Basic instrument design

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Instrument design steps

Science case → Primary requirements → Instrument layout / initial McStas → Define a figure of merit → McStas optimisation

Define a science case!!

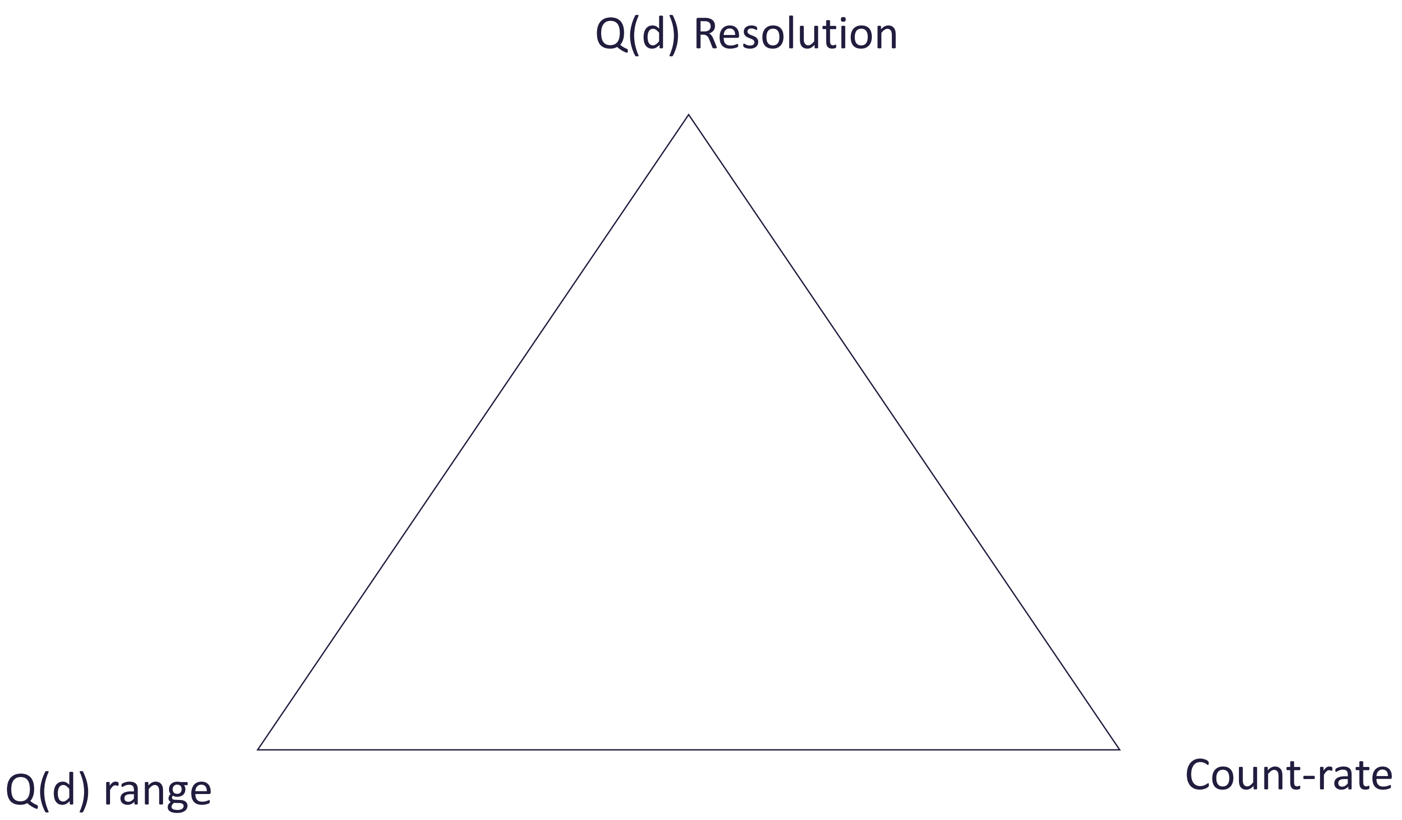
Instruments are designed and built to perform defined science

The science case generates the primary requirements

McStas is a tool. If used incorrectly it can be dangerous

Primary requirements

Defining primary requirements



But also:

- Single crystal, powder, non-crystalline
- Unit cell volume
- Sample environment restrictions
- Need for *in situ* capability
- Sample size / geometry
- Detector type / coverage / stability
- Parasitic scattering
- Etc…

Which come from:

- Science case requirements
- Available technology
- Space limitations
- Budget
- Etc…

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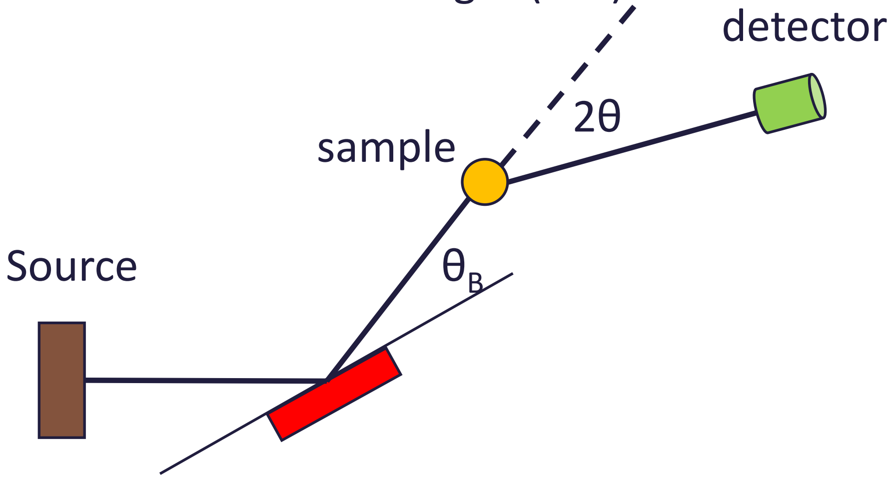
Diffractometer types

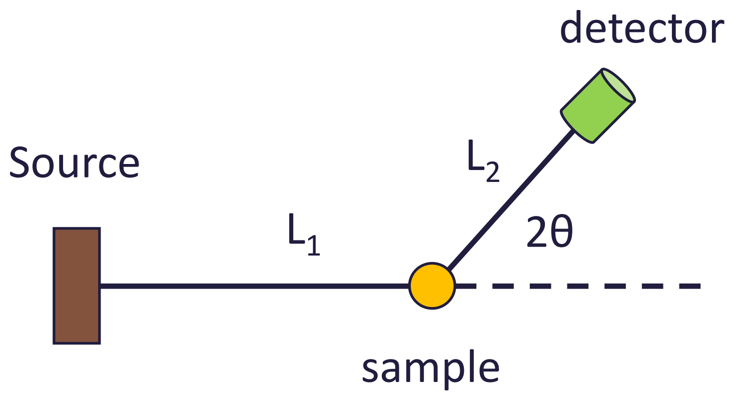
$$\lambda = 2d\sin\theta$$

Continuous wavelength (CW)



$$\lambda = \frac{2d_c \sin\theta_B}{n}$$

Time-of-flight (TOF)



$$\lambda = \frac{3956}{v} = \frac{3956\,(t - t_0)}{L_1 + L_2}$$

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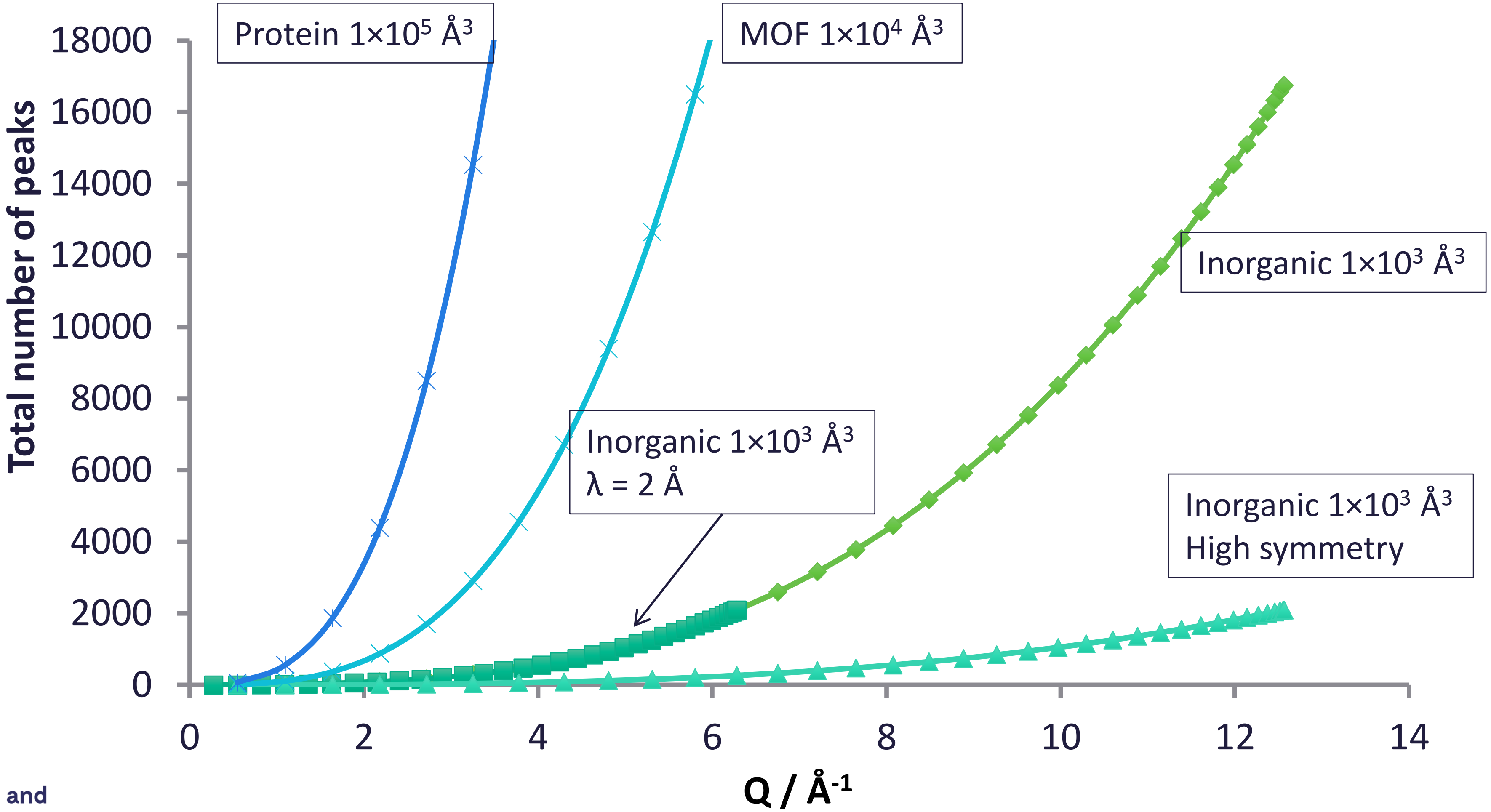
Diffractometer type

$$\lambda = 2d\sin\theta$$

- Monochromatic (CW)
  - Fix wavelength and scan detector angle
  - Multiple 2θ required to cover Q(d) spacing range
  - Q(d) spacing limit $4\pi/\lambda$ ($2\pi/d$)
  - Instrumental count rate factors: Source power, monochromator reflectivity, detector coverage and efficiency, etc
- TOF
  - Fix detector angle and scan wavelength
  - Single 2θ covers range of Q(d) space
  - Q(d range) determined by λ_{max}, λ_{min} and θ
  - Instrumental count rate factors: Source power, moderator performance, beam transport efficiency, detector coverage and efficiency, etc

Number of reflections



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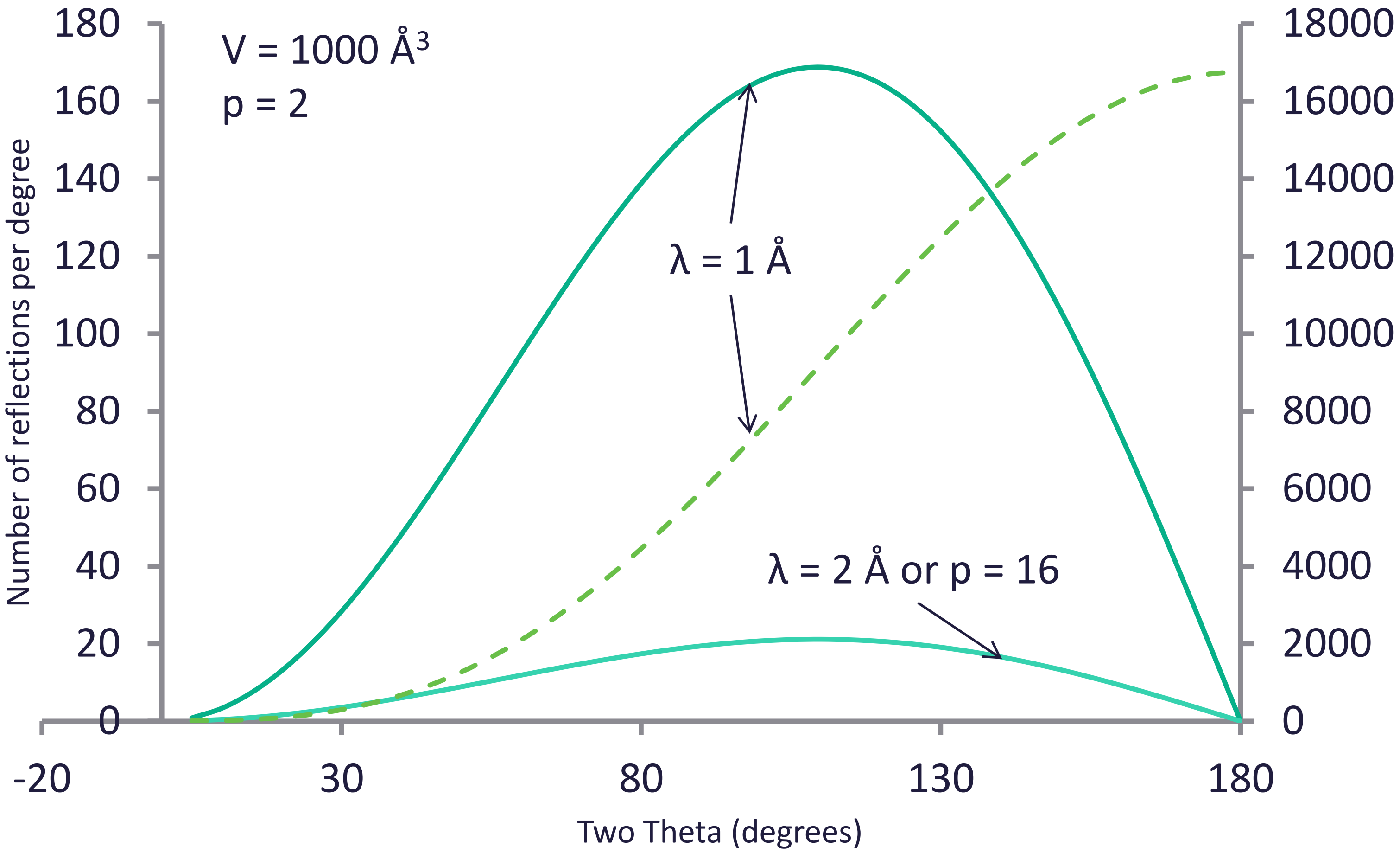
Reflection density (for CW)



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CW instruments designed to have best resolution at highest peak density

Resolution

Monochromatic

$$\frac{\Delta d}{d} = \frac{1}{2}\sqrt{U.\cot^2(\theta) + V.\cot(\theta) + W}$$

- U, V and W are functions of the collimation and U, V also takeoff angle to the monochromator
- Resolution minimum found near the takeoff angle of the monochromator $2\theta_B$
- Higher takeoff angle gives higher resolution for identical wavelength
- Wavelength produced by monochromator is takeoff angle dependent for any particular hkl plane

