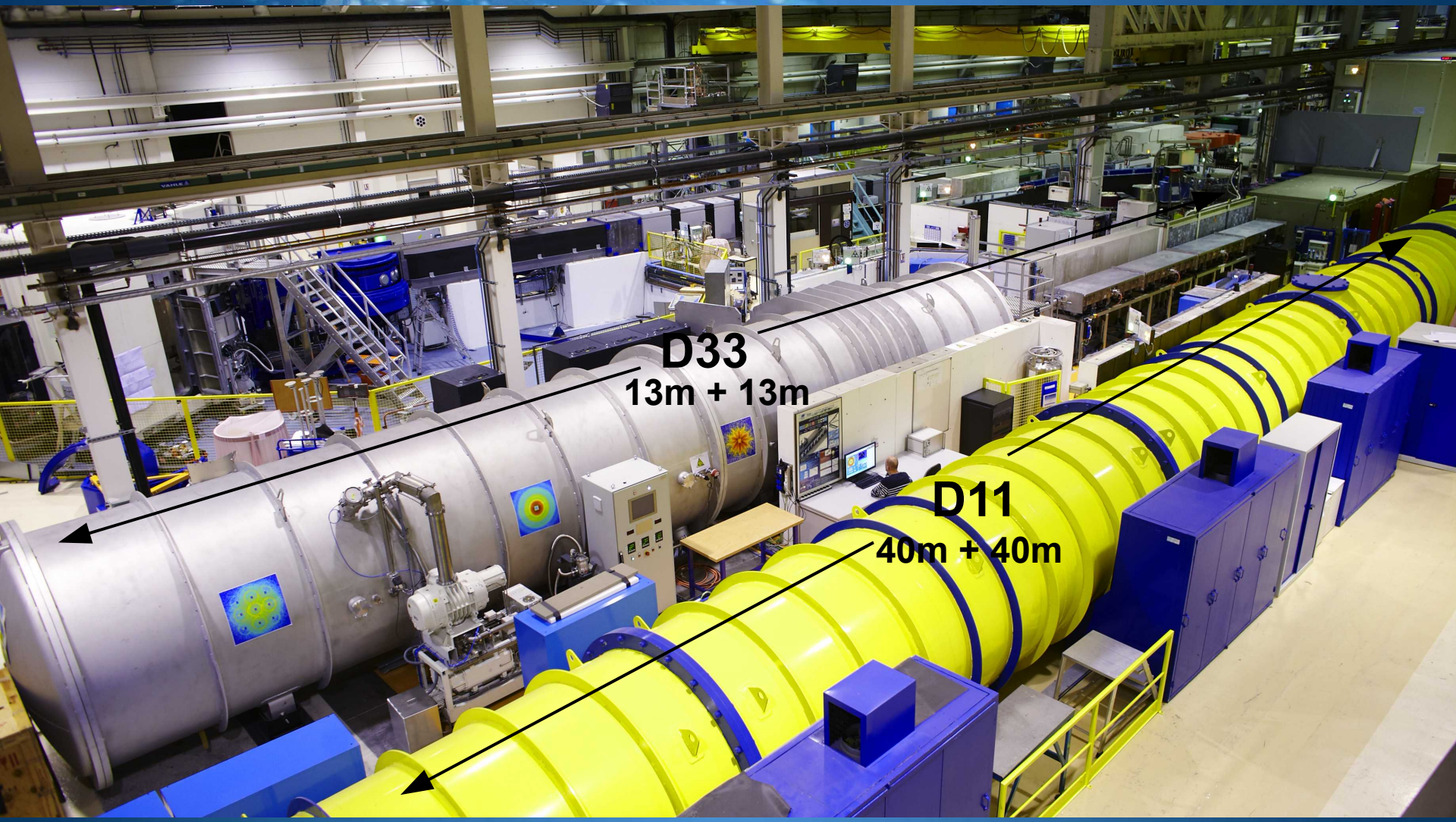
- Instrument not only considerate of magnetism / materials community but broad application over all scientific domains

- Developed the full instrument conceptual design
- Simulations and test experiments to prove principle

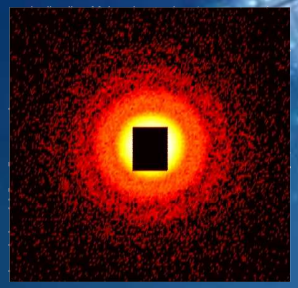
- Construction costs : ~ 3.3 M€
  - accompanied by H14 guide rebuild and ILL7 guide hall

- Concepts developed for D33 are inspiring new instrumentation approaches elsewhere: e.g. VSANS (NIST), Bilby (ANSTO)

Instrumentation: D33 Project

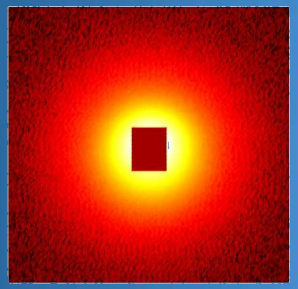


Instrumentation: D33 TOF vs. Mono



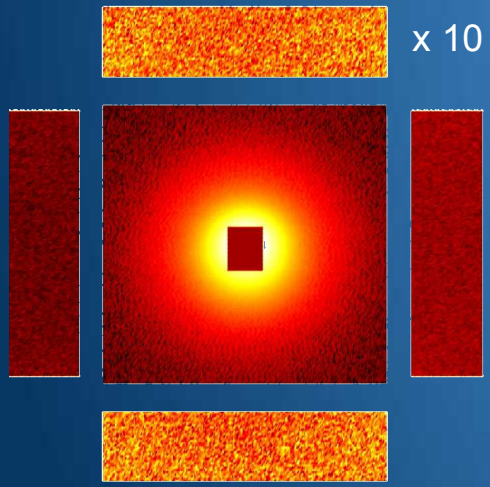
Monochromatic
1 Detector
$q_{max} / q_{min} \sim 10$

x 10



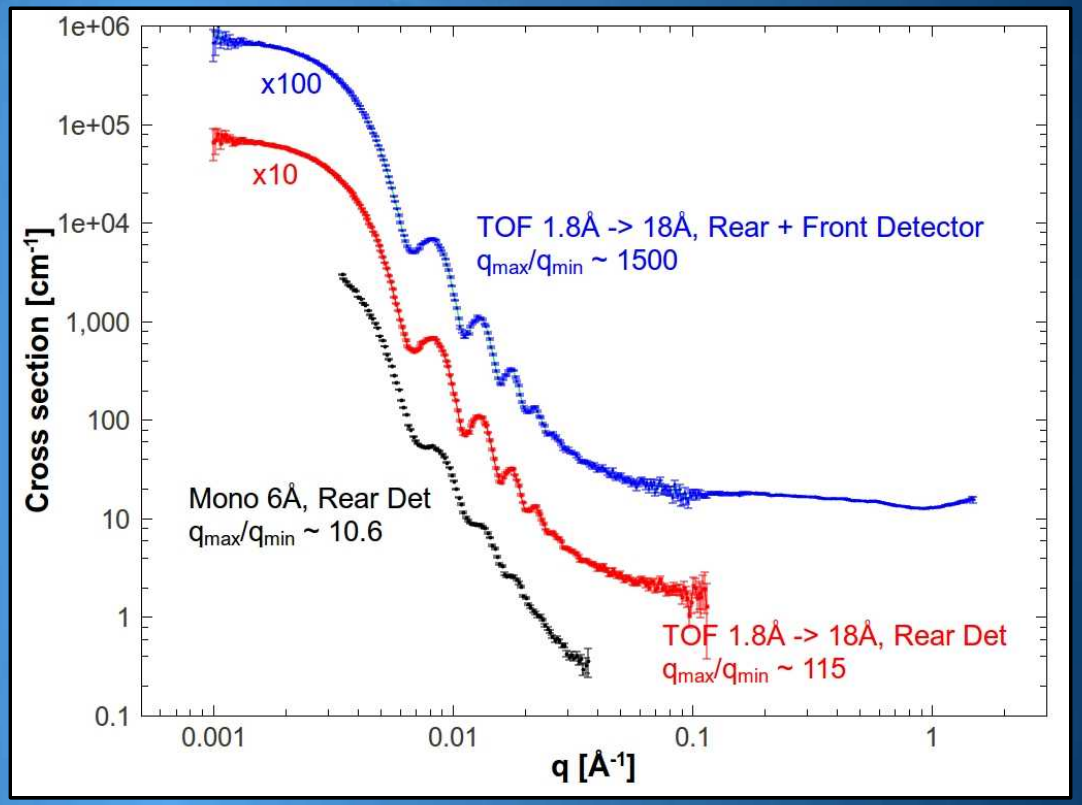
TOF,
1 Detector
$q_{max} / q_{min} > 100$

x 10



TOF + D33's Front & Rear Detectors
$q_{max} / q_{min} > 1000$

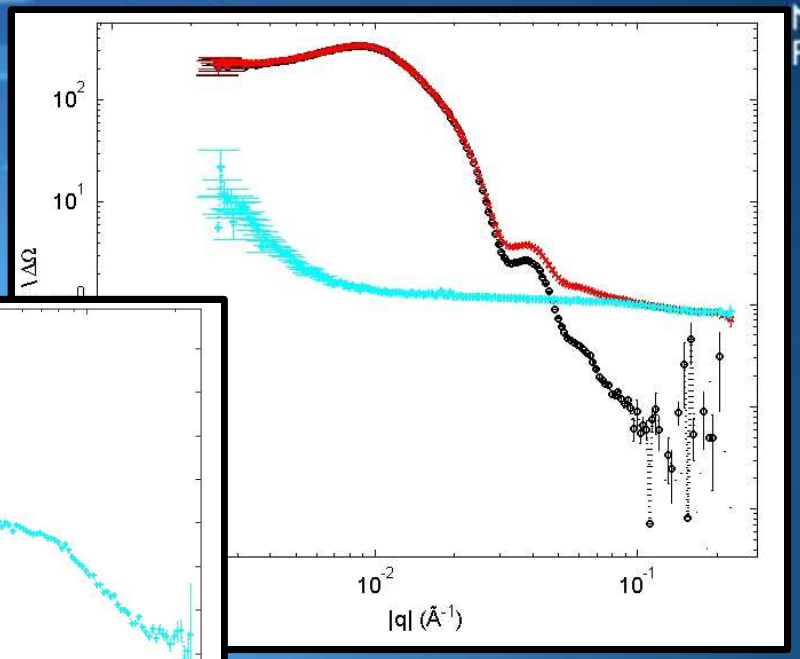
Massive dynamic *q*-range, q_{max} / q_{min}



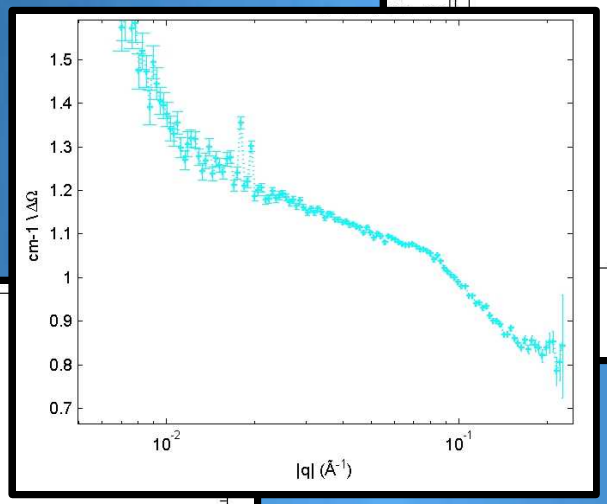
Latex Spheres in D_2O, r~700Å
Det1=1.2, Det2=12.8m
9.2% Δλ/λ
20 minute count time

How does TOF mode Compare to Mono?

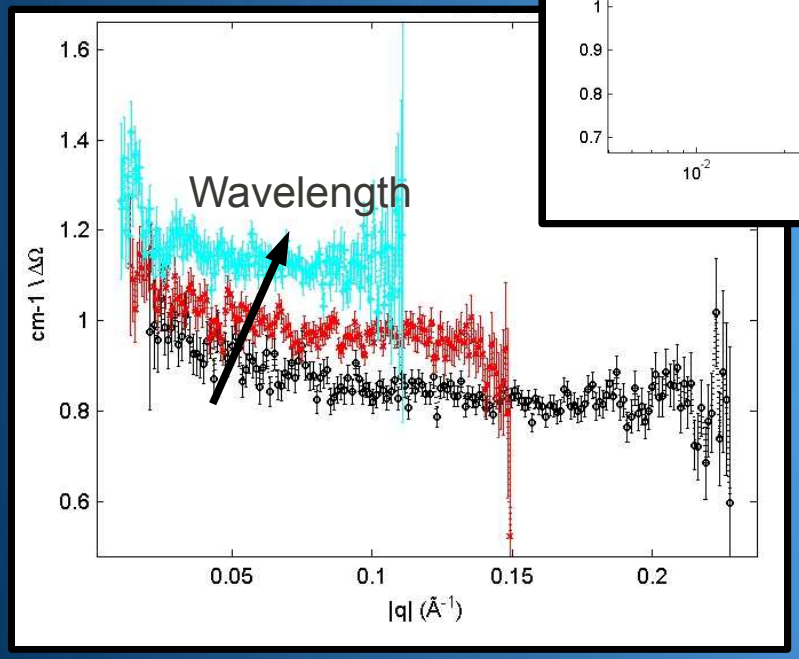
Hydrogenated materials &
Inelastic Scattering



Silica Spheres in H_2O



H_2O Background

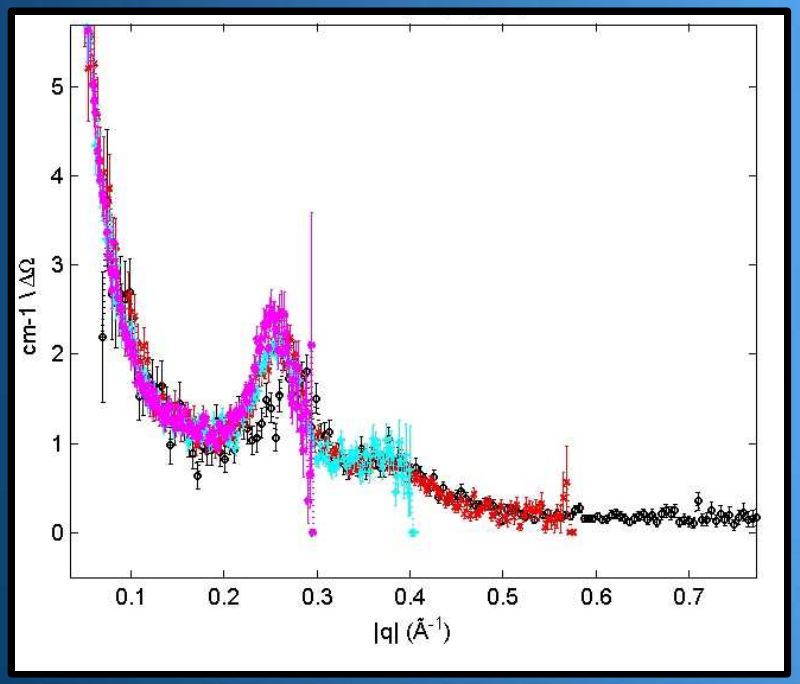


H_2O TOF time frames 2Å, 3Å, 4Å

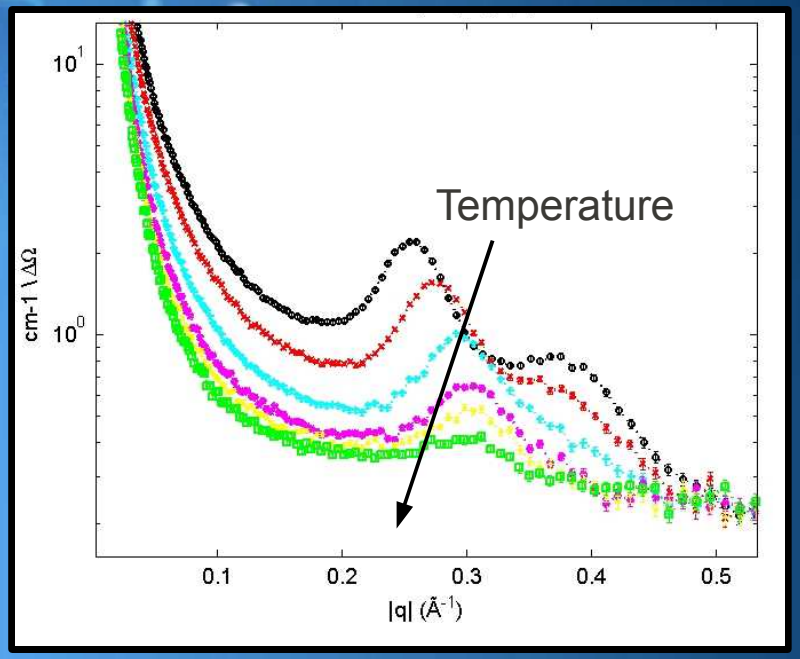
- Inelastic scattering from H
  - show up in 'wrong' time channels
- Cross-section of H_2O not constant with λ
- OK for dilute samples - background

How does TOF mode Compare to Mono?

Hard Matter & Magnetism



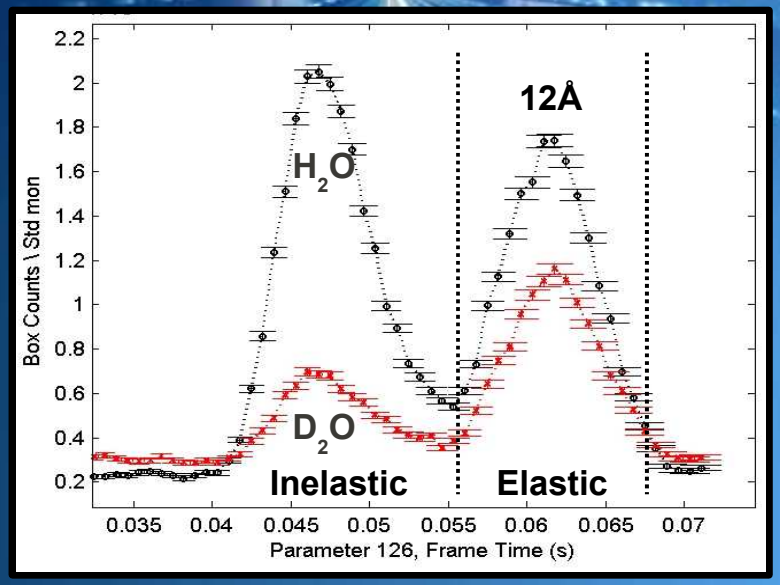
Holmium TOF time frames 1Å, 2Å, 3Å, 4Å



Nano-crystalline Holmium

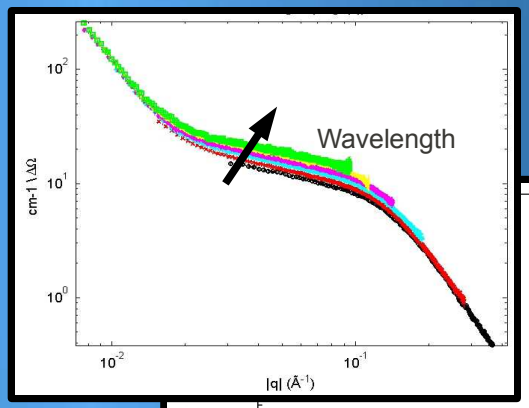
- Wide dynamic *q*-range
- Access to higher *q*'s using small λ
  (useful for restricted sample env.)
- No problems of inelasticity

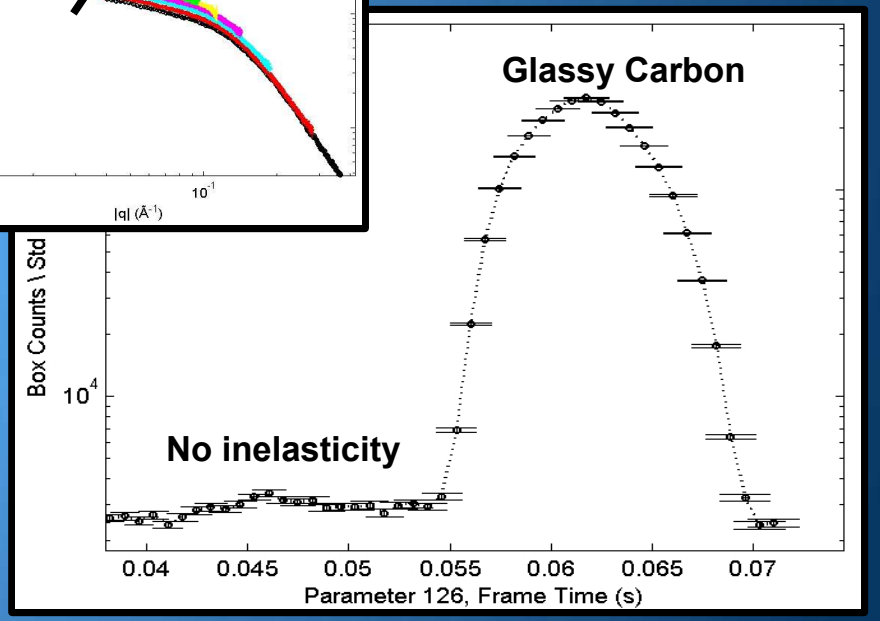
Instrumentation: D33 Enormous Flexibility = New Possibilities



- Mono + TOF

  → can easily look at the inelastic effects i.e thermalisation





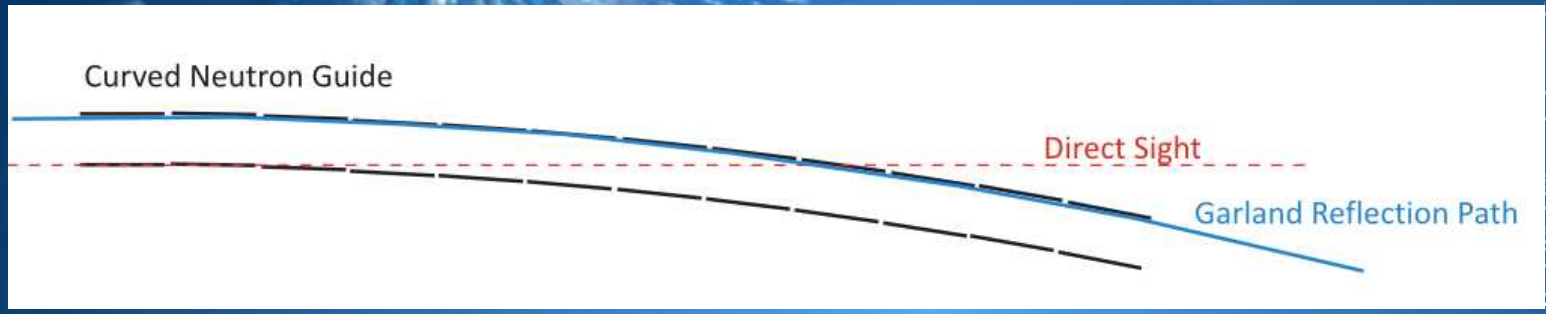
- TOF + Mono to remove much of the inelastic (incoherent) background

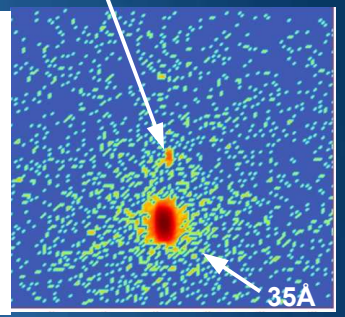
.....or at least .....