Time-of-flight

$$\Delta d/d = \left[\Delta\theta^2 \cot^2\theta + \left(\Delta t/t\right)^2 + \left(\Delta L/L\right)^2\right]^{1/2}$$

- $\Delta\theta$ is the angular uncertainty
- The main component of Δt is the moderation time of the neutron
- ΔL is the flight path uncertainty of the neutron mainly due to the finite width of the moderator
- First term can be minimised by moving to higher scattering angle
- Second and third terms minimised by increasing instrument length

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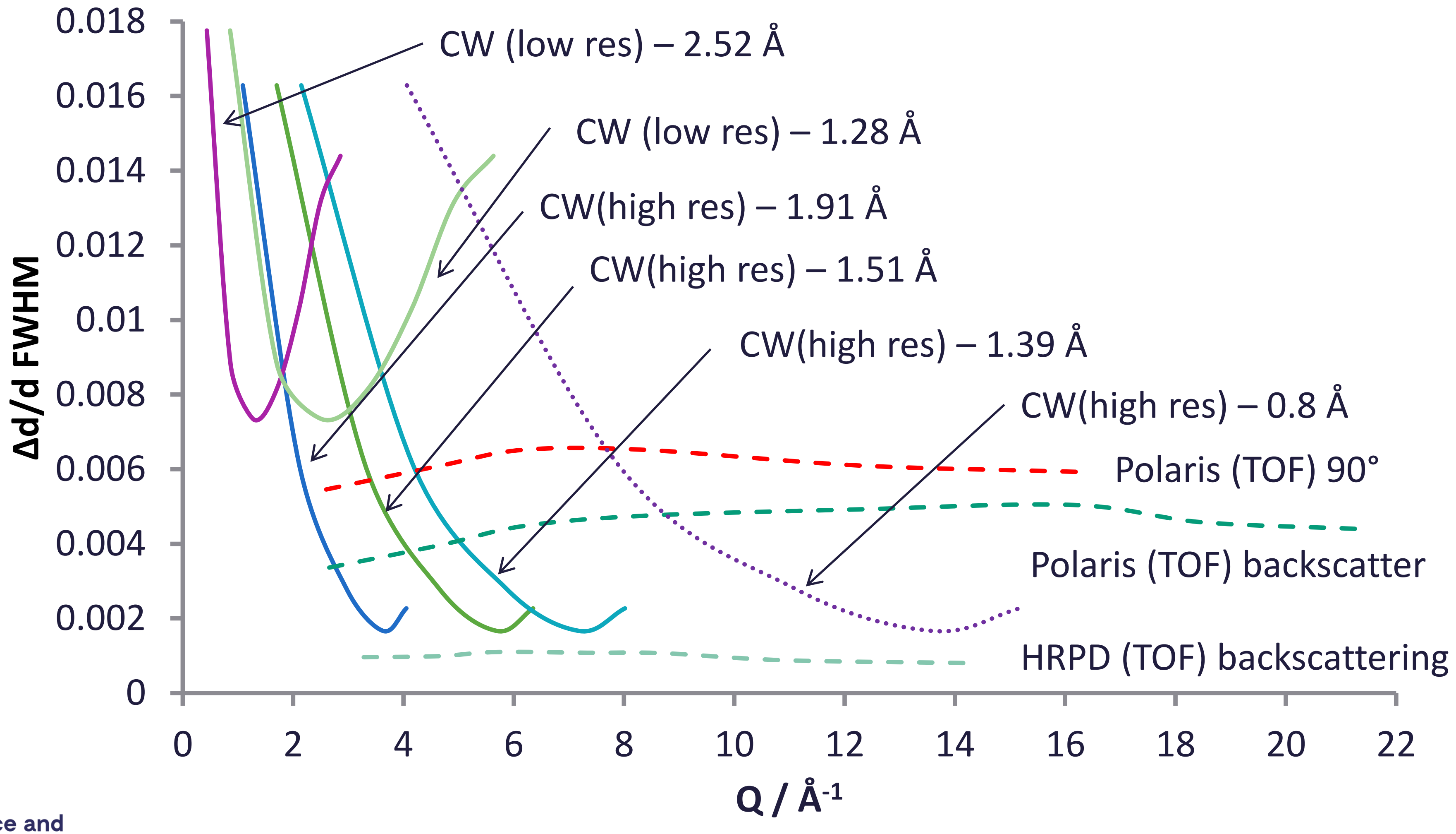
Resolution functions: CW v TOF examples



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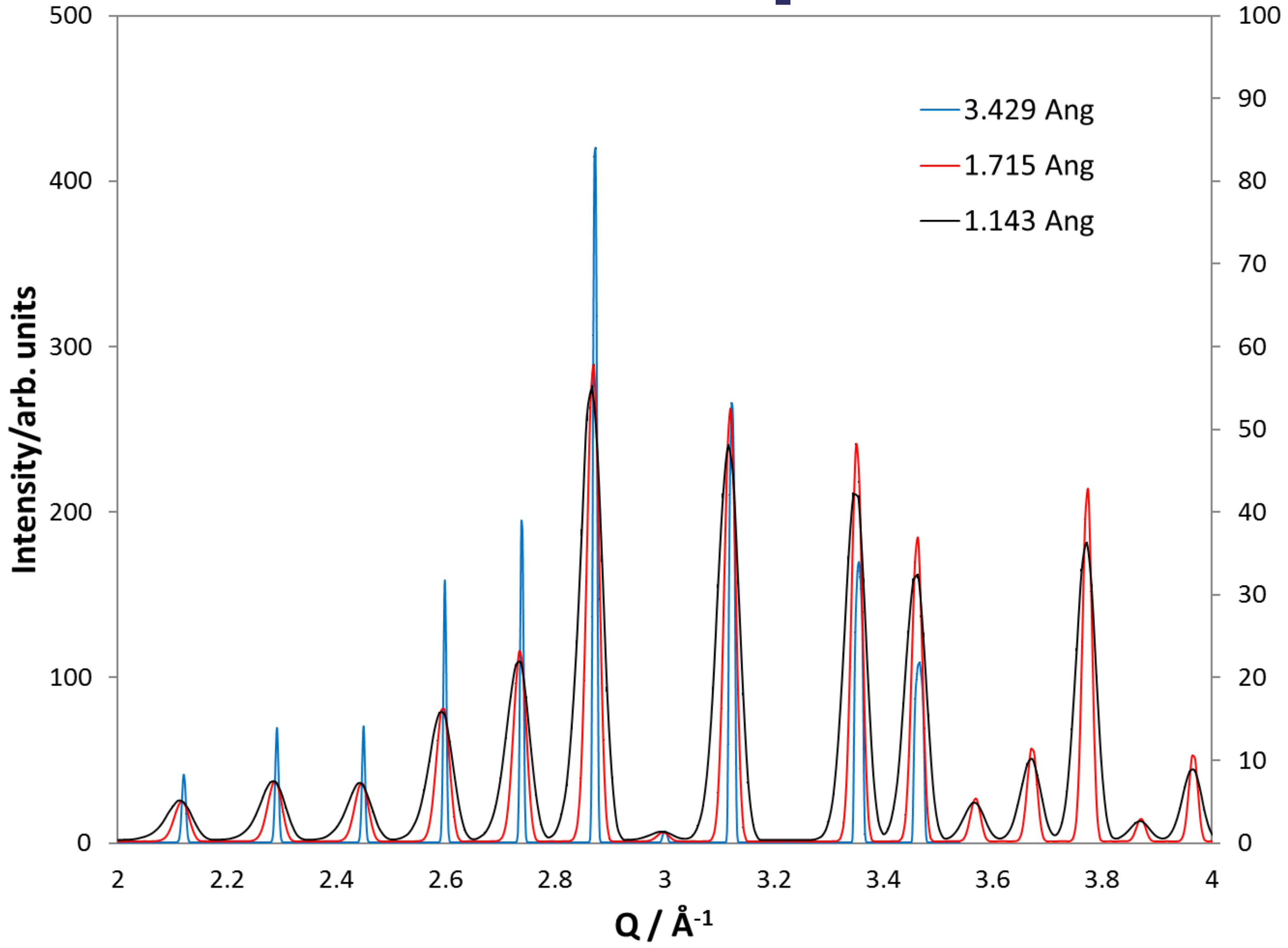
TOF Q-resolution tends to be flat, change at high Q caused by moderator residence time

Resolution function example: CW



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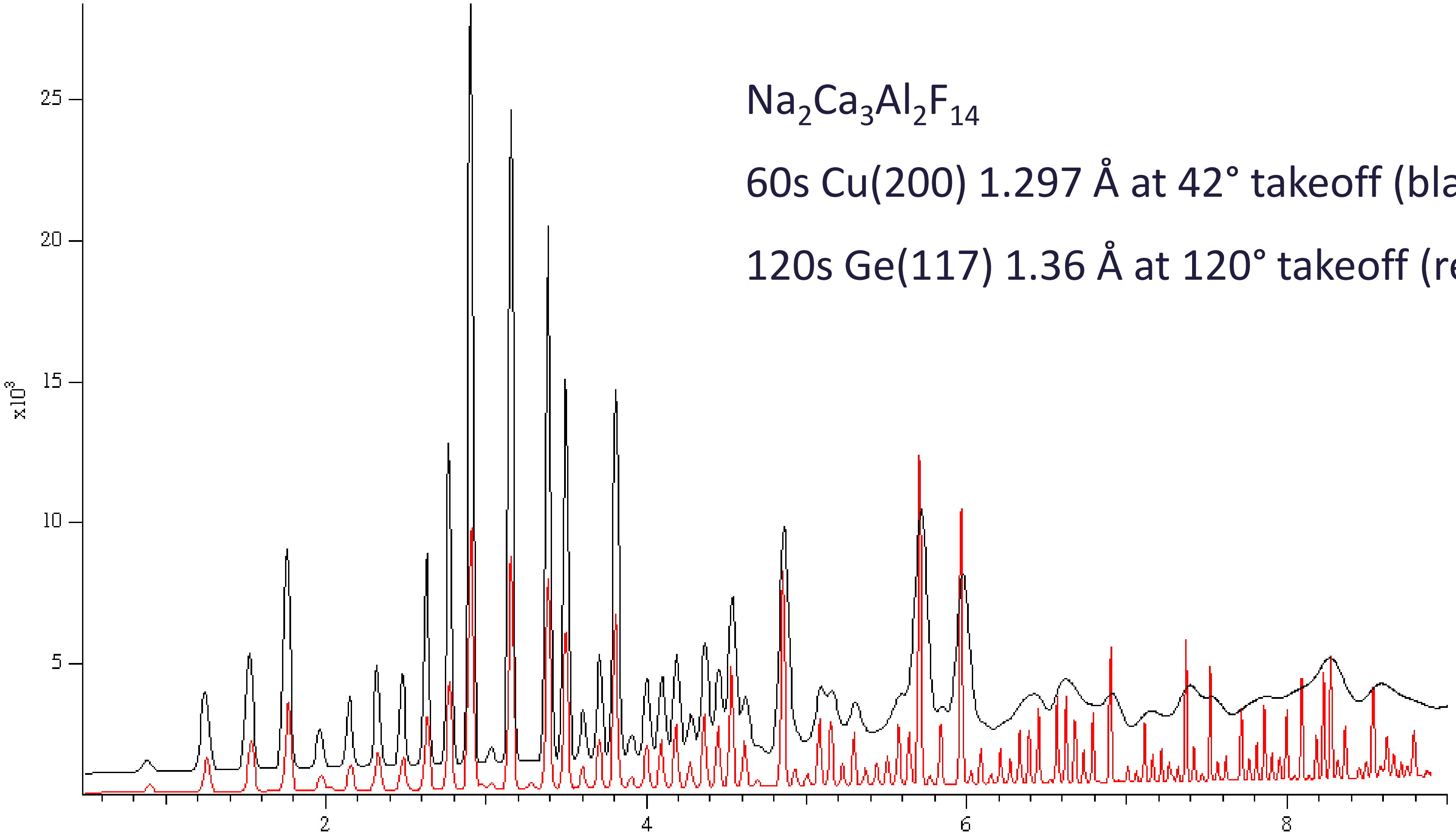
Choose wavelength to match Q resolution required by science in a given Q range

Resolution function with θ_B: CW

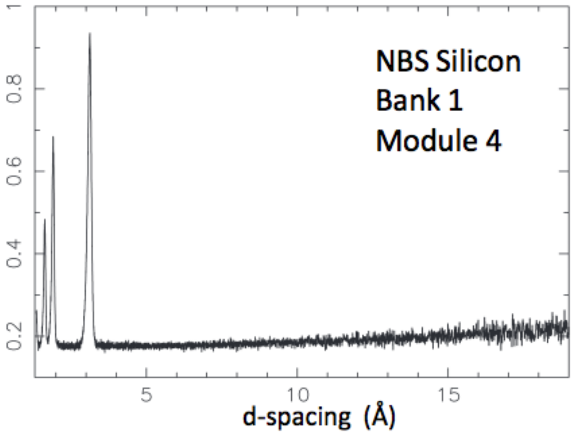


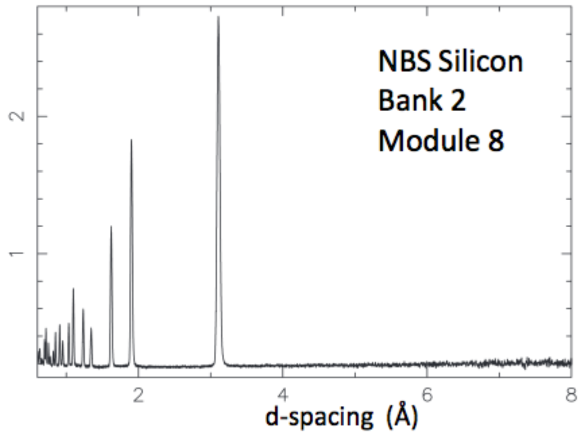
$Na_2Ca_3Al_2F_{14}$

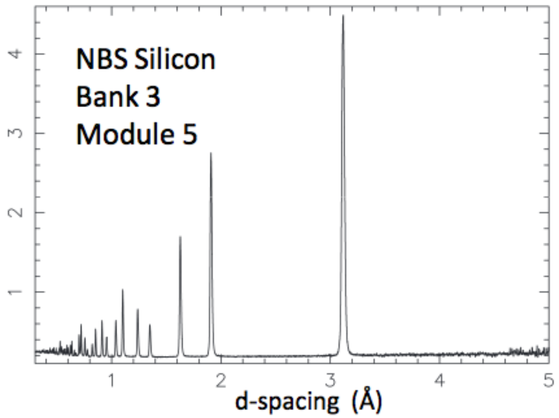
60s Cu(200) 1.297 Å at 42° takeoff (black)

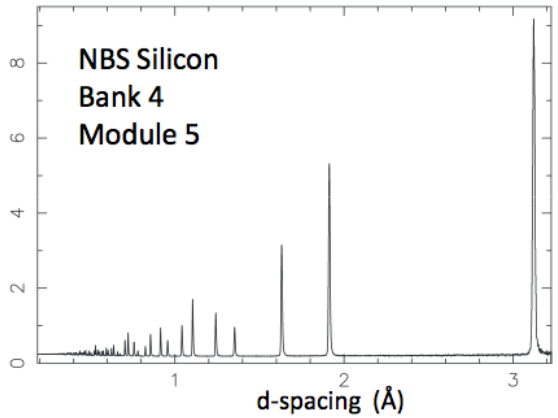
120s Ge(117) 1.36 Å at 120° takeoff (red)