- Diagnose where issues with data, samples, measurements, might come from
- D33 is de-bugging data issues from both Reactor and Spallation sources!

Instrumentation & Neutron Optics

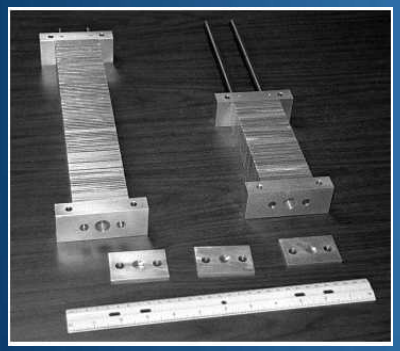
- Fast Neutrons down a curved guide (D22)

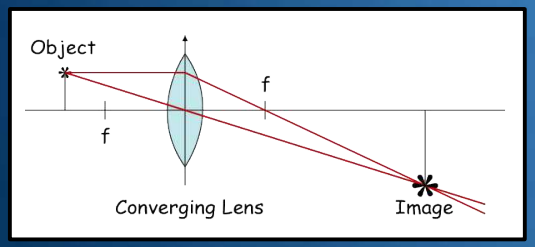




Garland reflections, i.e. glancing incidence neutrons around the curved guide
e.g. R = 3000m, L = 30m, 1m guide sections → 0.019° /m section. m = 1.2 (^{58}Ni) → λ_c = 0.16Å

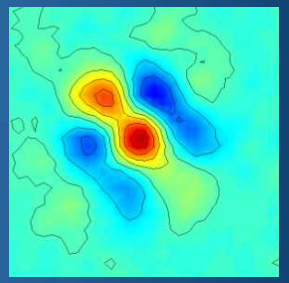
- Imaging with a refractive neutron lens (D22)



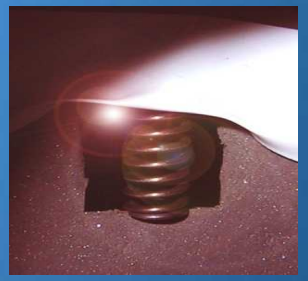


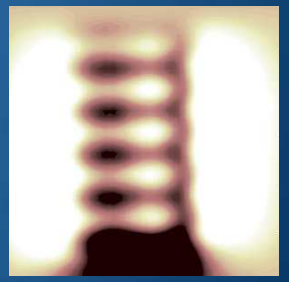
- Instrumental opportunities for increased flux, resolution & lowest ***q***

Plastic mesh



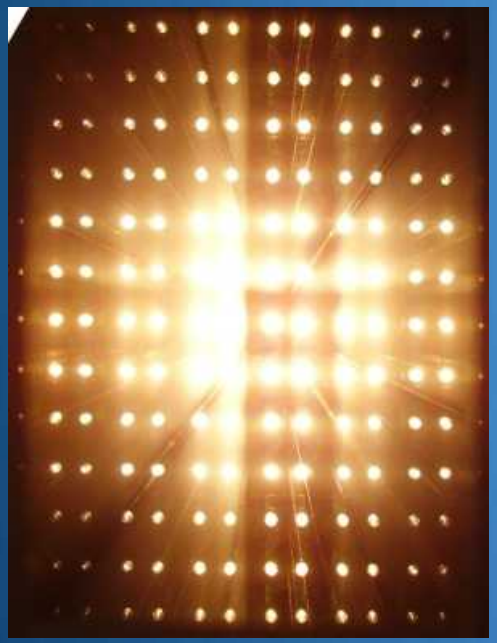
Steel Spring





Instrumentation & Neutron Optics – problems with D22

- By May 2008 D22 flux was ~50% that when it was commissioned in May 1995
  - Simulations of the D22 & D11 Flux loss
  - Spurious reflections
  - Inhomogeneous beam profile
  - Neutron Guide Problems!

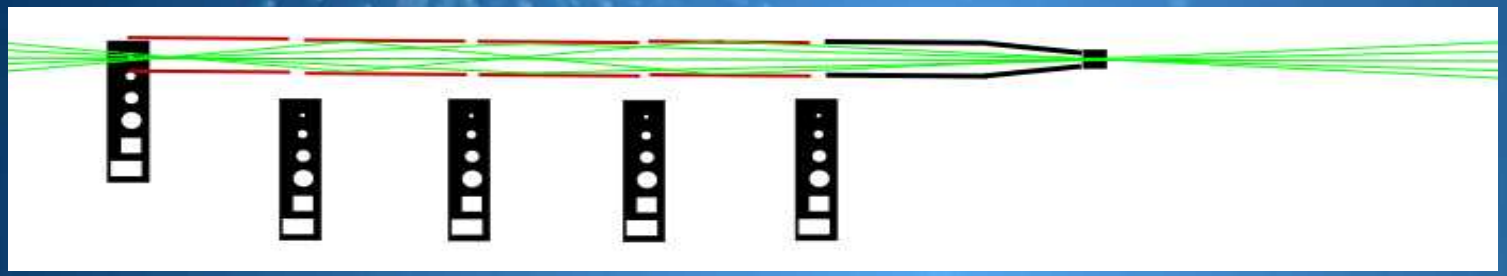


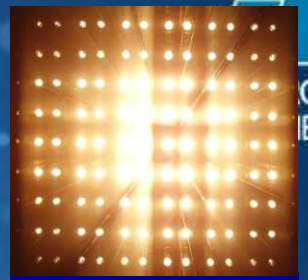
What's this got to do with guide problems?

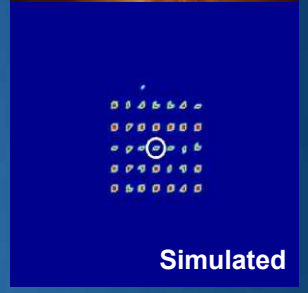
- Torch at the end of a 1.2m neutron guide
- Neutron guide 'kaleidoscope'
- Eye (or camera) is forming the second 'pin-hole' to form the image ....
  .....multiply reflected by the walls of the guide

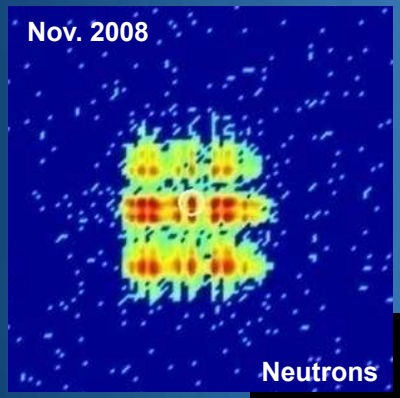
Instrumentation & Neutron Optics – problems with D22

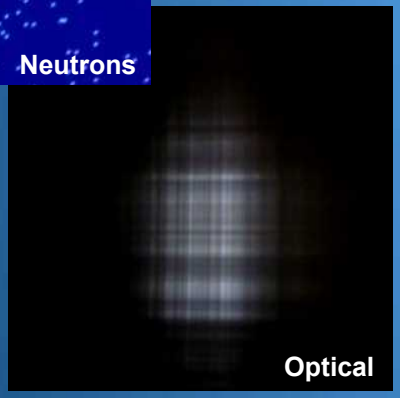
- Pin-hole imaging of neutron guides (D22)
  – a trick showed to me by Bob Cubitt, way back



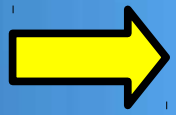


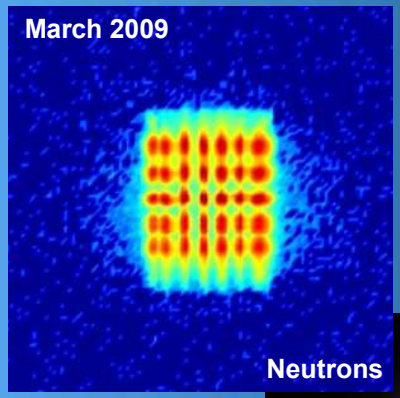


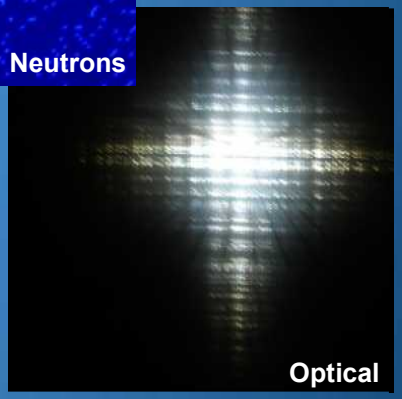




Guide realignment



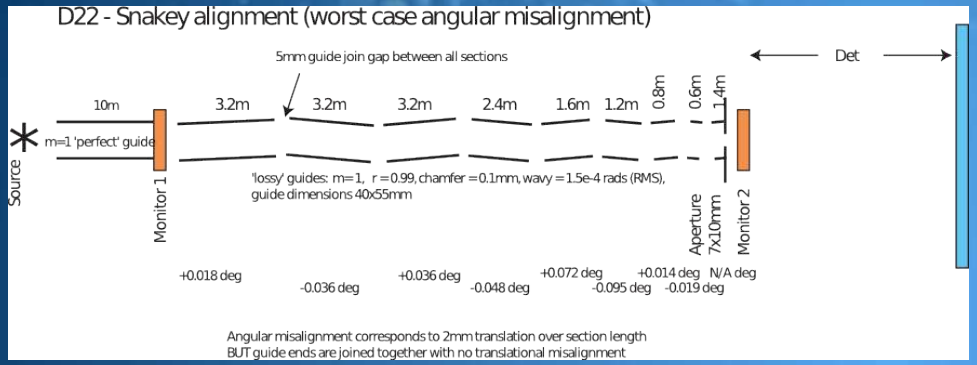


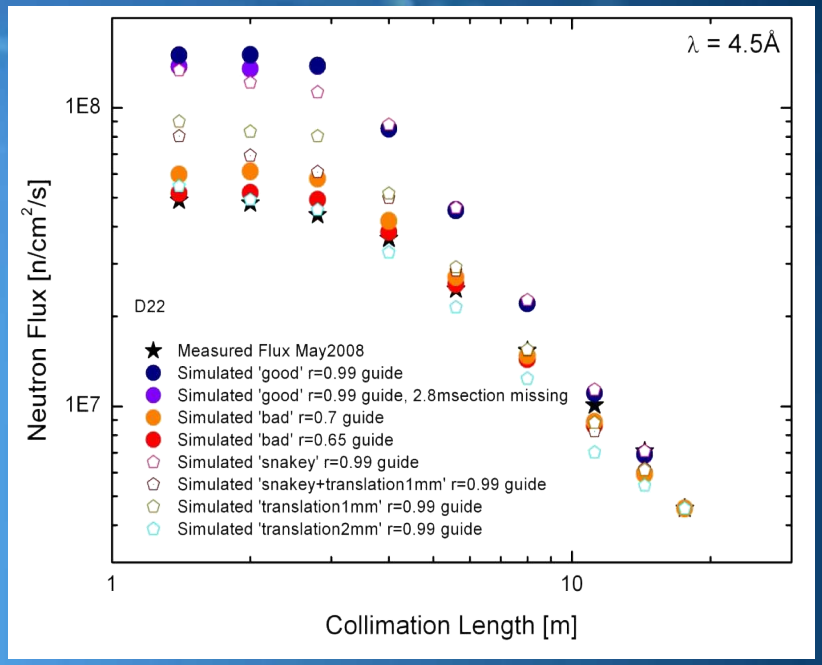


Can we make more use of optical alignment tools?