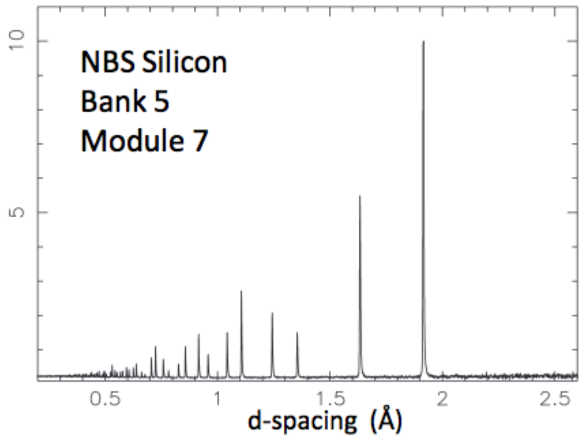
Resolution function example TOF: Polaris

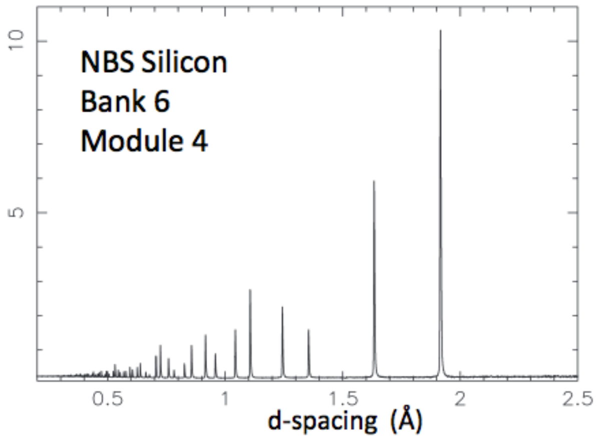


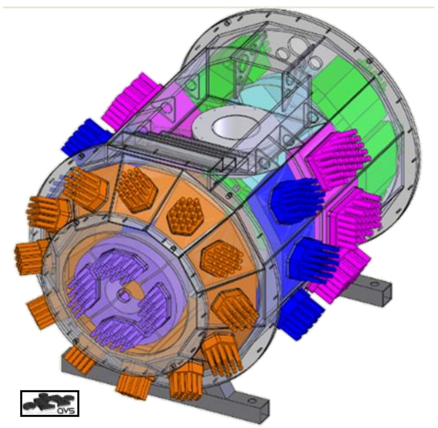












Bank 1 – cyan
Bank 2 – green
Bank 3 – pink
Bank 4 – blue
Bank 5 – orange
Bank 6 - purple

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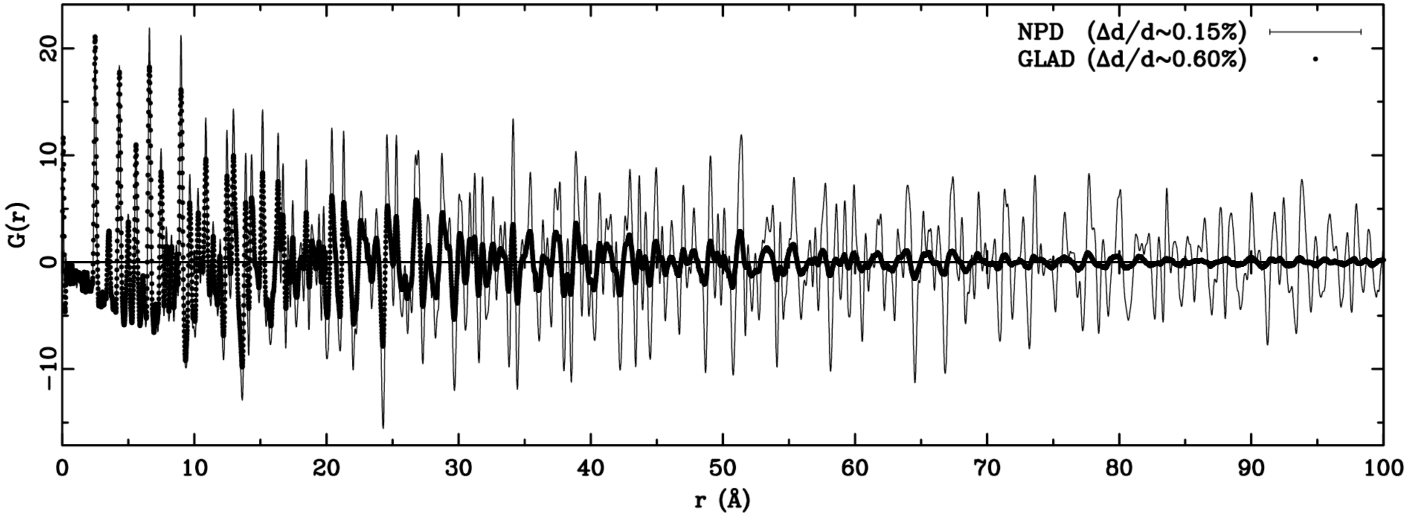
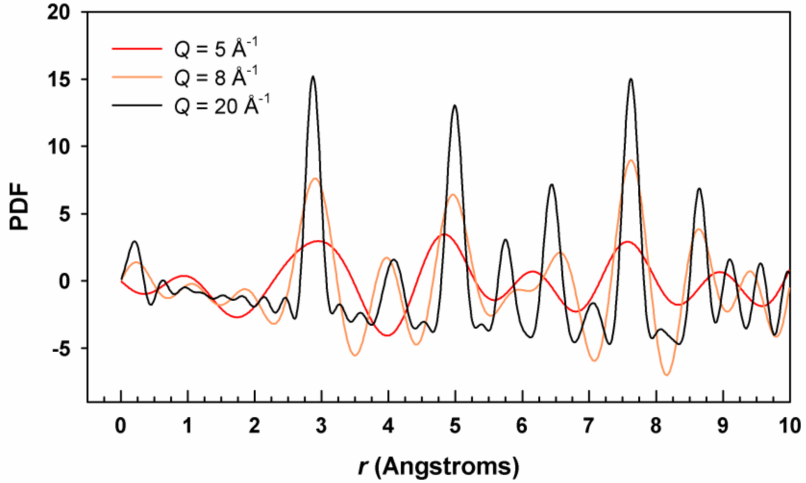
Importance of Q-max and Q-resolution



(reproduced from Proffen *et al.* (2003). *Z. Kristallogr.* **218**, 132-143) showing Ni G(r) from 2 instruments with different Q-resolution with Q_{max} cut-off of 35 $Å^{-1}$



Reproduced from Michel, SSRL workshop (2010)

- Good Δd/d resolution at low d (ΔQ/Q resolution at high Q)
- Access to as low d (high Q) as possible

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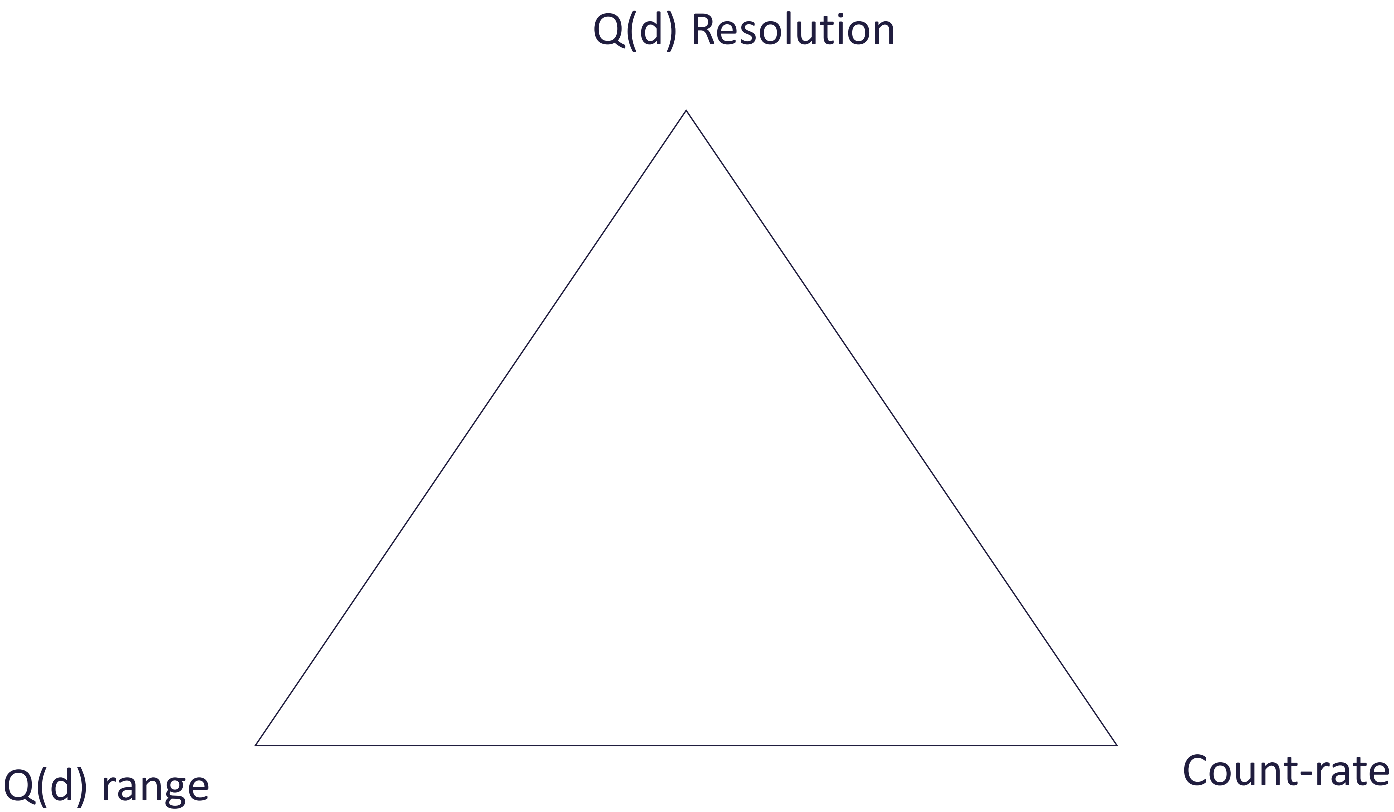
Summary of Q resolution and range

- CW:
  - Simple, symmetric peakshape function
  - Best resolution where diffraction peak density is highest in scattering angle
  - Different wavelength can be used to give Q resolution where required
  - Different takeoff angle can be used to change resolution function and wavelength
  - Instrument can have high Q resolution over a very limited Q range

- TOF:
  - Complex asymmetric peakshape related to moderator characteristics
  - Instrument length and moderator give wavelength band and overall resolution
  - Q resolution almost constant for a given detector bank so increasing peak density with Q can be an issue
  - Q resolution improved by moving to higher scattering angle detector bank
  - Q range determined by scattering angle of detector bank

Defining primary requirements



But also:

- Single crystal, powder, non-crystalline
- Unit cell volume
- Sample environment restrictions
- Need for *in situ* capability
- Sample size / geometry
- Detector type / coverage / stability
- Parasitic scattering
- Etc…

Rank them in importance to the proposed instrument role

Instrument layout

Instrument layout: follow the neutrons

Source → Beam transport → Sample area → Detectors

Understand the impact of complexity on performance v cost

Identify potential issues early

Identify necessary development / proof of concept studies

Prepare yourself for discussions with engineers and vendors

Source

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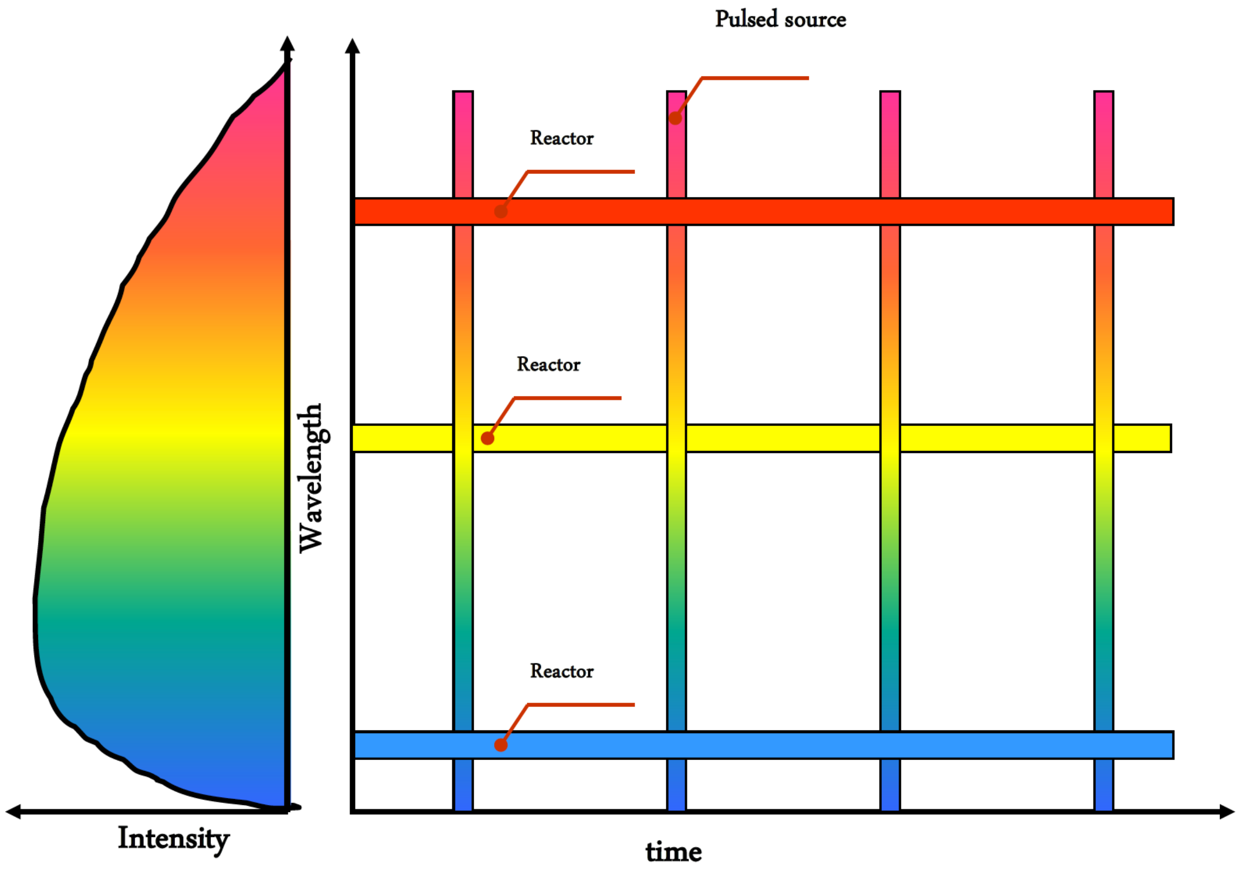
Source influence on CW or TOF



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Some of the neutrons all of the time or all of the neutrons some of the time

Moderators

	cold	thermal	hot
moderator	liquid D_2	Liquid D_2O	graphite
moderator temperature	20K	300K	2000K
neutron wavelength	3→20Å	1→3Å	0.3→1Å
sample lengthscale	1Å→100 nm	0.3→5Å	0.1→2Å
sample timescale	1kHz→1 THz	0.1→10 THz	1→100 THz

- Wavelength range
- Peak-shape (residence time)
- Temperature stability
- Viewing angle
- Viewing multiple moderators
- Poisoning
- Moderator development