Instrumentation & Neutron Optics – problems with D22

• Simulations: Try to image the worst possible, yet reasonable, alignment or guide reflectivity to try to understand the flux loss on D22





• Extremely low reflectivity r < 0.65 ?

• Massive guide misalignments ~ 2mm ?

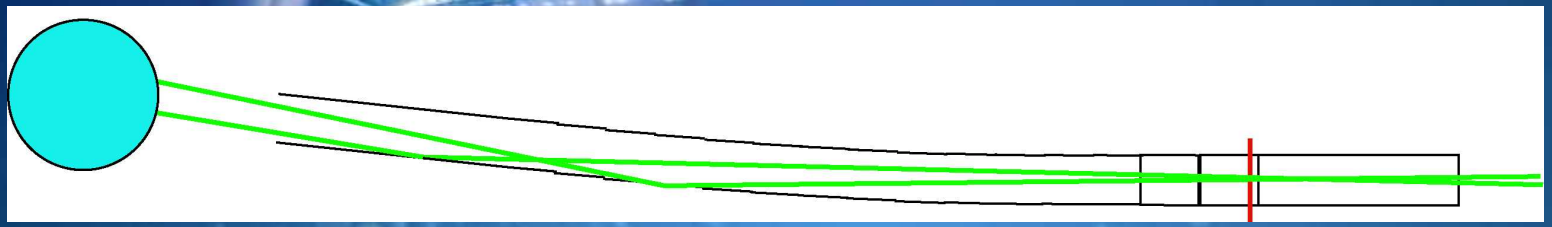
• Results presented at the ILL outdoor guide meeting, Chateau de Sassenage, Nov. 2008

Feedback: “That's ridiculous, impossible!”

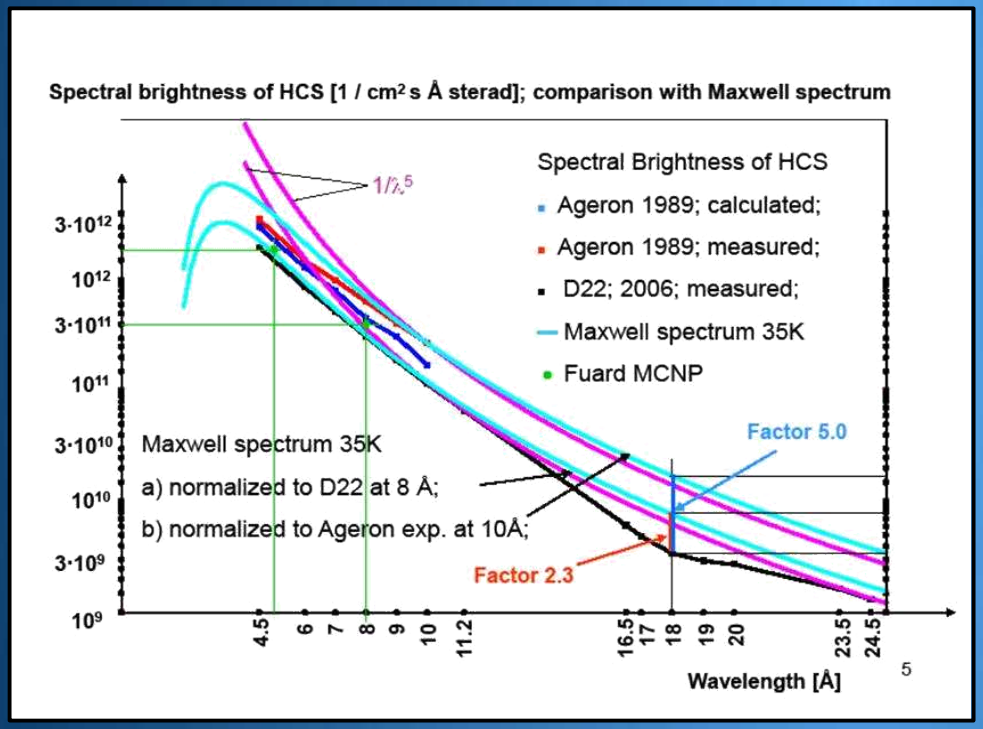
• No one had considered:

- 9mm 'sag' in the centre of the D22 collimation
- 3mm Horizontal & 5mm Vertical displacement in the casemat
- 7mm Vertical mismatch at the beam shutter ...etc...etc.

Instrumentation & Neutron Optics – Imaging of the Horz. Cold Source

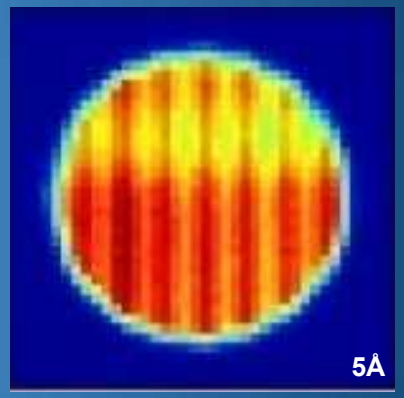


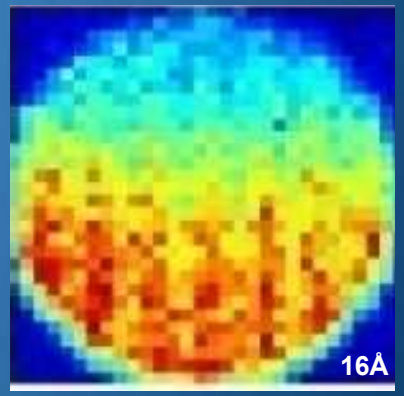
- Brightness & imaging of the Horizontal Cold Source
- 5mm @~20m → 40mm @80m back from sample
- Only 1 bounce (in horz plane) due to guide curvature



- H5 Brightness data used for the H5 guide project
  ..... it is some of the few measured data we have

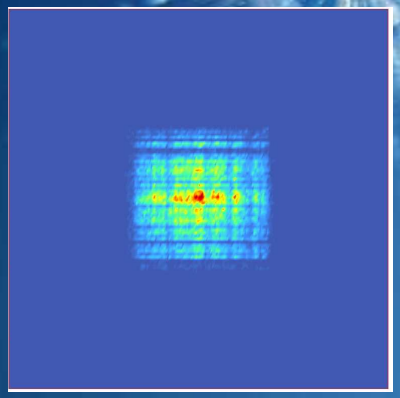
Images of the Horizontal Cold Source





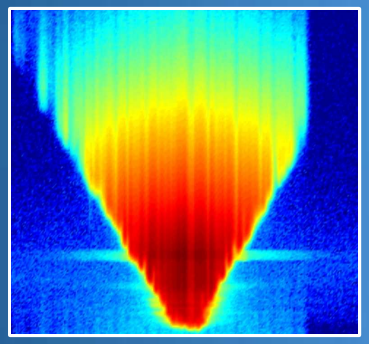
Characterising Guide Systems

- Pin-hole image of D33 + H14 Neutron guide

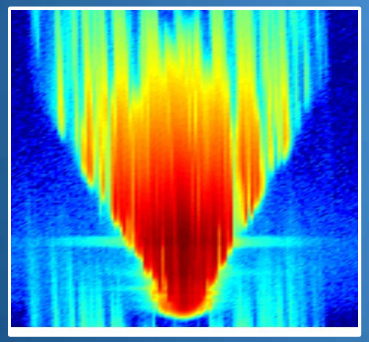


- Raster Scan across surface of guide
  0.5mm aperture, ~10 000 measurements of 1s
  ~ ½ Day
- Construct phase-space diagrams normally only seen in Simulations