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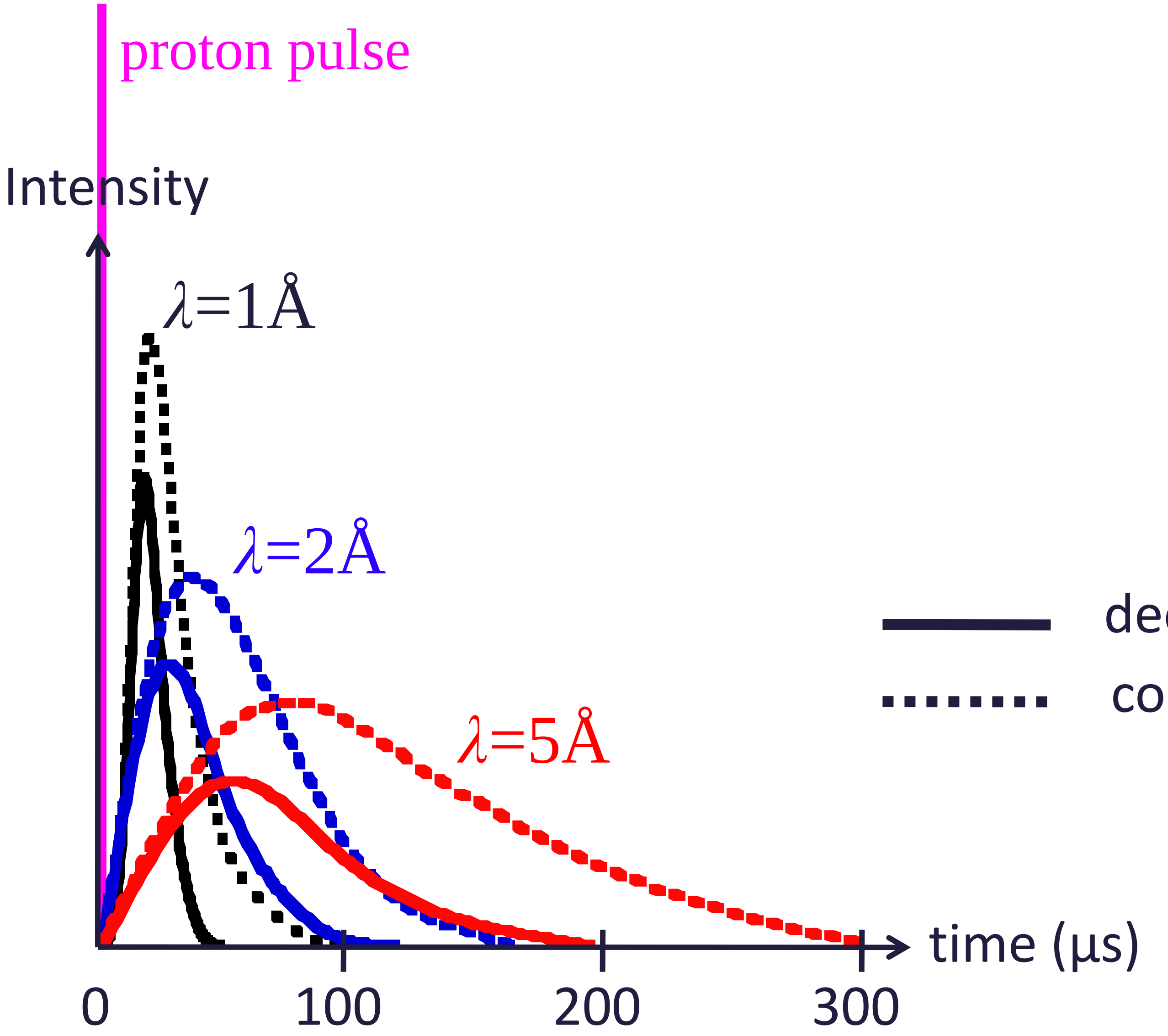
Moderators: short pulse



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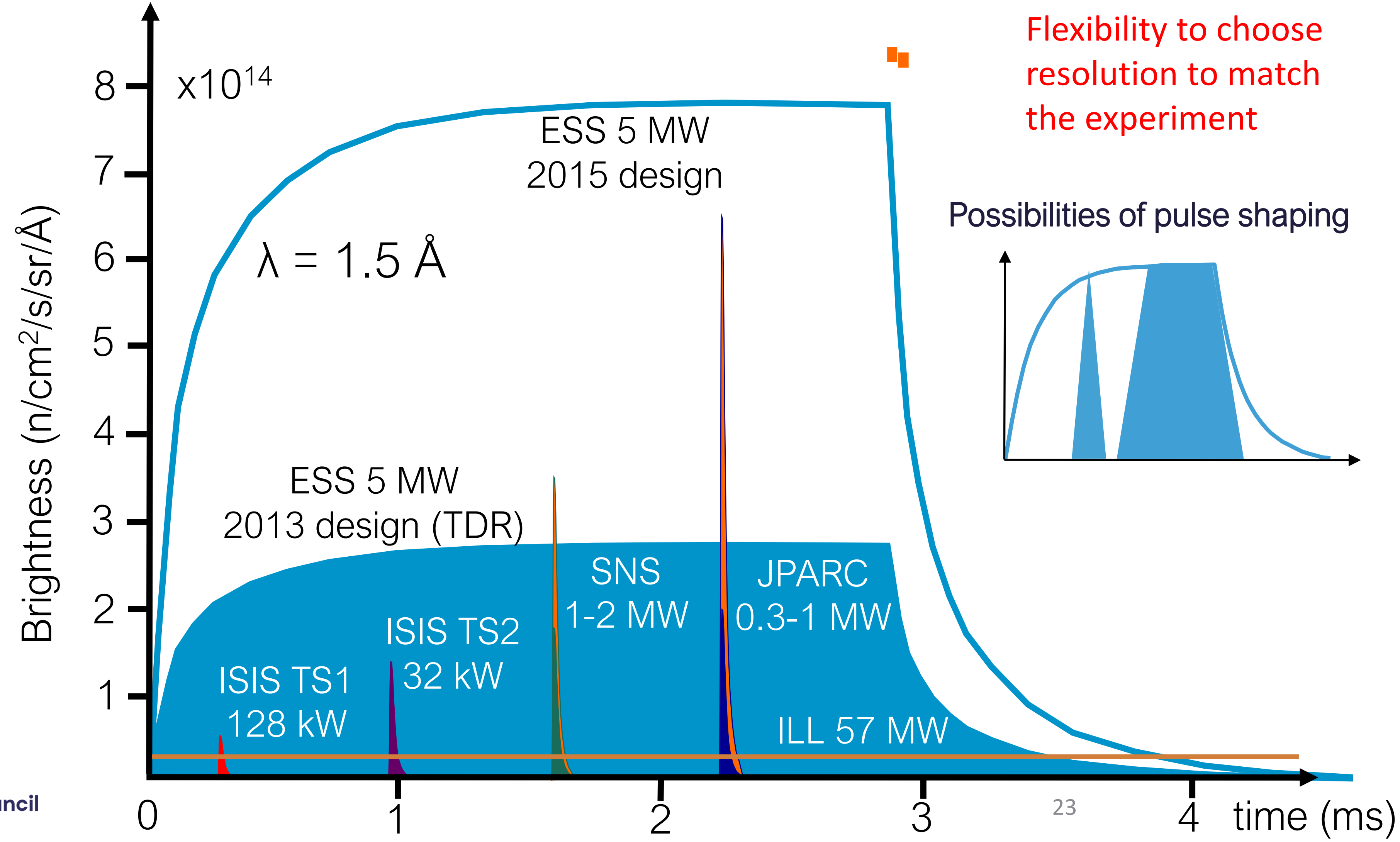
Moderators: long pulse



Flexibility to choose resolution to match the experiment

Possibilities of pulse shaping

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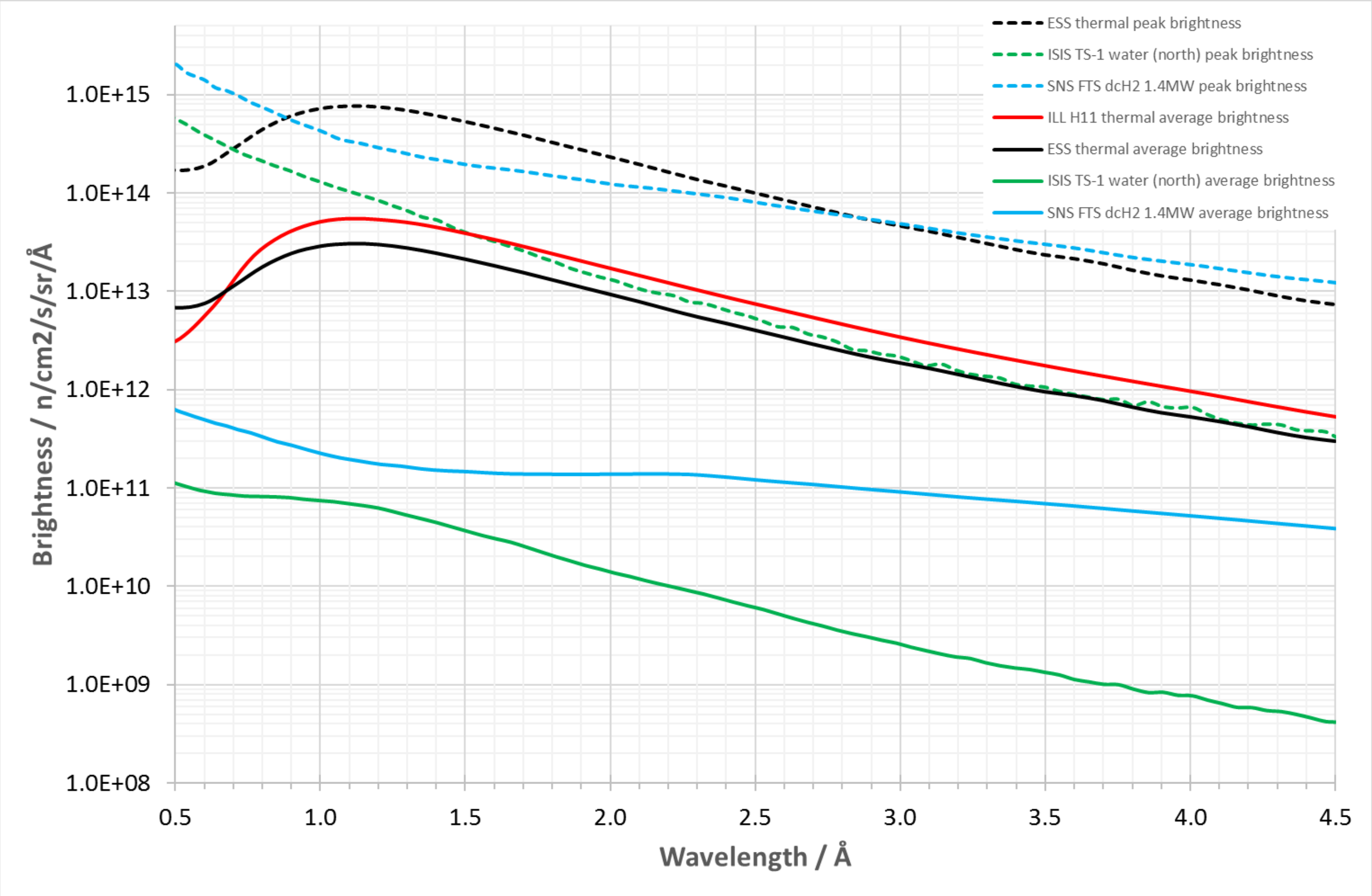
Source brightness for CW or TOF



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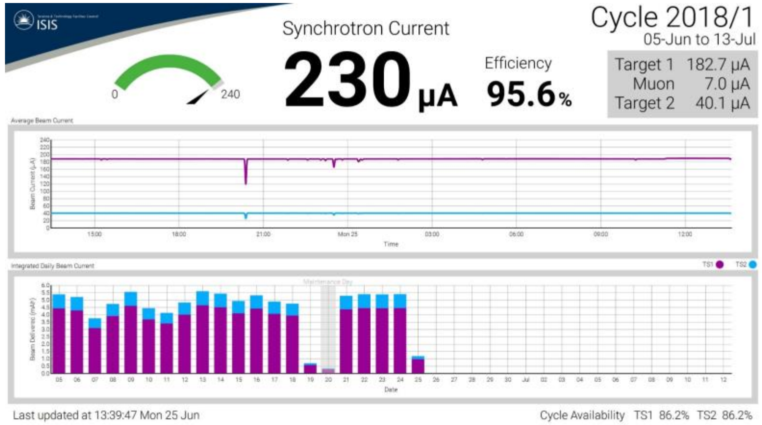
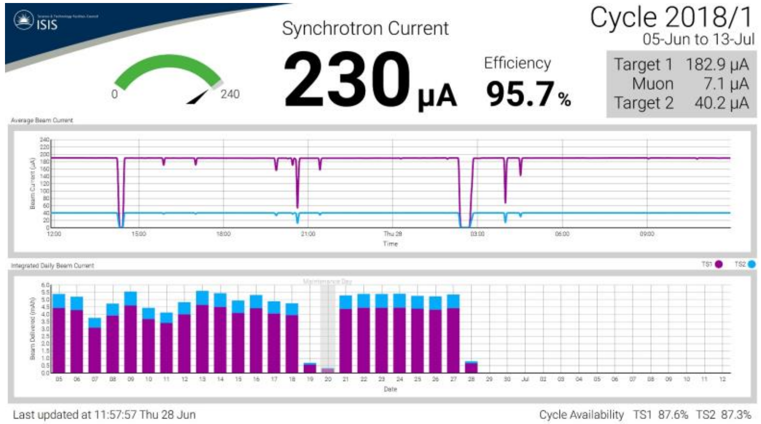
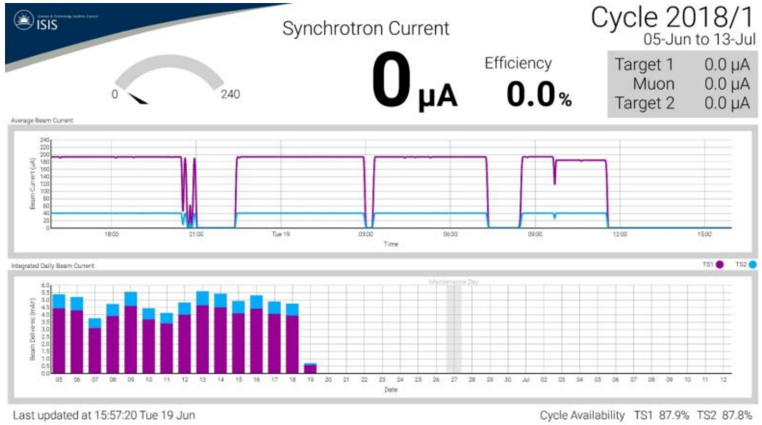
High peak brilliance good for TOF
High time-average brilliance good for CW

Source stability / availability







Spallation sources have lower availability than reactors. Does this compromise science case?