- Wavelength vs Divergence

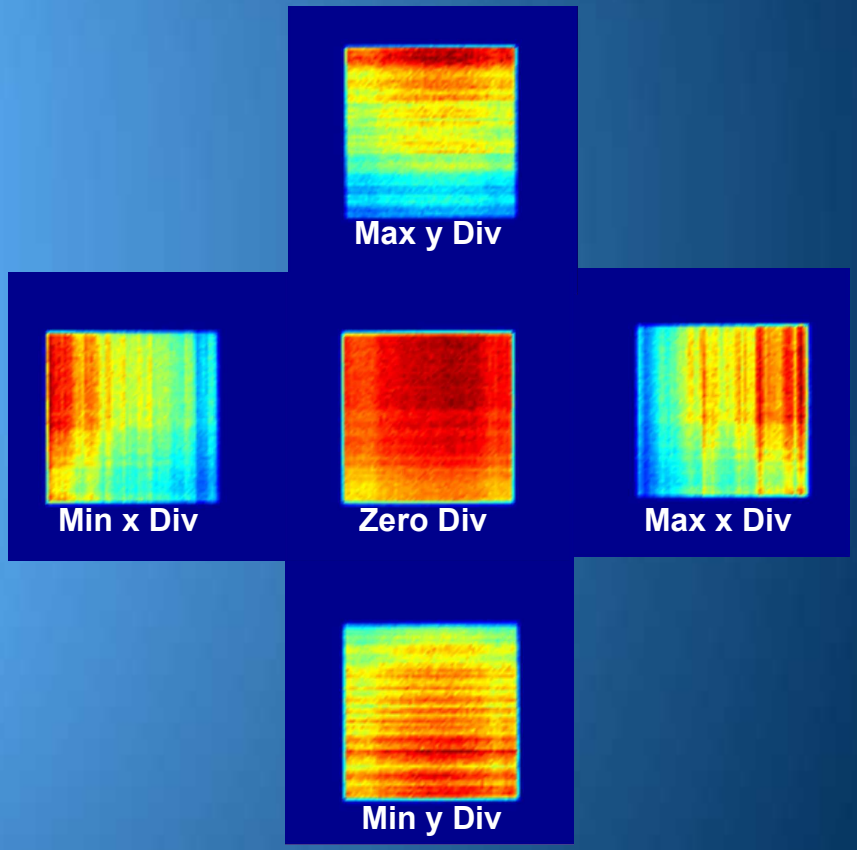


x Div

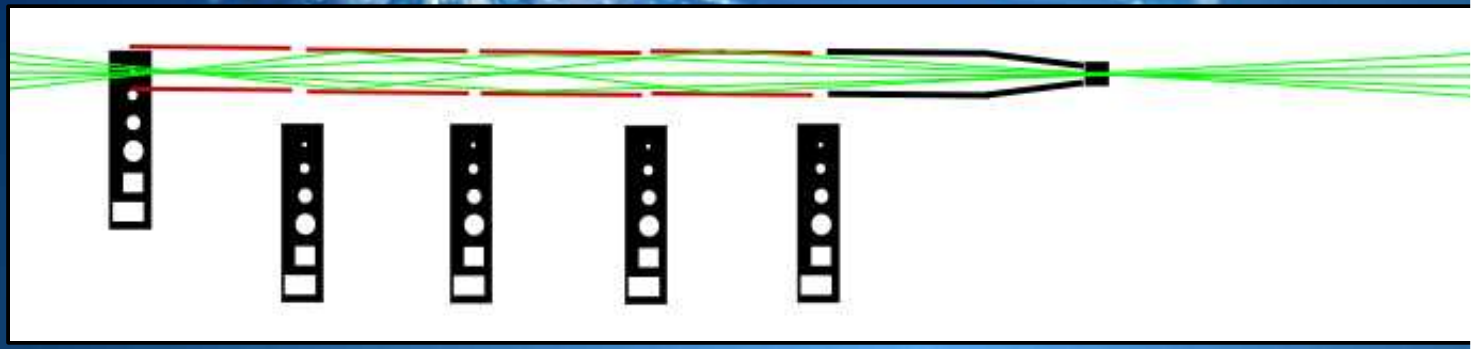


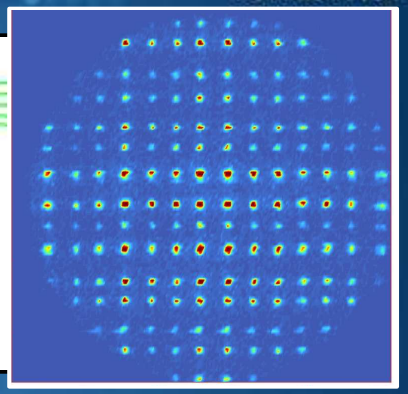
y Div

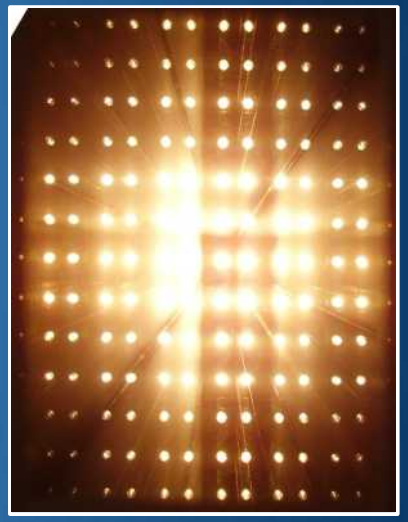
- Position vs. Divergence



Multiple Beam SANS: D33 – Enormous Flexibility = New Possibilities







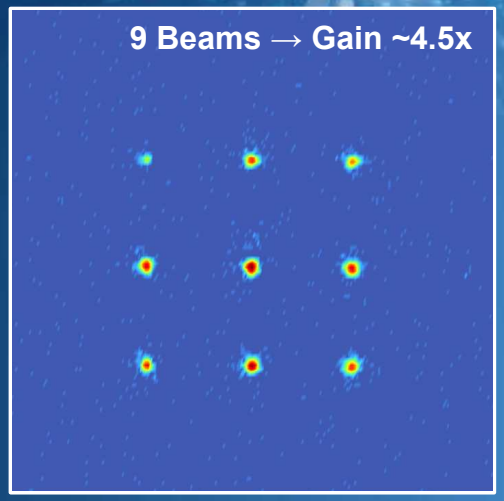
- Many 'quantized' reflections from pin-hole guide imaging
- Good check of guide alignment

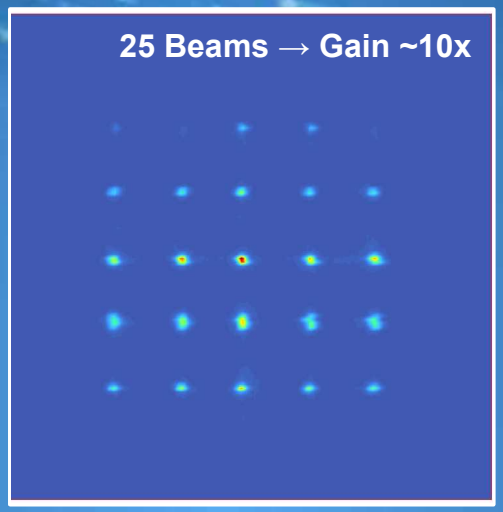
Isabelle: *"Looks a bit like multi-pin-hole SANS"*

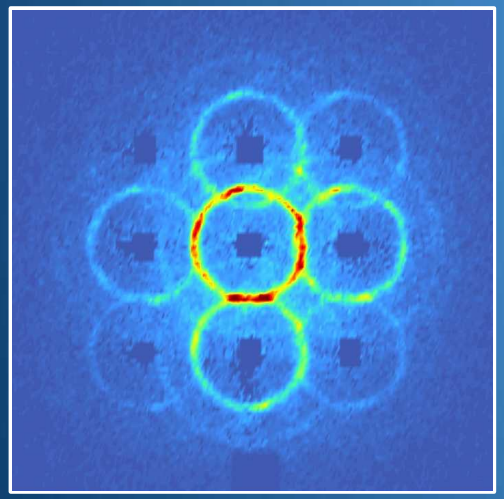
Charles (1hr later): *"That's a brilliant idea – put a sample in"*

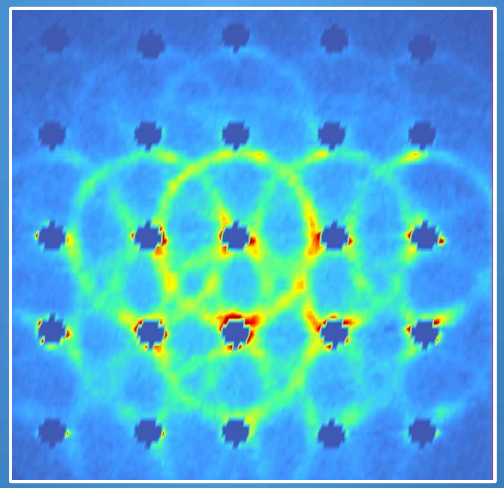
Multiple Beam SANS: D33 – Enormous Flexibility = New Possibilities

- After some playing around with apertures and guides









OPAL sample

Bragg ring at $q \sim 3.7 \times 10^{-3}$ Å^{-1}

$q_{min} \sim 3 \times 10^{-4}$ Å^{-1} (VSANS)

Intensity gains from multiple beams

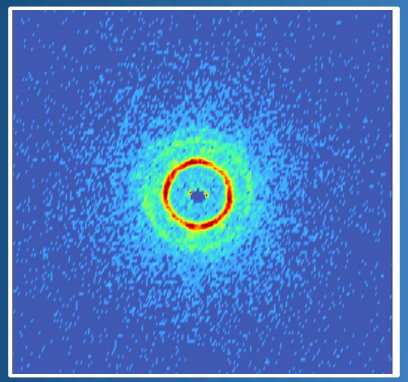
Complexity in analysis

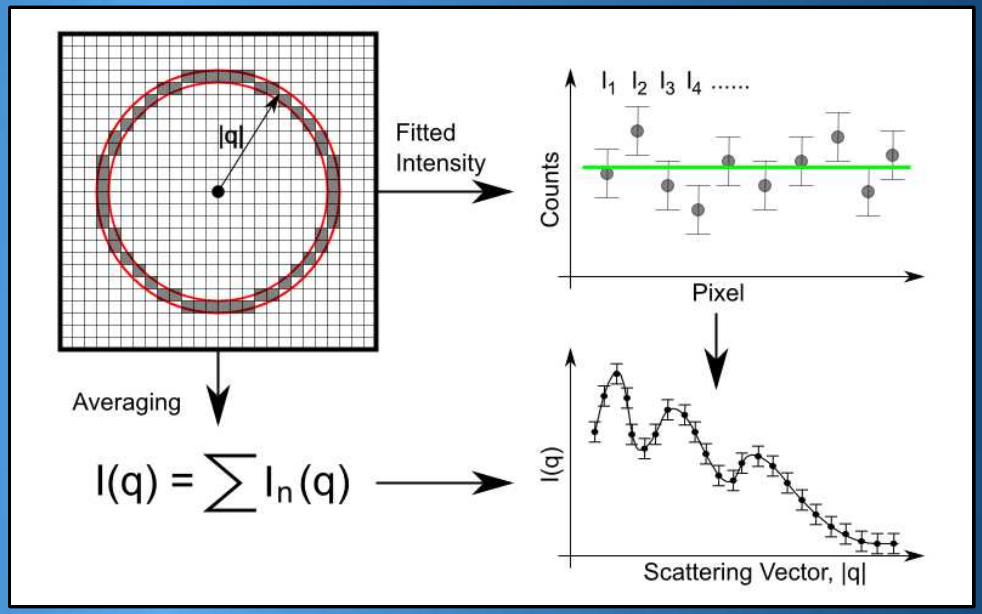
...but all of this was for free!

Publication: ***"Novel multiple-beam very small angle neutron scattering (VSANS) using a conventional SANS instrument"***
C. D. Dewhurst, J. Appl. Cryst. 47, 1180 (2014)

Multiple Beam SANS: D33 – Enormous Flexibility = New Possibilities

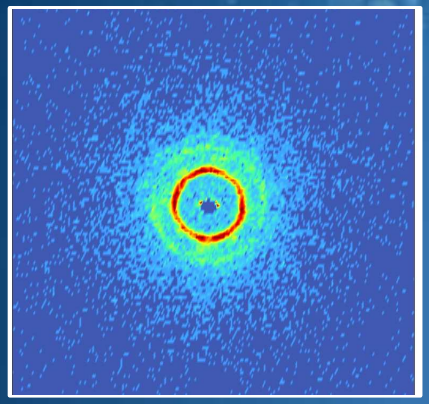
- How to treat multiple beam data?
- Reminder: Single beam usual SANS data treatment, reduction & analysis

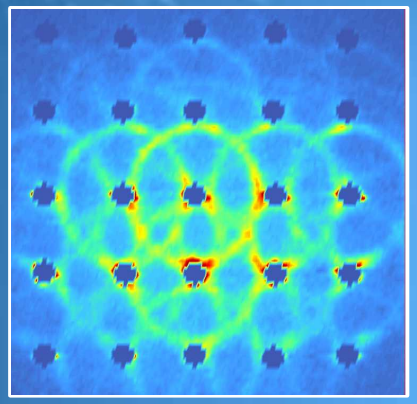


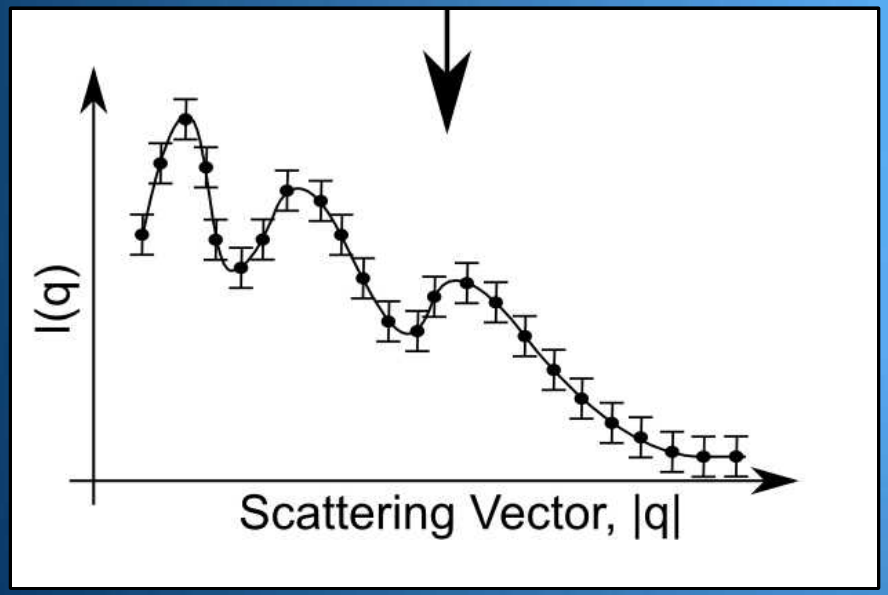


Multiple Beam SANS: D33 – Enormous Flexibility = New Possibilities

- How to treat multiple beam data?
- Complexity in Analysis:







Possible Methods:

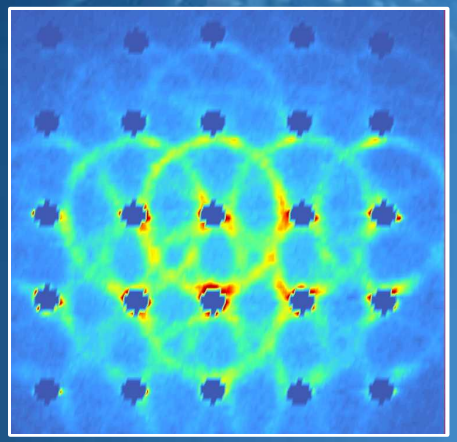
· Direct (multiple) fitting to multi-beam 2D data
→ only useful if scattering function is well known

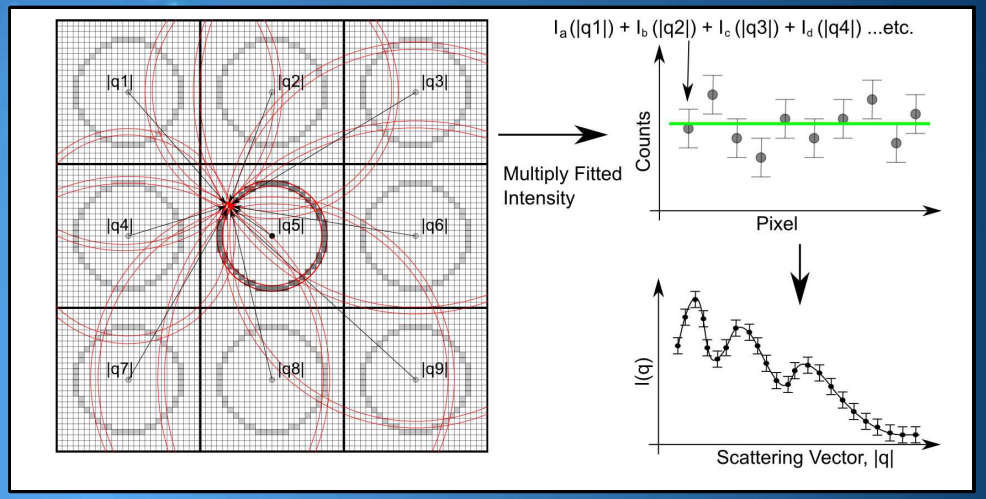
· Simple cut-and-paste then usual SANS reduction
→ neglect contamination due to overlap of patterns

· Fit to find the unknown 2D function that satisfies the data when expanded to 2D and weighted for intensities
→ An ill-posed problem:
A great many simultaneous equations = # detector pixels, noisy data, and a number of parameters, e.g. 200, to solve for

Multiple Beam SANS: D33 – Enormous Flexibility = New Possibilities

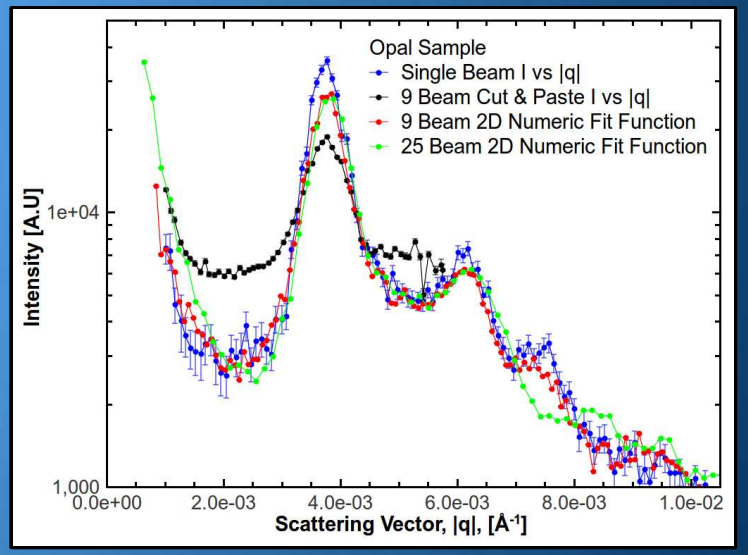
- How to treat multiple beam data?
- Complexity in Analysis: Possible methods:



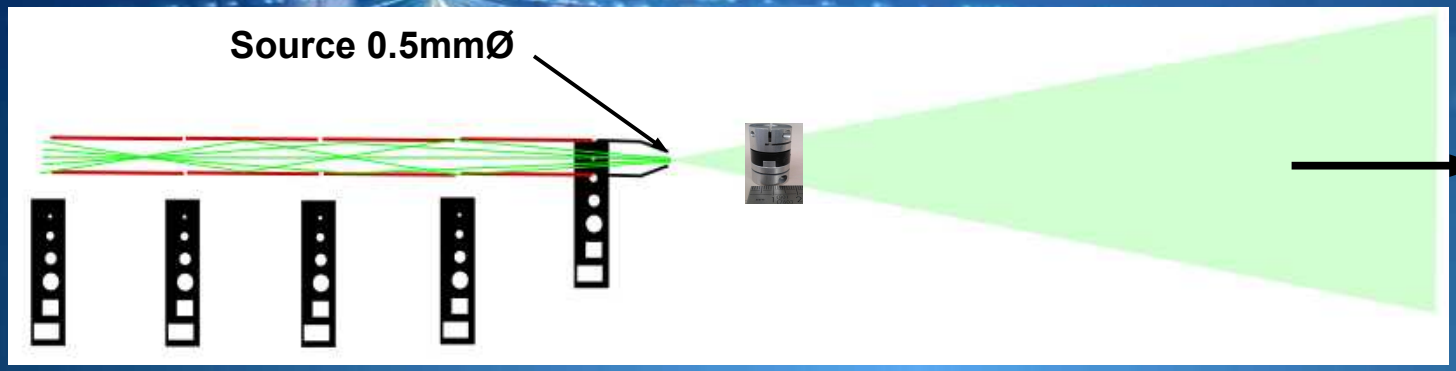


· Fit to find the unknown 2D function that satisfies the data when expanded to 2D and weighted for intensities
→ An ill-posed problem: A great many simultaneous equations = # detector pixels, noisy data, and a number of parameters, e.g. 200, to solve for

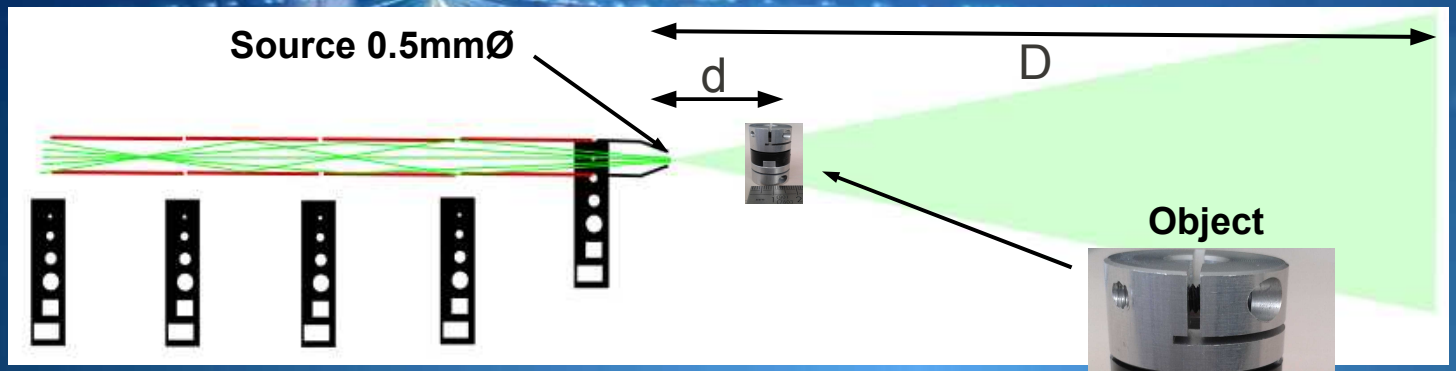
· I am confident there is someone smart out their who knows about information theory, statsitics, Bayesian analysis, coded aperture imaging etc. ....or something like that who knows how to do this best

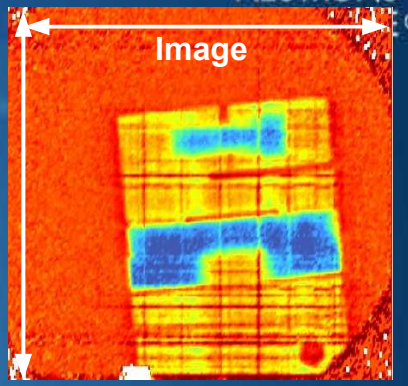


Magnified Neutron Imaging:



Magnified Neutron Imaging:





SANS Detector:
64cm x 64cm
2.5 x 5mm resolution

· Magnification: $M = D / d$ ~ x5 → x25

· Field of view:
Depends on $\theta_{c\text{-}guide}$ (λ) and M, Objects ~ mm → few cm