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Instrument type v source type

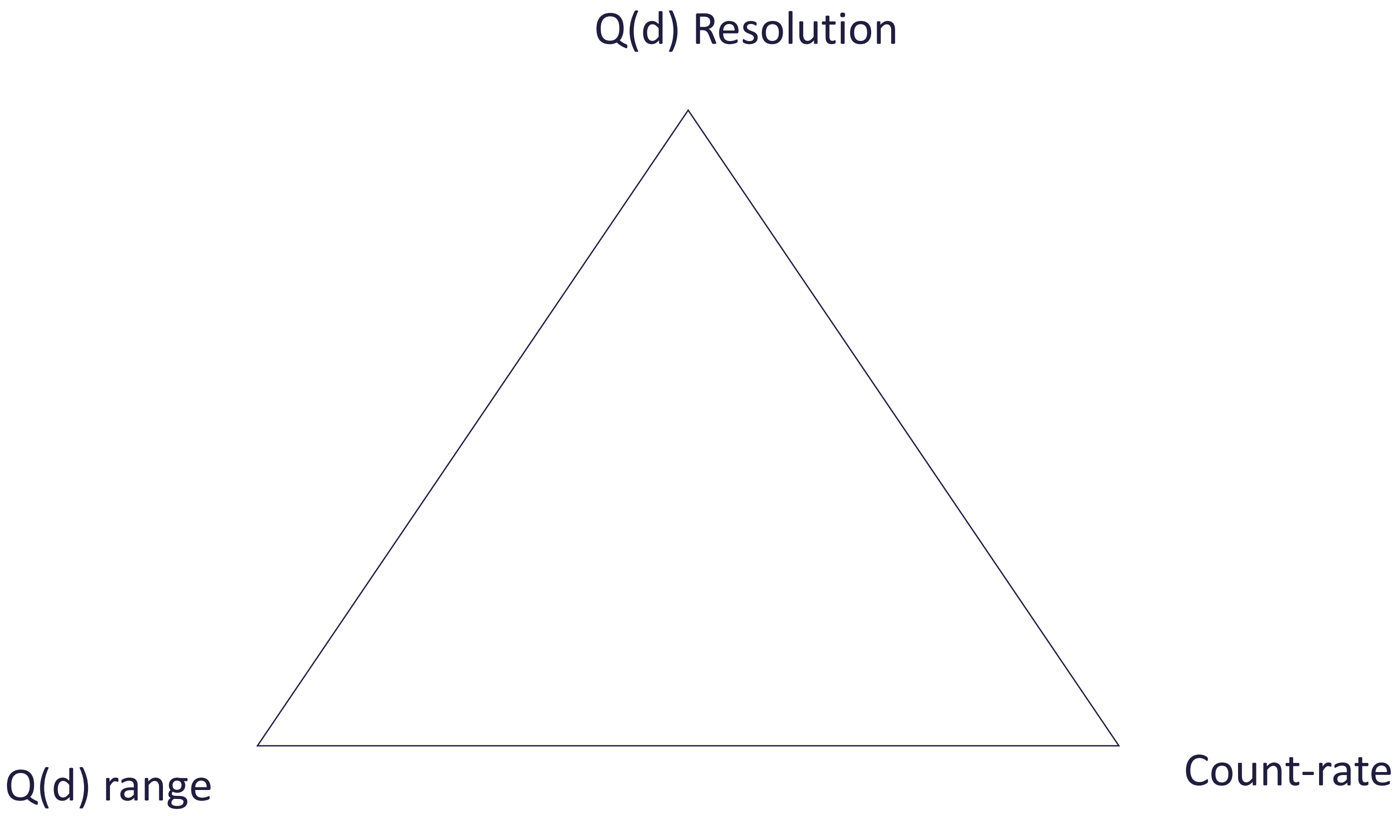
- Reactors build CW instruments*
    - Low peak brilliance, high time-average brilliance
    - Variable reflectivity from monochromators limit low λ use
    - High Q not easily reached
    - Match moderator and monochromator take-off angle to Q range and resolution
    - Beam always on

*Except when significantly restricted geometry constraints from science case necessitate use of TOF

- Pulsed sources build TOF instruments#
    - High peak brilliance, low time-averaged brilliance
    - Require efficient beam transport
    - High Q possible
    - Increase instrument length to improve resolution at expense of bandwidth
    - Variable Q range and resolution from detector angles
    - Beam availability can compromise science

#Remains to be seen for long pulse sources

Summary



- Different source types offer complementary possibilities
- Don’t limit yourself to a particular source type without good reason

It may be that our spallation source is not ideally suited to your science case requirements!

Beam transport

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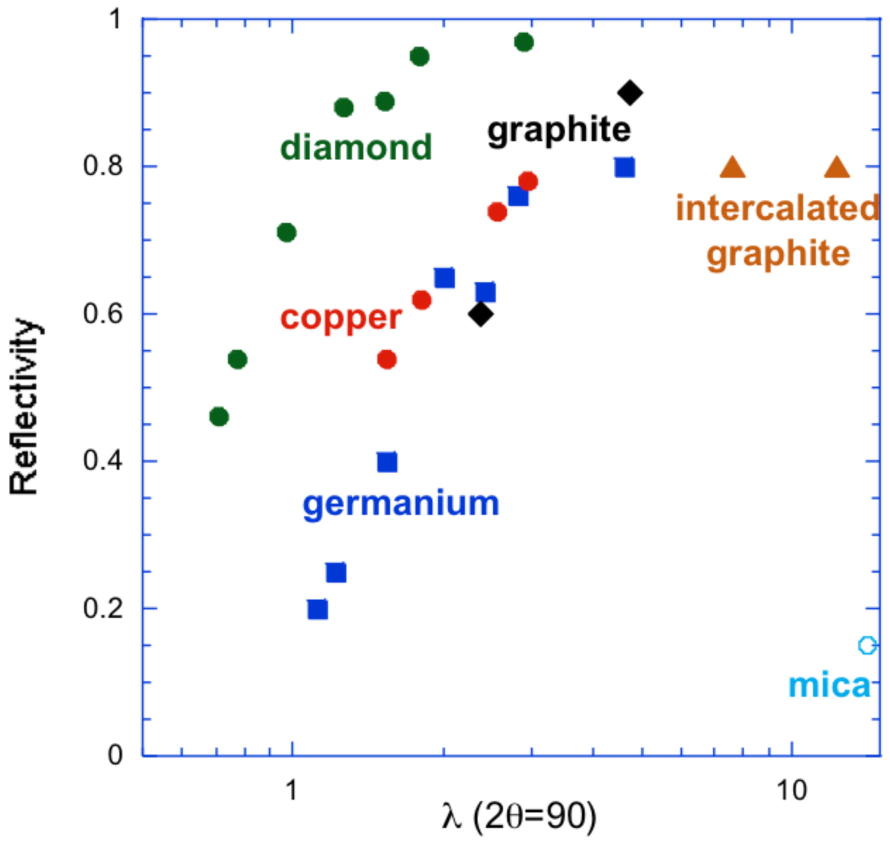
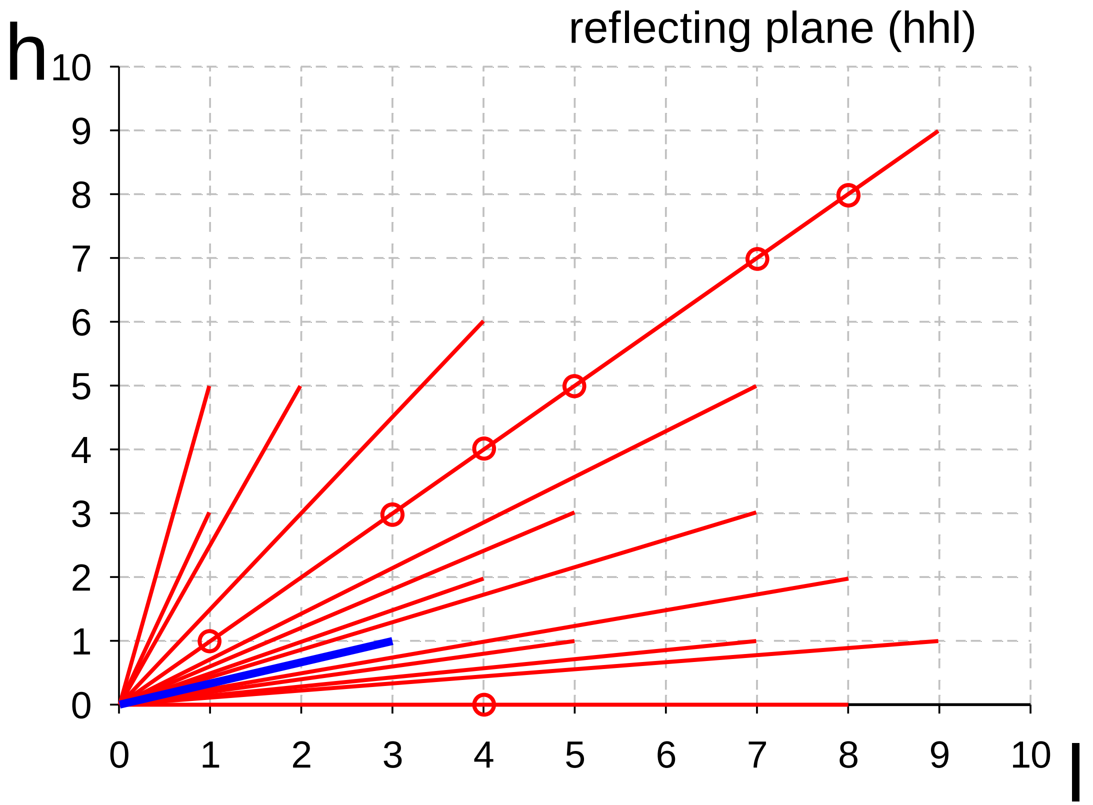
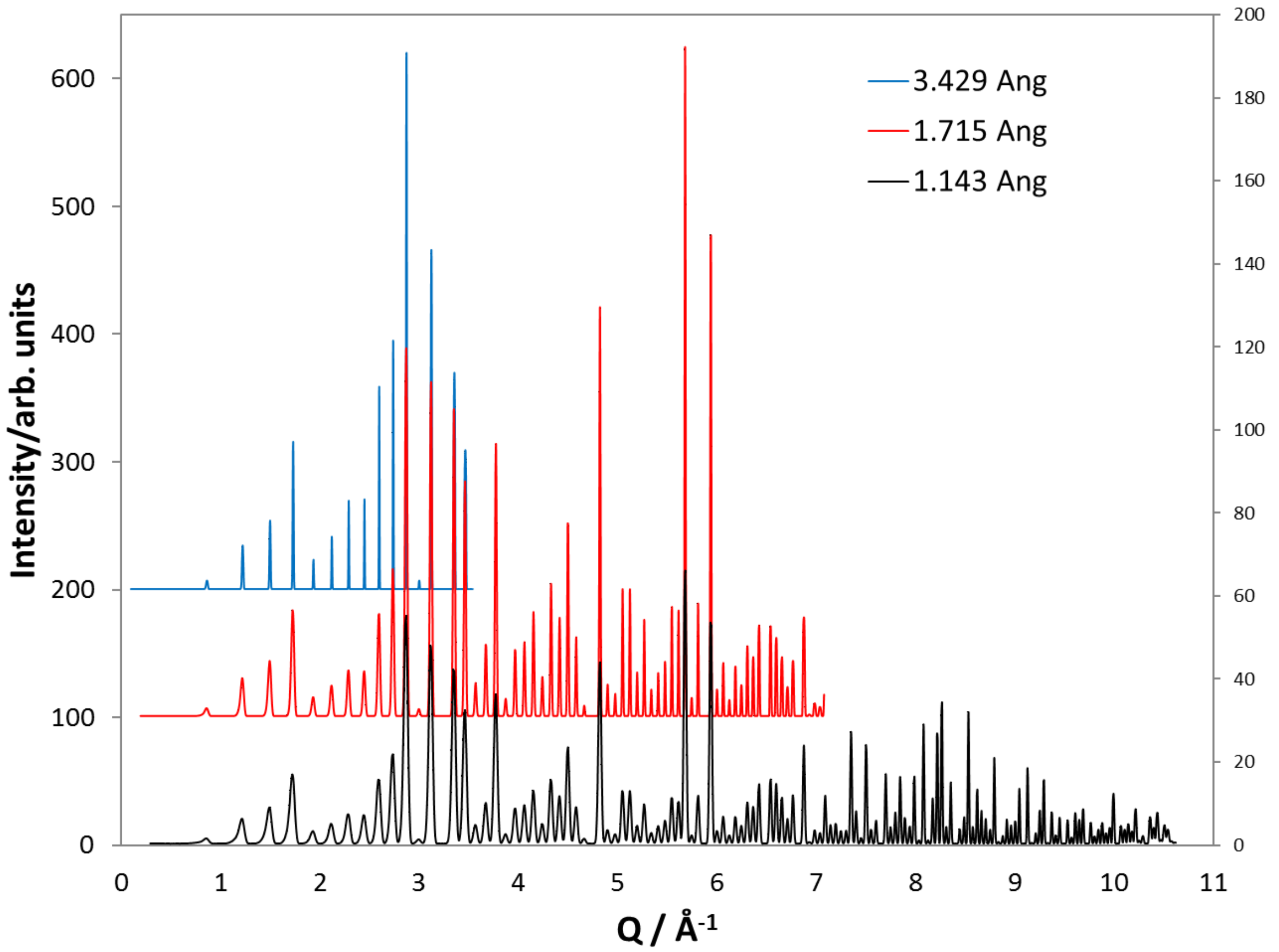
Monochromator reflectivity for CW





Choose a material and plane to access necessary Q-range
Reflectivity falls as wavelength decreases

Q-range accessible with CW



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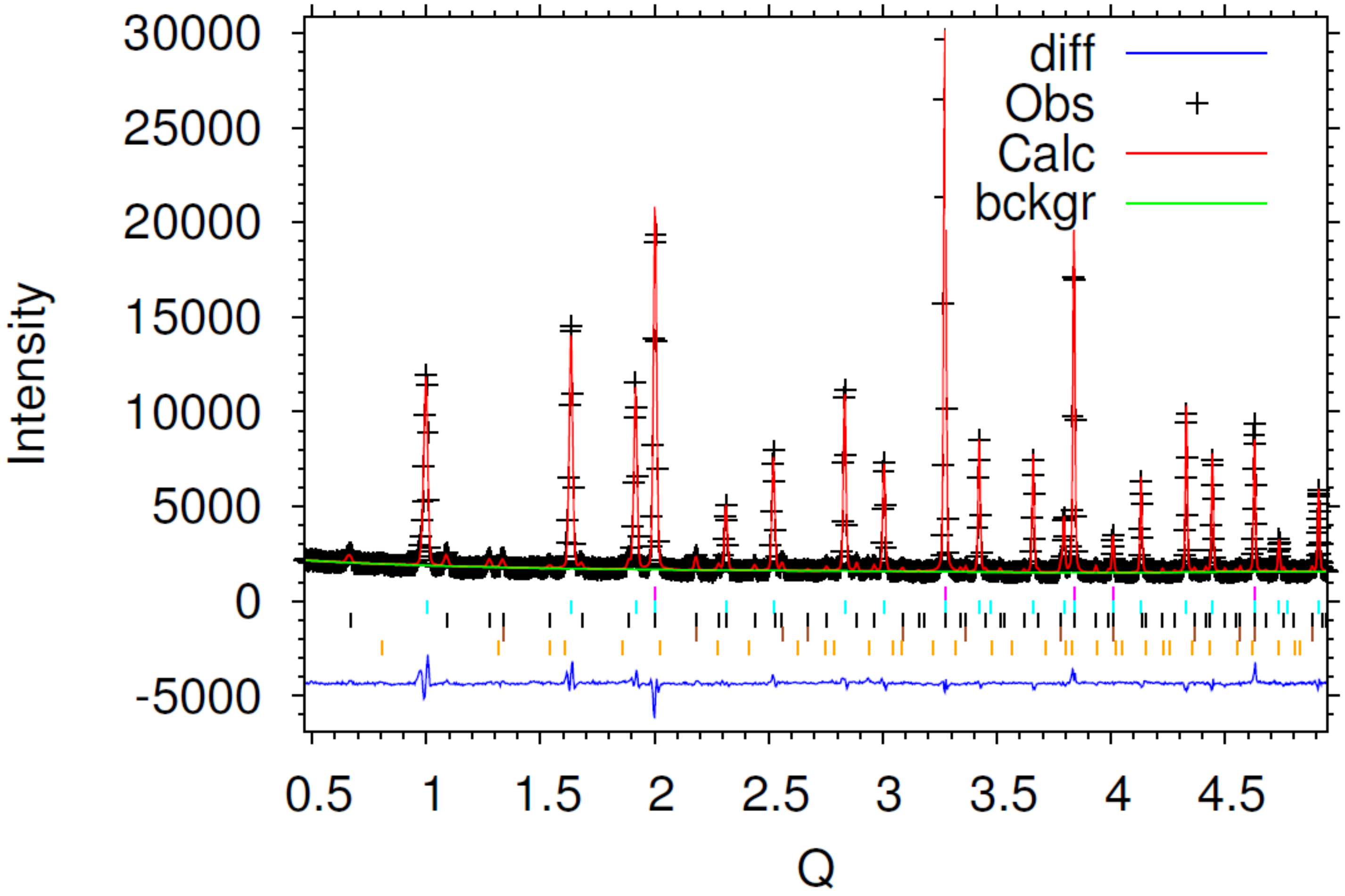
Shorter wavelengths access higher Q but have lower reflectivity