· Spatial resolution: Down to ~ 200µm
Limited by Det. Res. / M or Source Ø

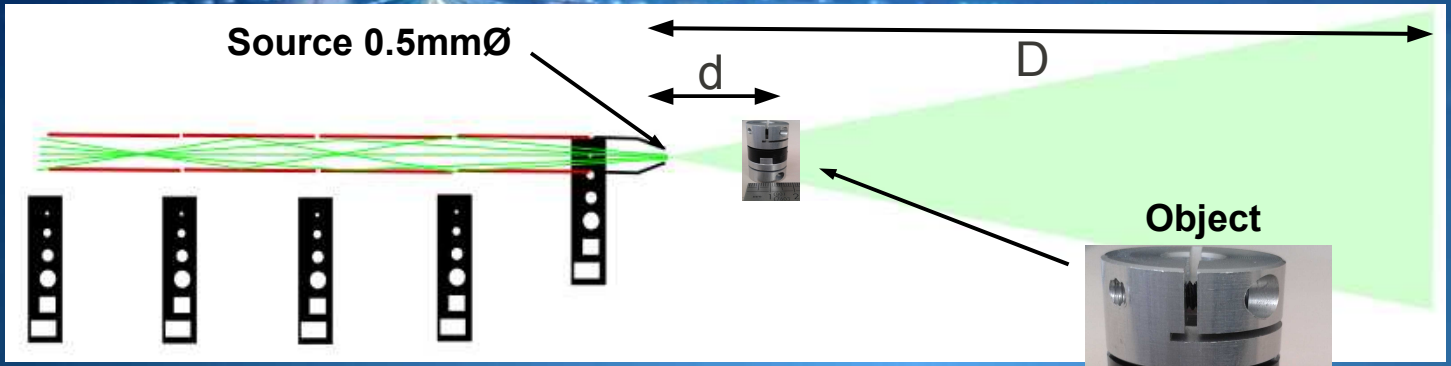
· Absorption & Scattering Contrast

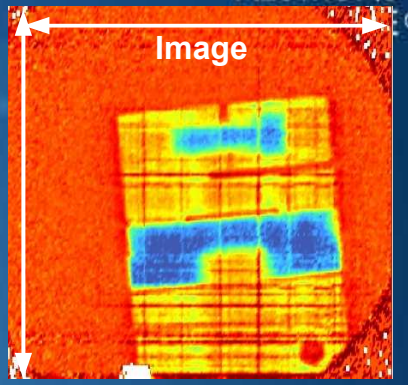
· Wavelength selectivity

· Monochromatic or TOF

· Not bad .....and for free!

Magnified Neutron Imaging:





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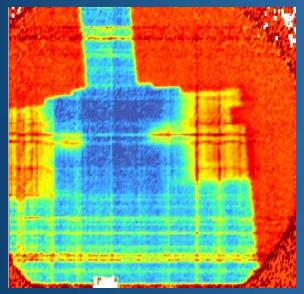
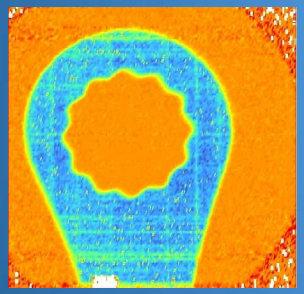
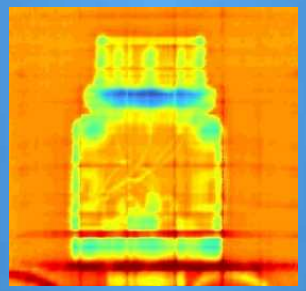


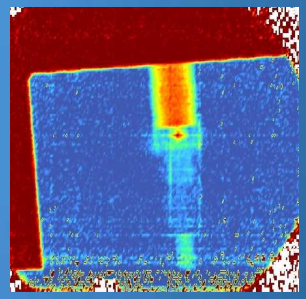
Coder



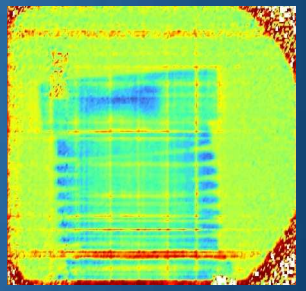
Ratchet Spanner



Cryostat Plug



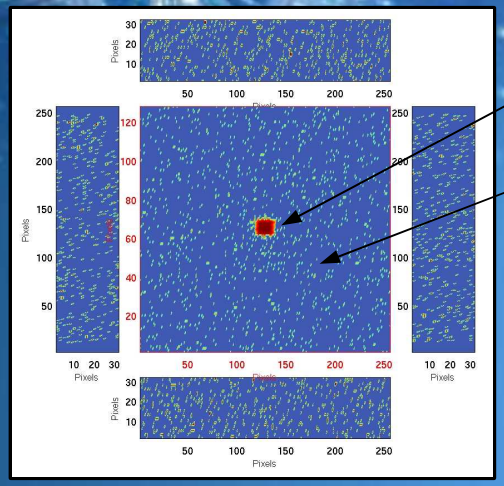
Steel Bolt in 5mm Plexi



Bellows Coupling

Scanning Neutron Imaging:

Sample ....
.... and lab-book aid



Transmitted beam: Attenuation by absorption & scattering

A few counts ..... close to beam-off background level

· Raster scan a fine aperture over sample

· Reconstruct image from transmission and scattering data

· This example:

Mechanical Pencil

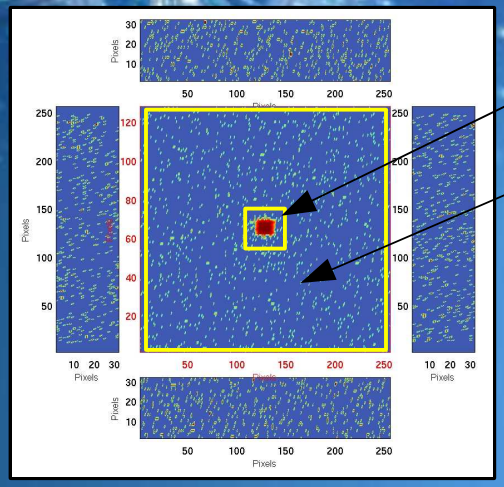
Sea Snail Shell

Sample ....
.... and Isabelle's holiday souvenir

· 200μm Ø aperture (determines resolution). Possible down to ~ 50μm
· Scan size: x: 51 * 0.2mm = 10.2mm, y: 186 * 0.2mm = 37.2 mm
· Total pixels = 9486 ...or individual measurements
· Each measurement = 5s data + 1.5s deadtime for moving & data storage
· Total time = 17.1 hrs

· D33: λ = 6Å, Col = 2.8m, Det1 = 2m, Det2 = 3m

Scanning Neutron Imaging:



Transmission

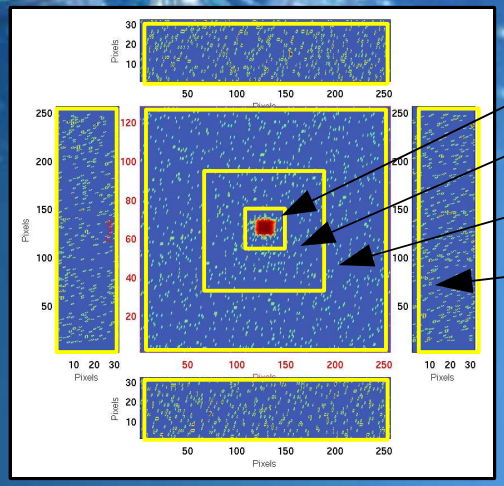
Scattering

Sample ....
.... and Isabelle's holiday souvenir

Transmission

Scattering

Scanning Neutron Imaging:



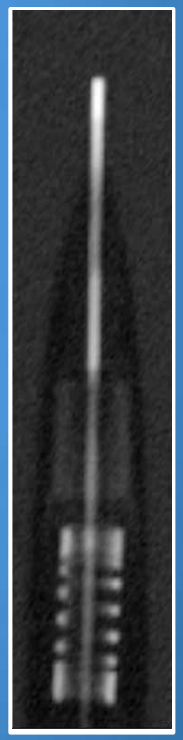
Transmission

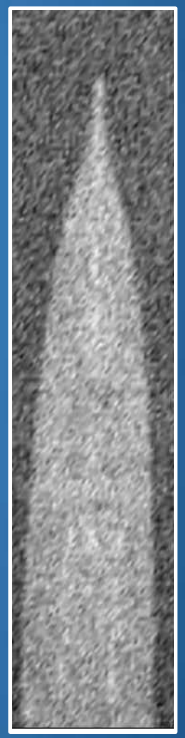
Low q

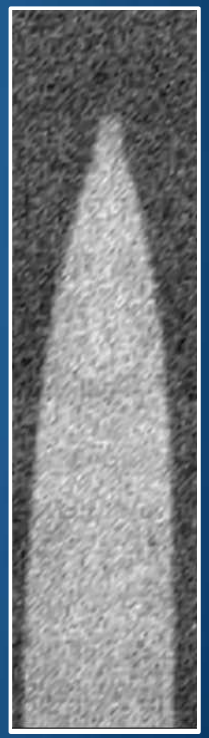
Medium q

High q

Sample ....
.... and lab-book aid



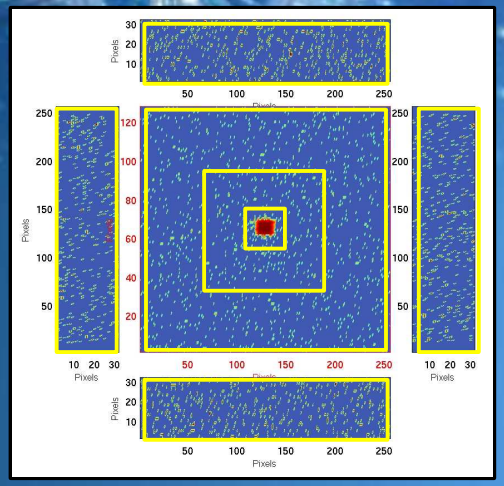




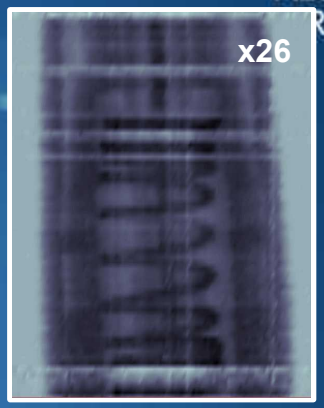
Transmission **Low q** **Medium q** **High q**

· Imaging shows us there is definitely 'lead in my pencil'

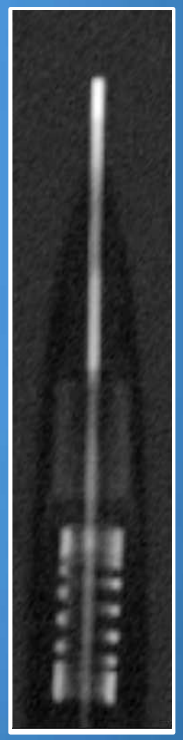
Scanning Neutron Imaging:



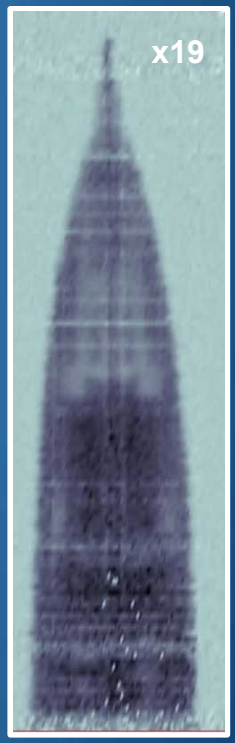
Sample ....
.... and lab-book aid



Transmission



Low q

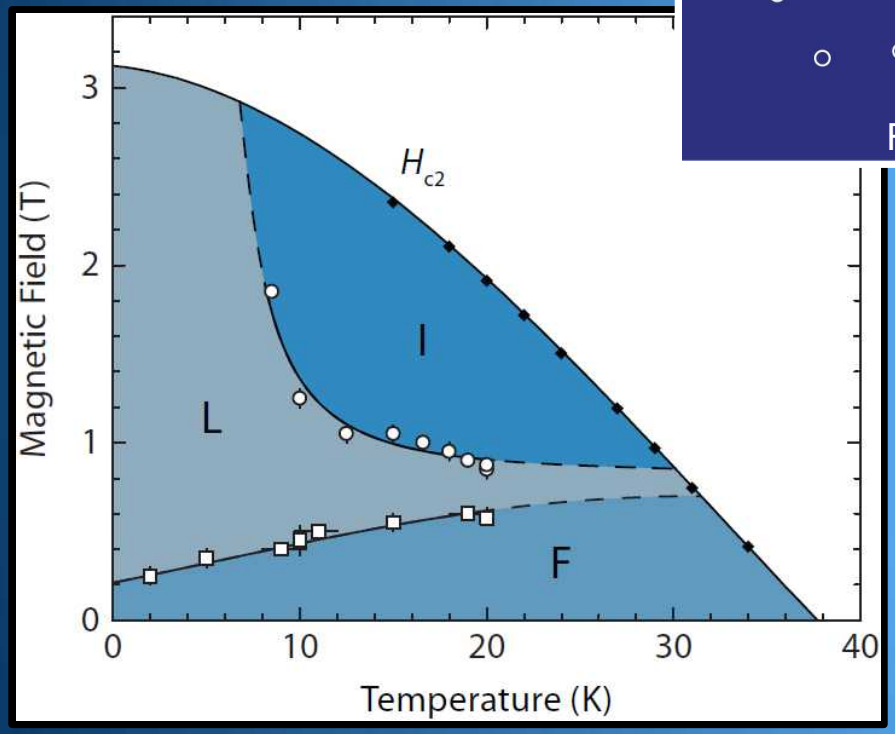


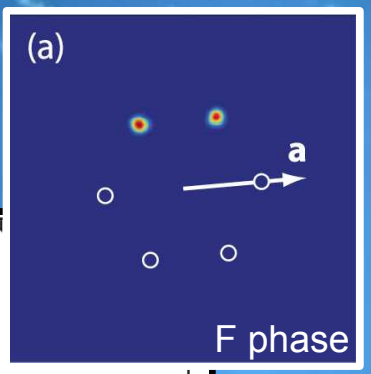
Magnified Imaging

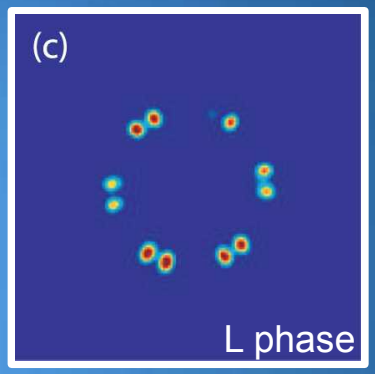
· Imaging shows us there is definitely 'lead in my pencil'

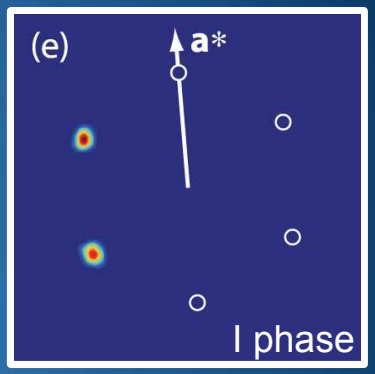
Instrumentation: Multiple Beams → Scanning SANS Microscopy

- MgB_2: Equilibrium Vortex Lattice Phase Diagram
- Three hexagonal V-neck VL phases separated by 2 second order transitions

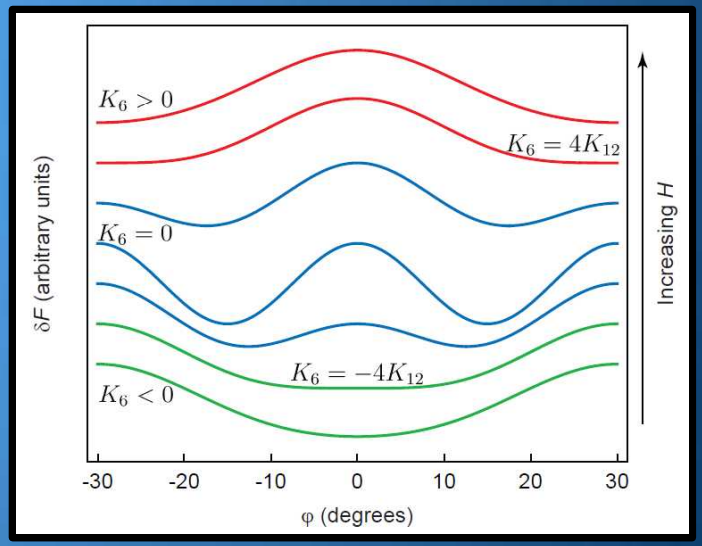








$$\delta F(\varphi) = K_6 \cos(6\varphi) + K_{12} \cos(12\varphi)$$

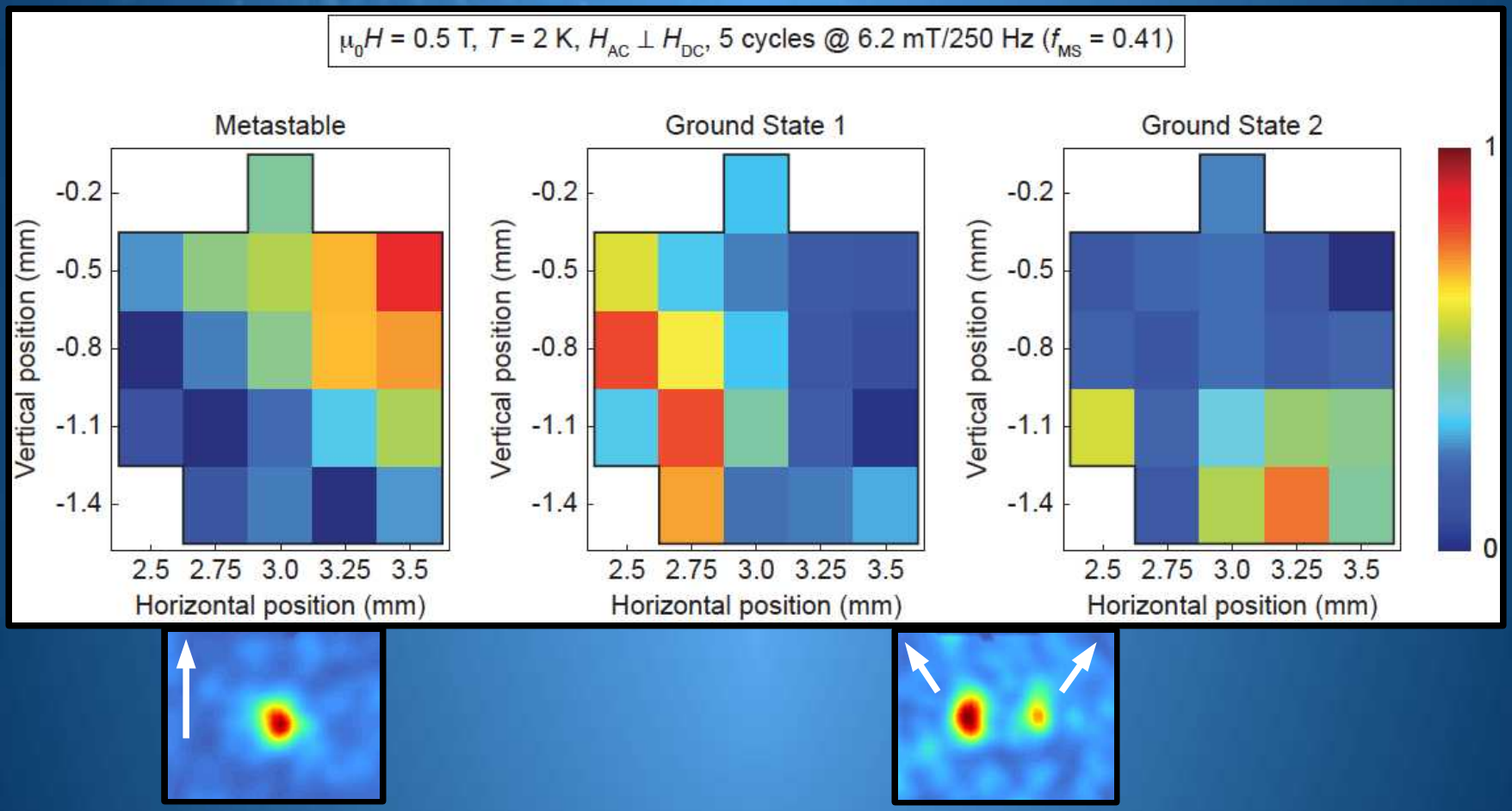


P. Das et al., PRL (2012)

T. Hirano et al., arXiv:1304:7314 (to appear in JPSJ)

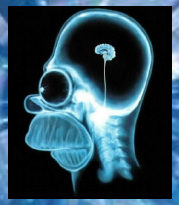
Instrumentation: Multiple Beams → Scanning SANS Microscopy

- Spatially resolved SANS < 0.1 mm resolution
- First attempt at domain size determination: Scanning SANS Diffraction Microscopy

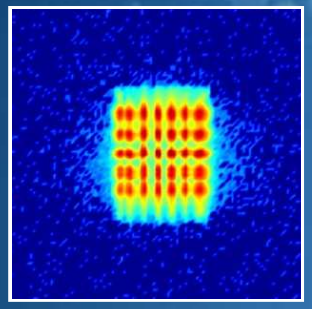
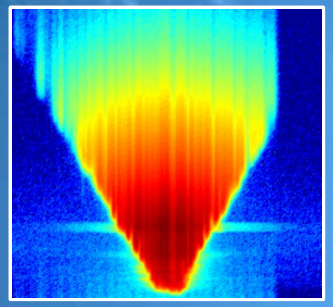
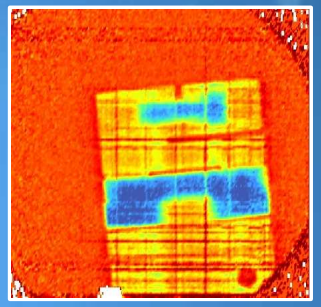
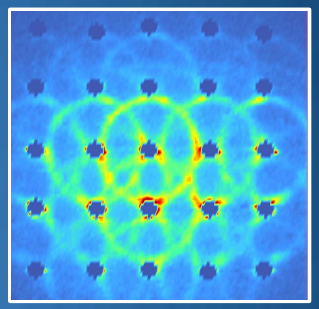


- Clear spatial separation between different (dominant) domain orientations

Summary:



Non-standard configuration of SANS instruments

· Flexibility in instrument configuration = New Possibilities

· Do not be afraid of some redundancy in components

· Use your imagination – there is lots that we can do

· Availability of custom software tools is crucial to pursue new ideas