Higher reflection order contamination: CW



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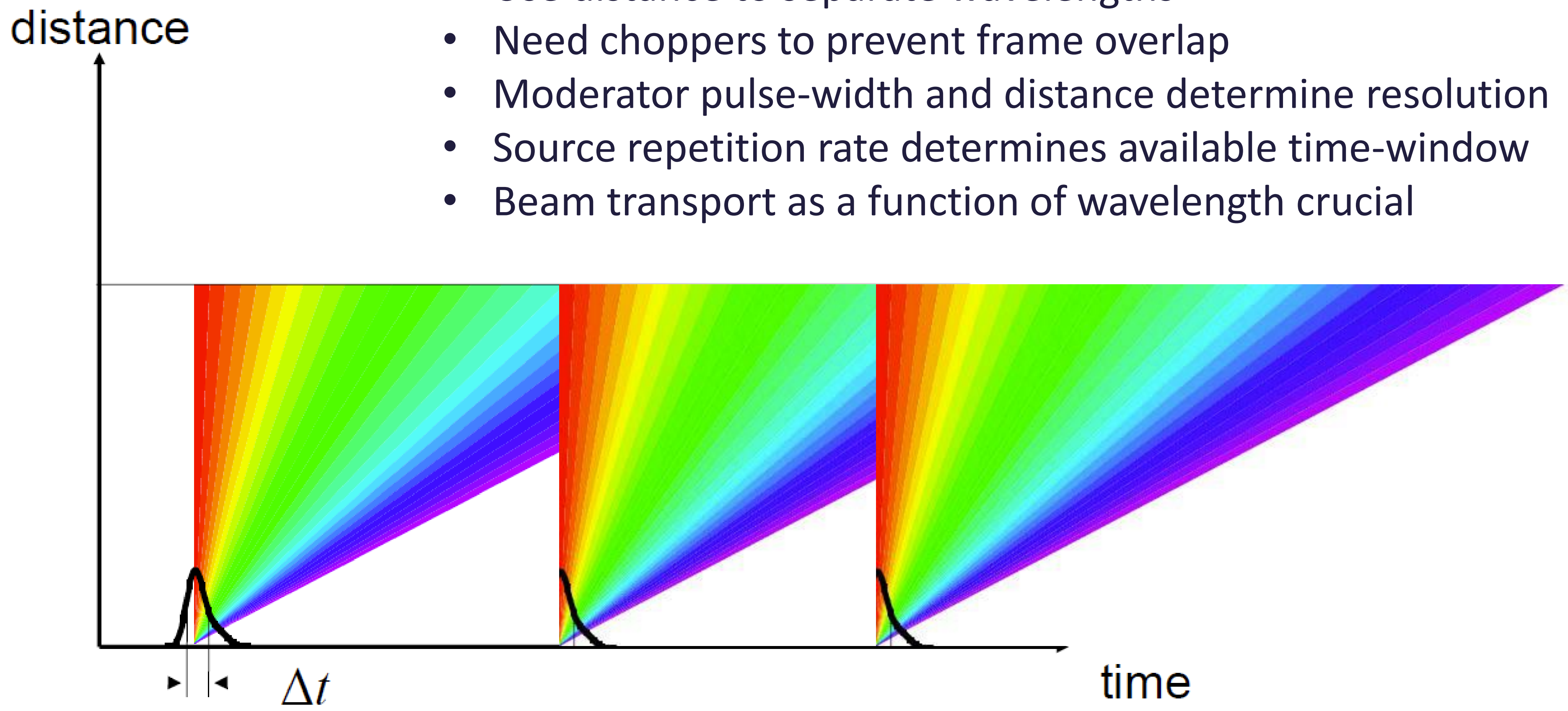
High reflection order contamination complicates analysis with CW data

Beam transport for pulsed sources

- Use distance to separate wavelengths
- Need choppers to prevent frame overlap
- Moderator pulse-width and distance determine resolution
- Source repetition rate determines available time-window
- Beam transport as a function of wavelength crucial



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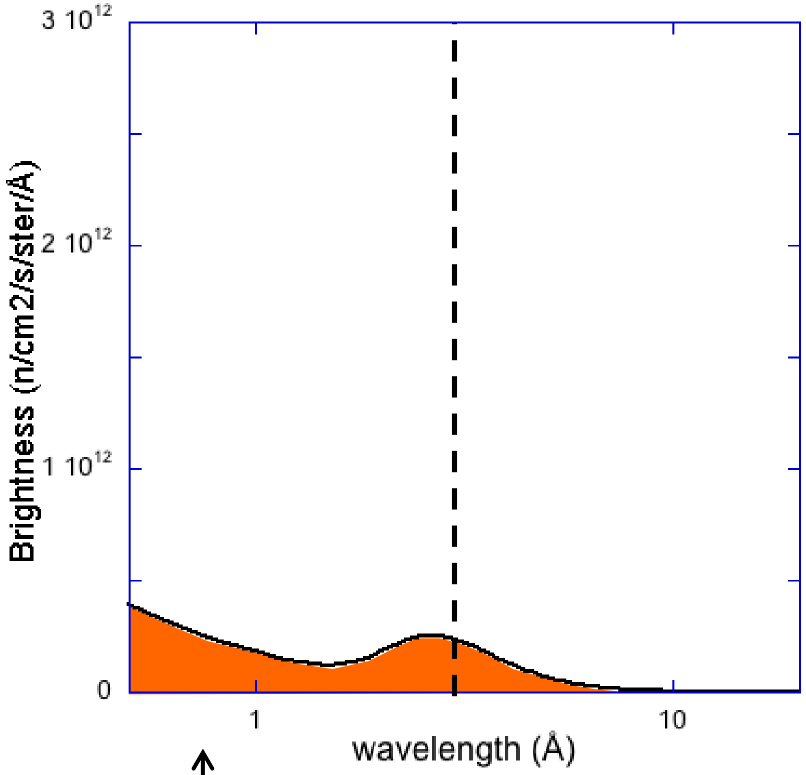
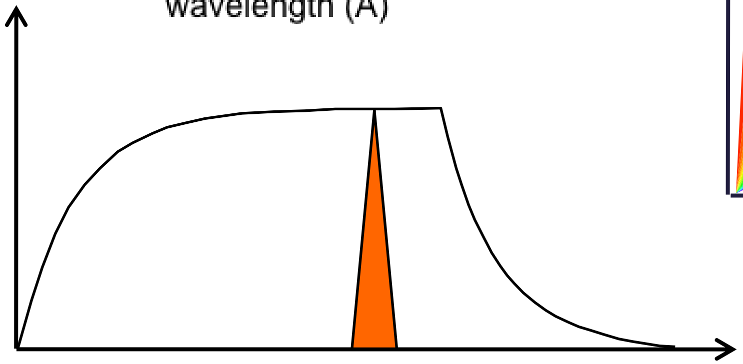
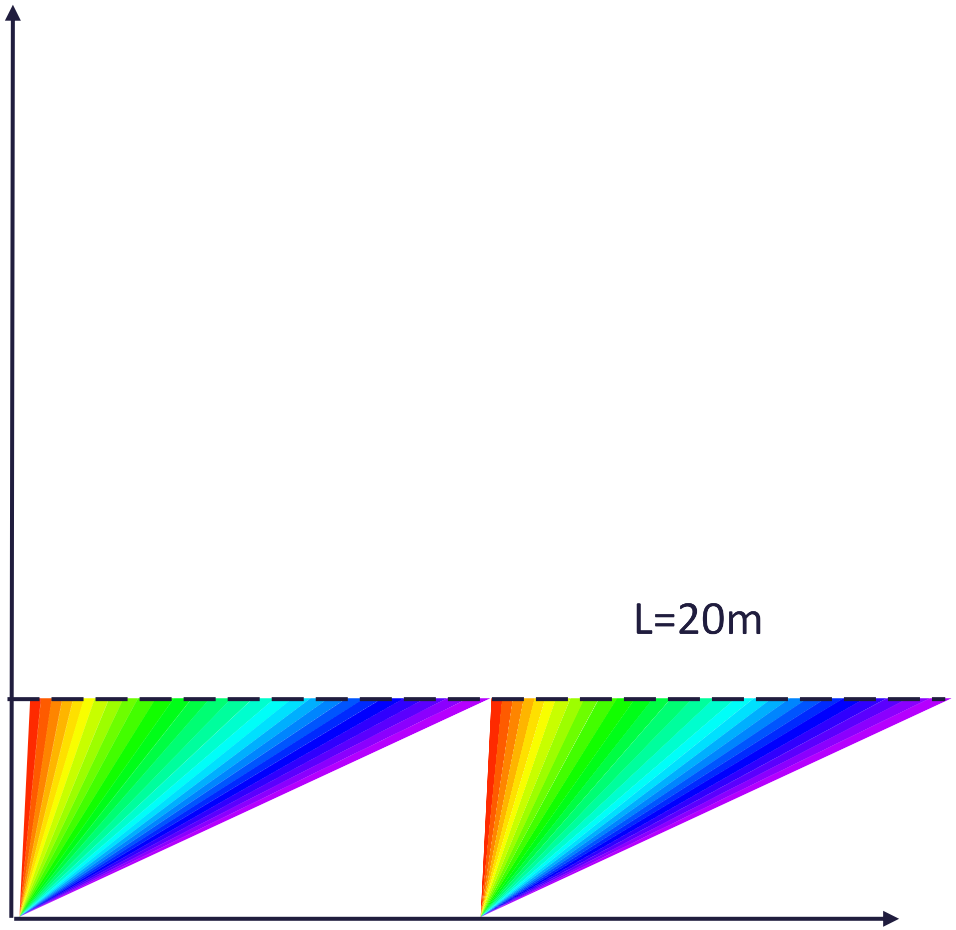
Q-range with TOF (available bandwidth)







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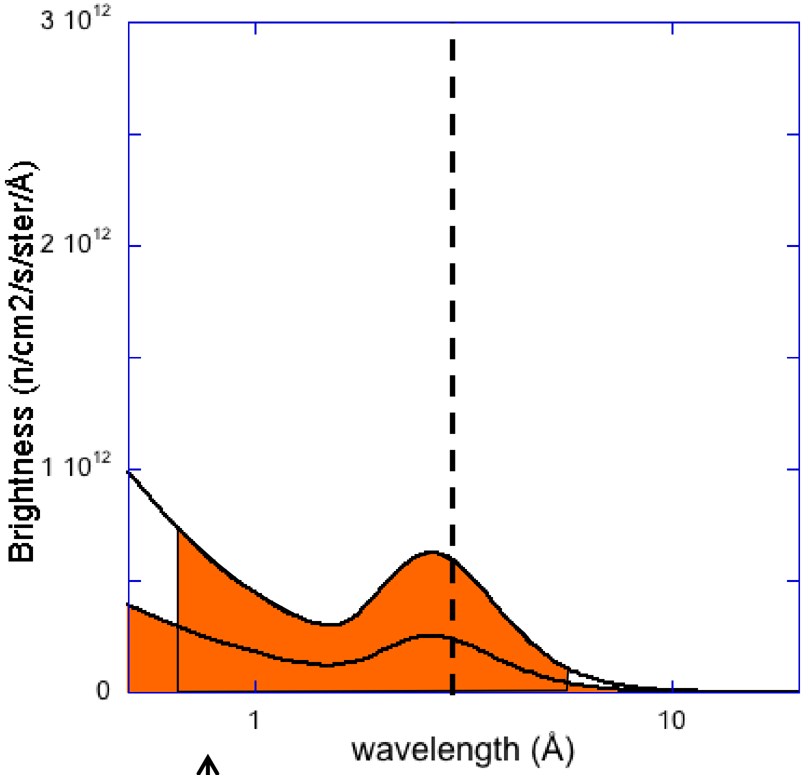
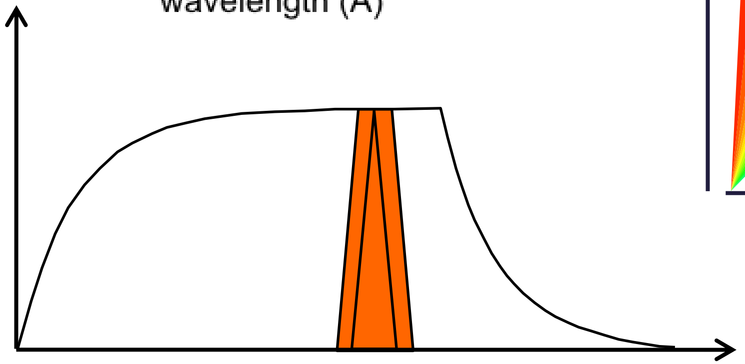
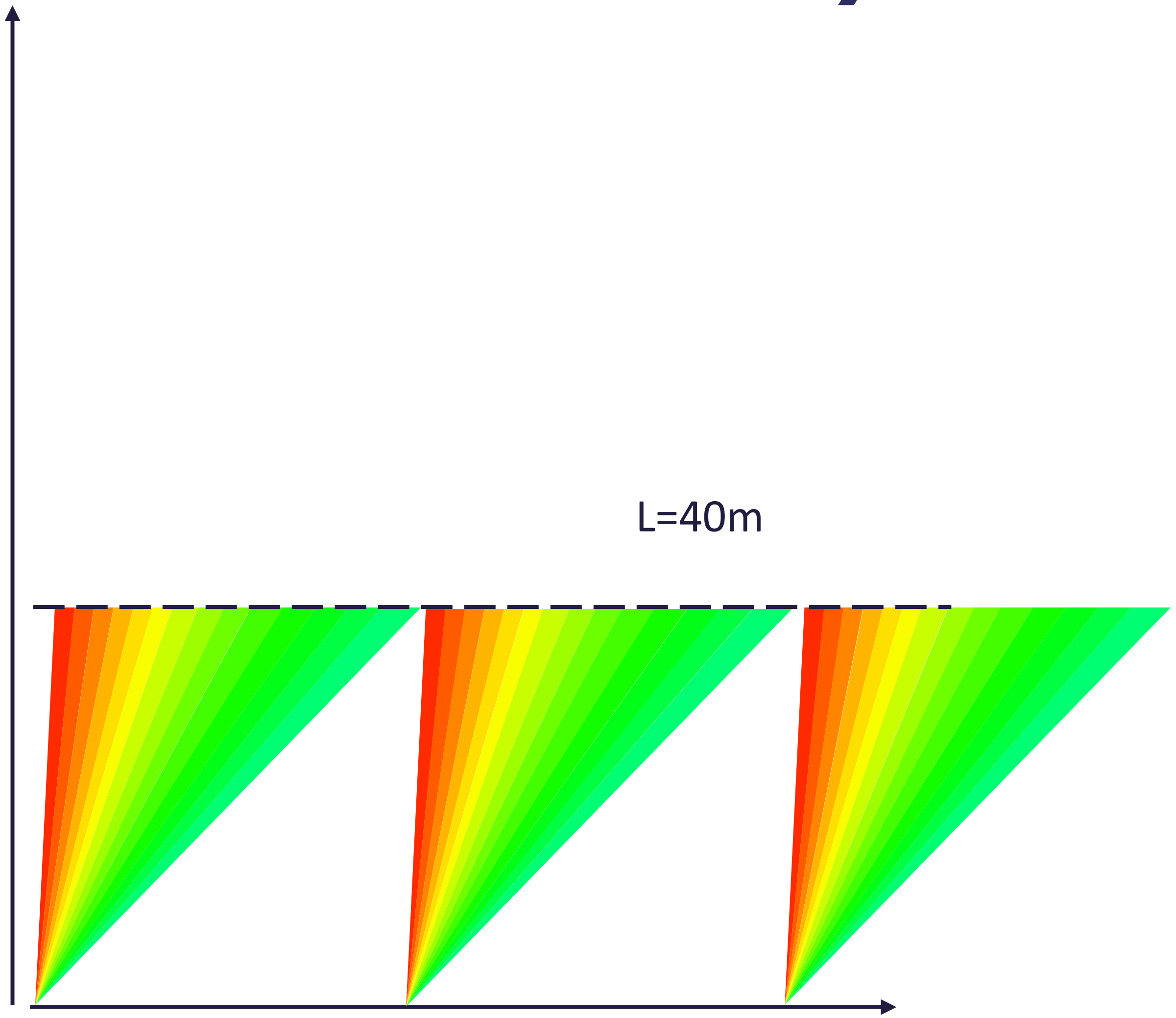
Q-range with TOF (available bandwidth)







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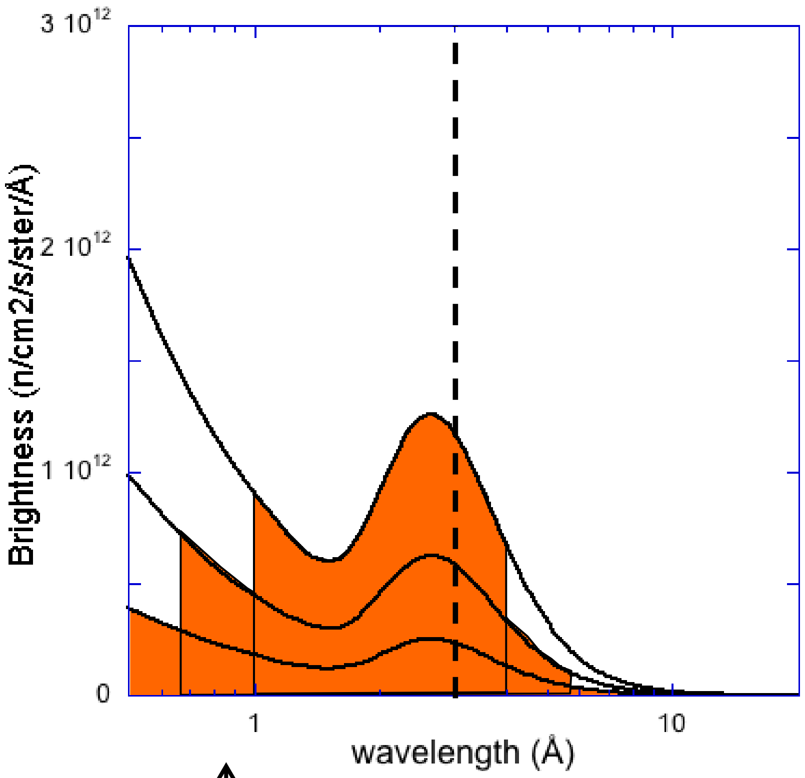
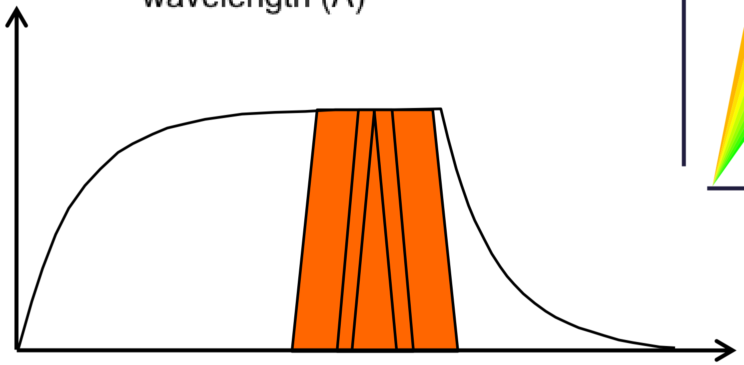
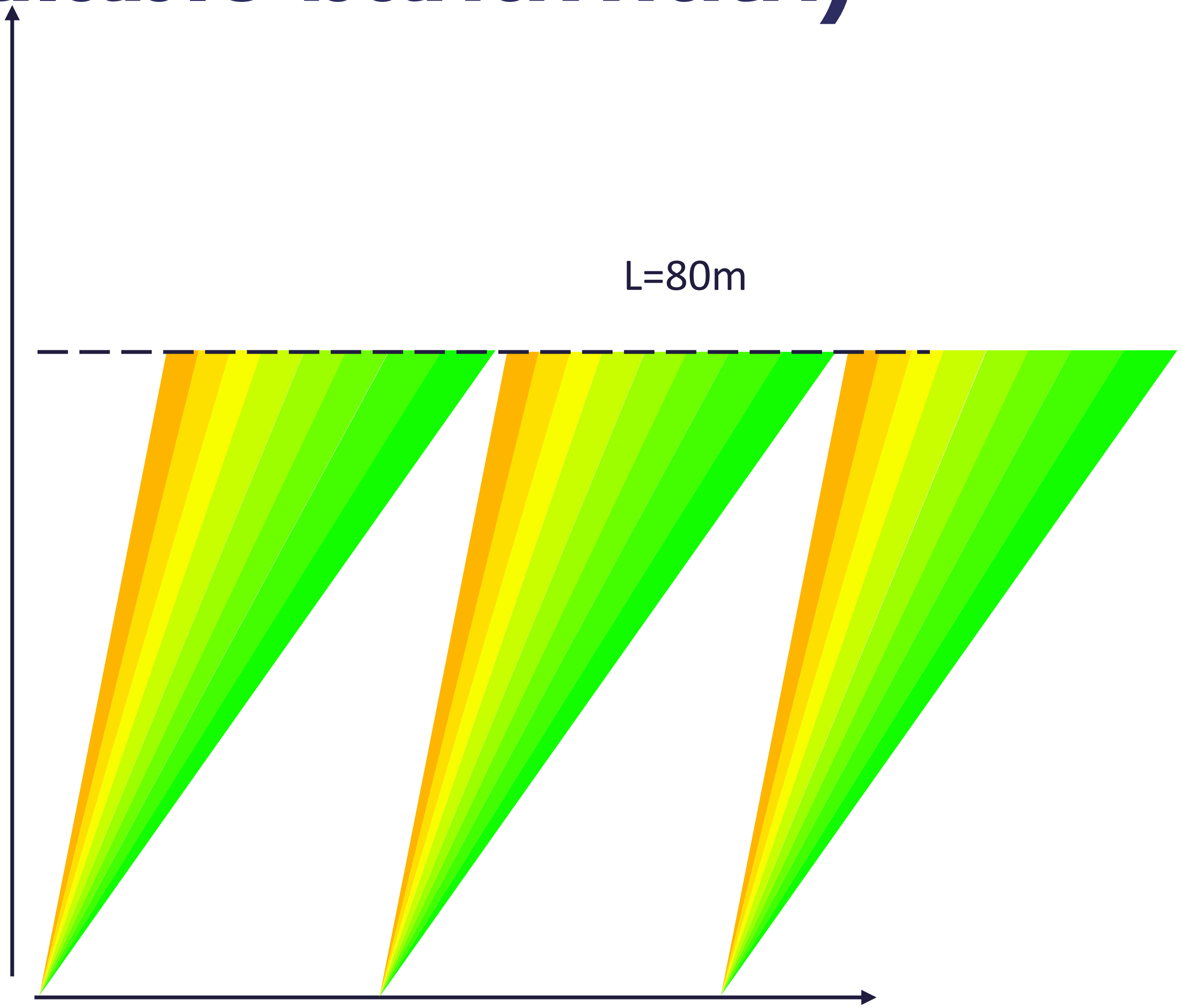
Q-range with TOF (available bandwidth)







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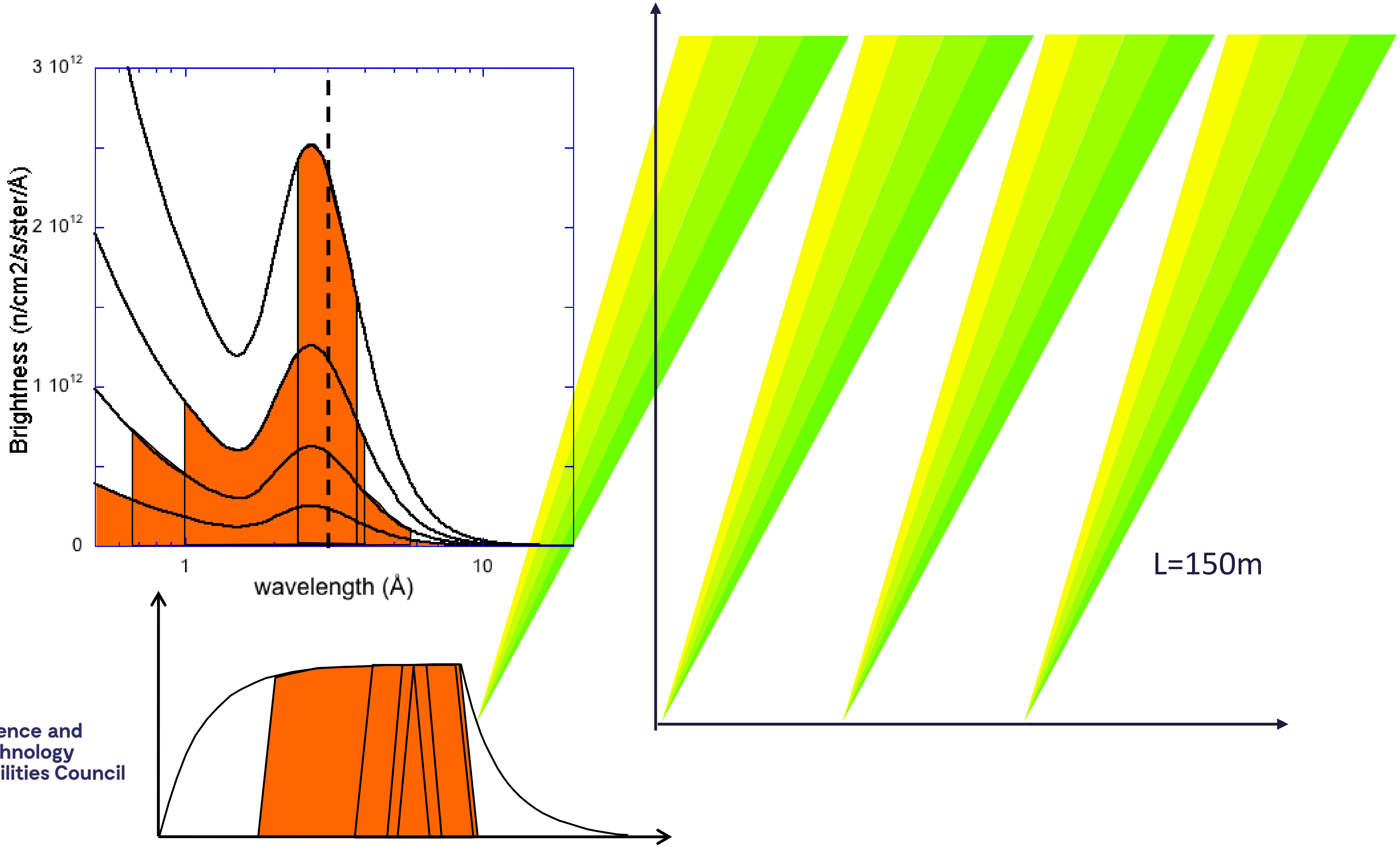
Q-range with TOF (available bandwidth)



Q-range and resolution for CW and TOF

For CW:

- For monochromatic instruments the Q_{max} is $4\pi/\lambda$ i.e. when $\sin\theta = 1$, $\theta = 90°$, $2\theta = 180°$
- If a high Q_{max} is required a shorter wavelength must be used.
- Shorter wavelengths are produced by higher order hkl planes
- Reflectivity is lower for shorter wavelengths
- Realistic Q_{max} of around 25 Å^{-1}

For TOF:

- Q_{max} depends on λ_{min} and detector θ.
- λ_{min} can be much lower than for the CW case allowing Q_{max} > 100 Å^{-1}
- λ_{min} determined by the moderator, transport characteristics of the guide and which frame the instrument is working in

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Other factors

- Line-of-sight loss v T_{zero} v beamstop shielding v background v etc…
- Phase space homogeneity (primarily divergence)
- Footprint of guide
- Need for /positioning of choppers
- Shielding requirements
- £ – longer = more expensive
- £ – higher M-coatings = more expensive
- £ – complex guide geometries = more expensive
- £ – large guide cross-sections = more expensive
- £££!

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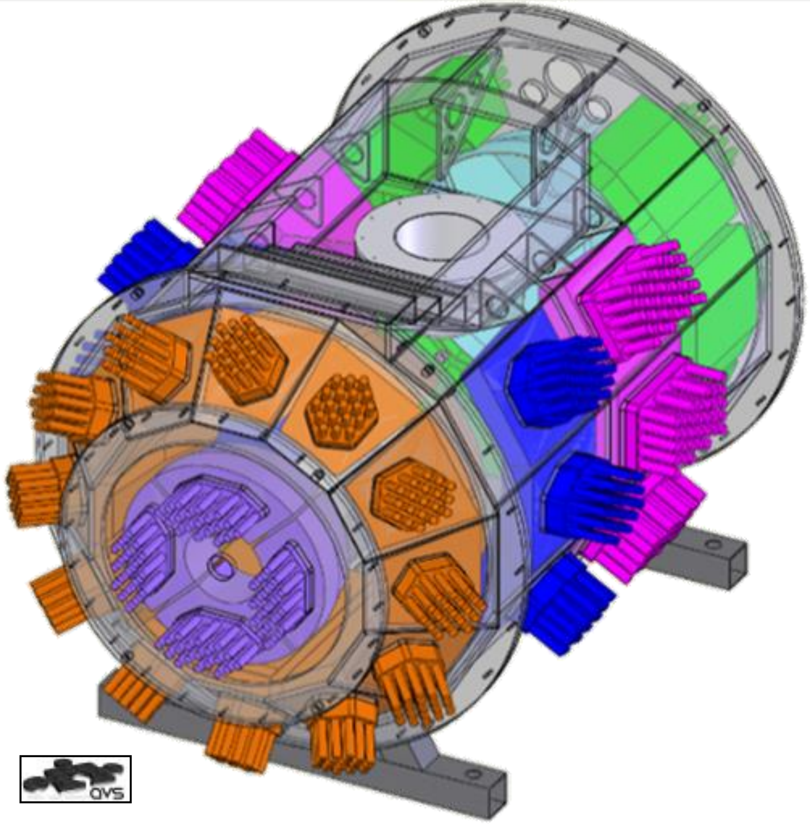
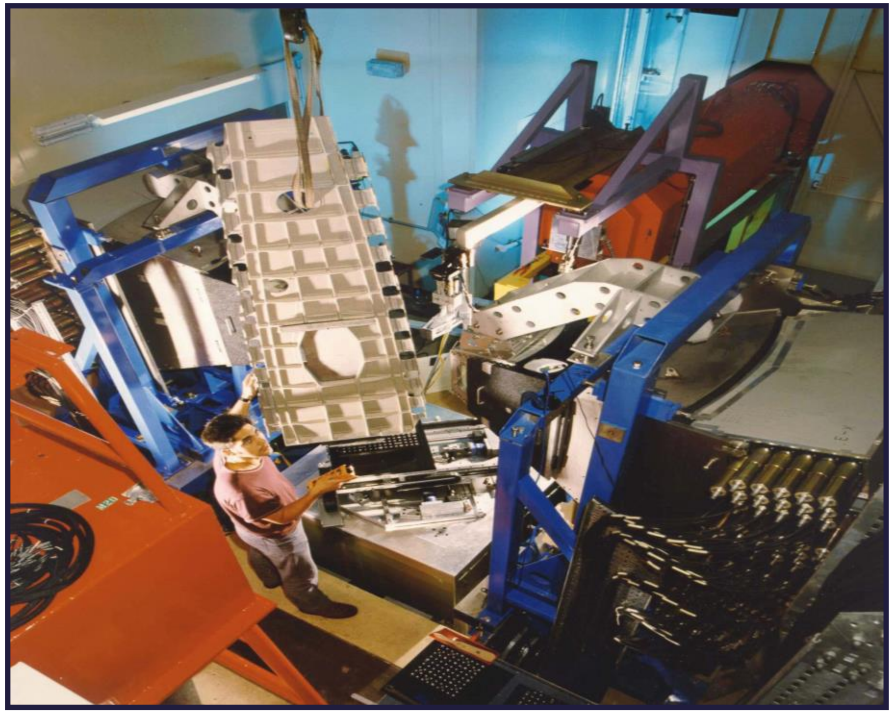
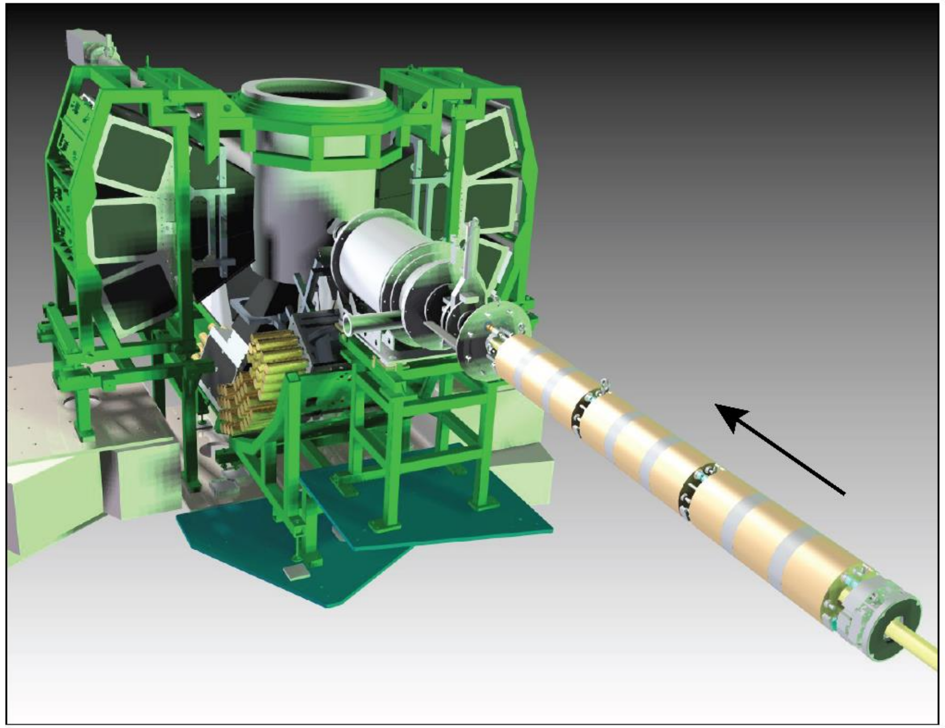
Sample area

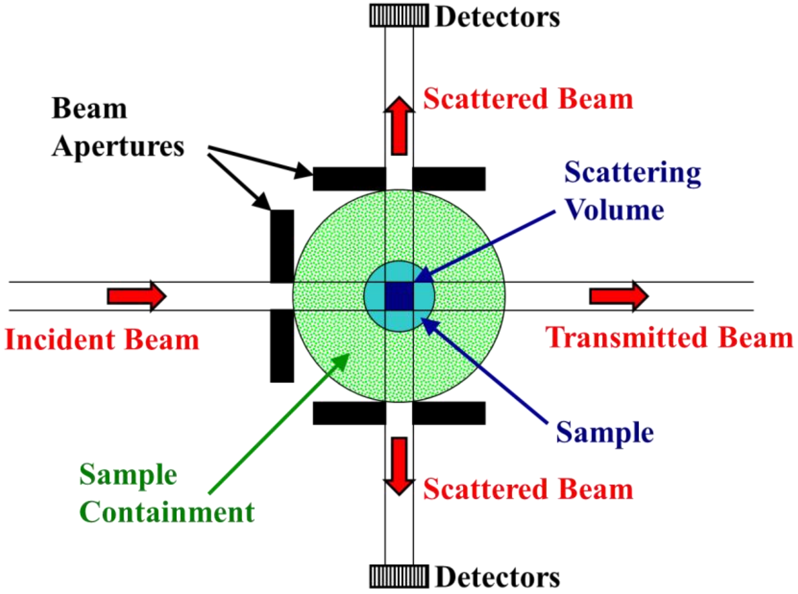
Vacuum v air?





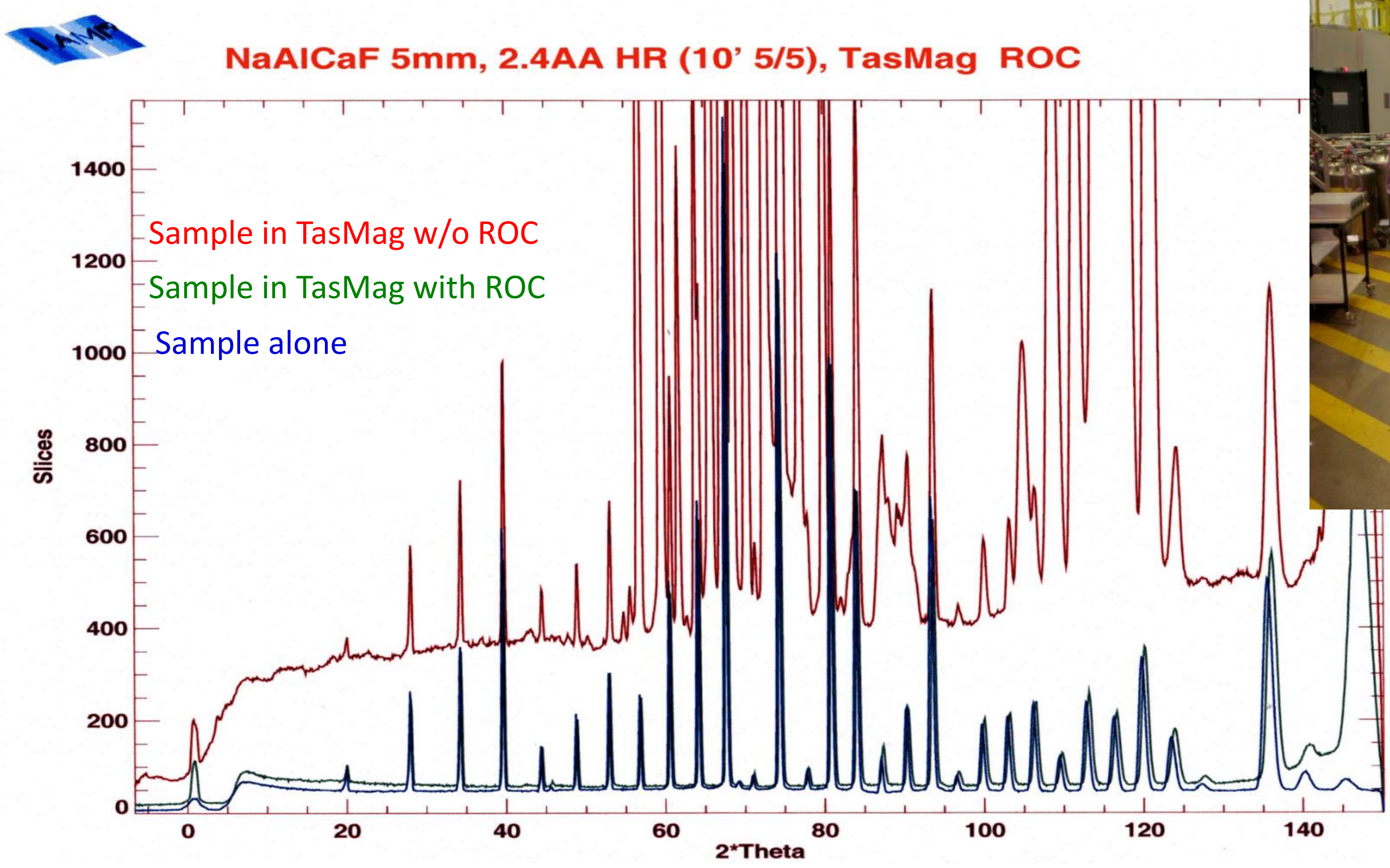
Restricted geometry: Pearl

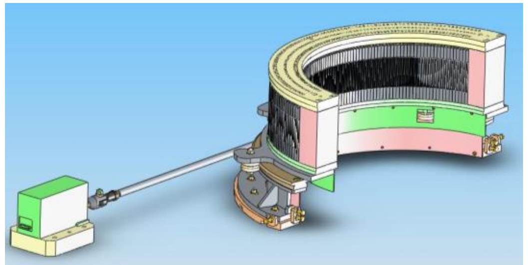


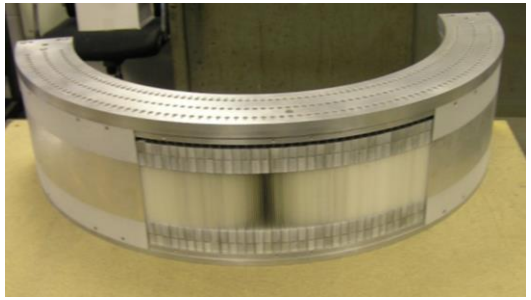


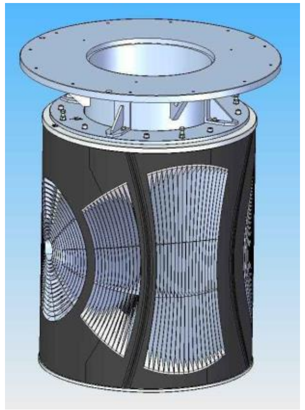
Instrument geometry designed to match sample environments

Parasitic scattering: collimation









Other factors

- Beam definition close to sample – slits and / or guide snouts
- Accessing sample environment during experiment
- Sample environment scattering / materials
- Difficulty running under vacuum v background / beam attenuation from air scattering
- Shadowing from collimation
- Sample geometry
- Non-magnetic components to allow magnetism studies
- Future upgrades – e.g. polarisation
- Etc…

Detectors

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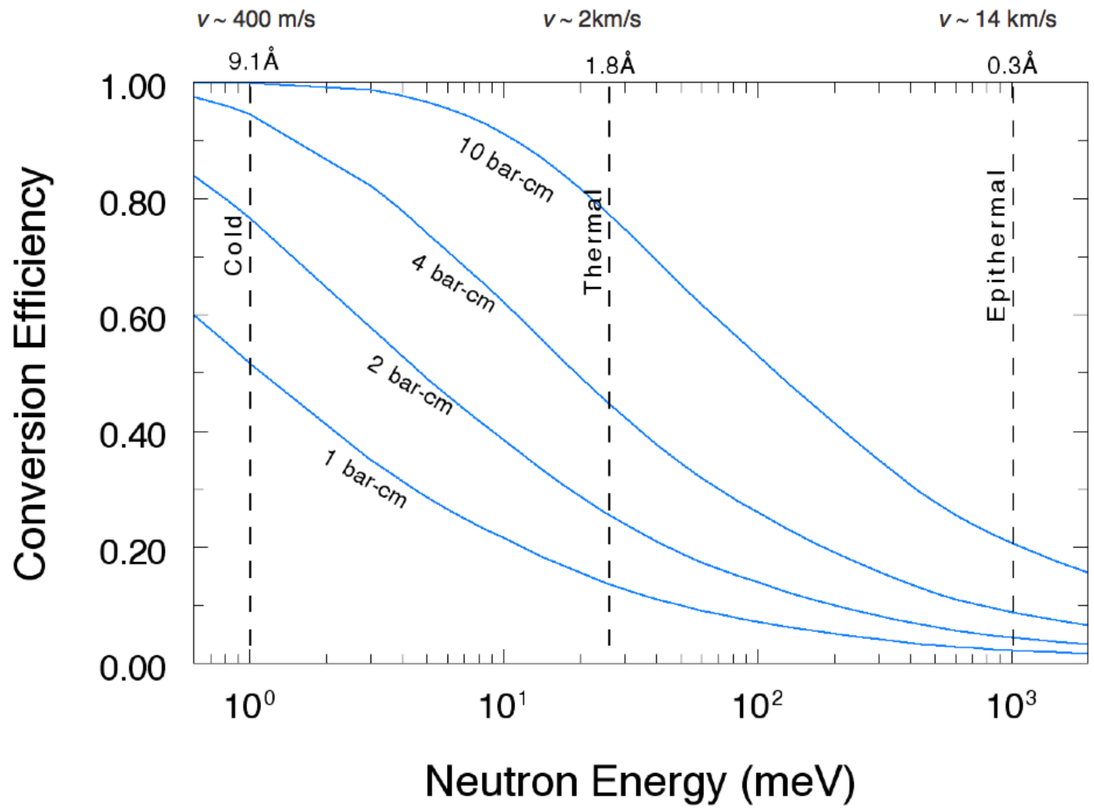
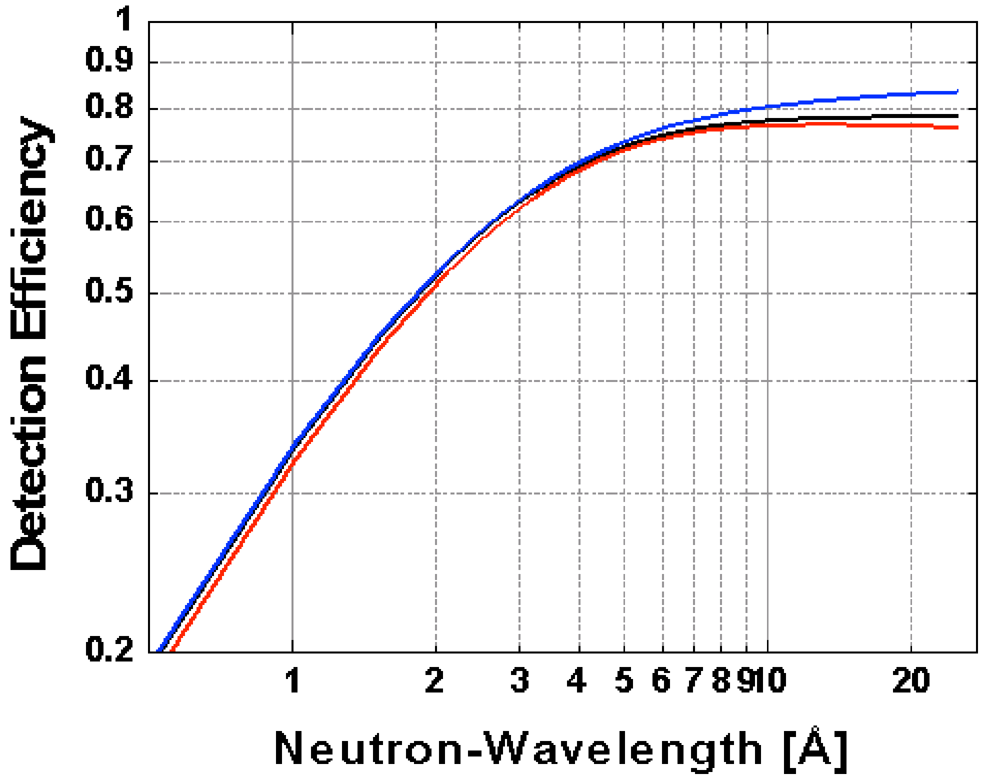
Detector efficiency



^{3}He detection efficiency as a function of detection depth



Predicted detector efficiency CASCADE-detector for 20 ^{10}B layers

Detector coverage v sample geometry

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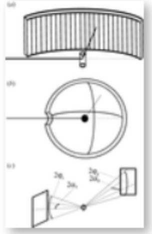

The ABC of powder diffractometer detector coverage

K. H. Andersen, **P. M. Bentley** and **L. D. Cussen**

This article addresses the question of the most effective detector configuration for neutron spectrometers using a discussion of a particular case - constant-wavelength powder diffractometers at continuous neutron sources. A first variation uses an essentially one-dimensional `banana' detector coupled with out-of-scattering-plane beam divergence before and after the sample. A second variation uses an incident beam tightly defined both in- and out-of-plane coupled to a `4π' detector covering all possible scattering angles after the sample. It is widely believed that the 4π arrangement is superior for most varieties of neutron spectrometer but is more difficult and more expensive to implement. Starting from a commonly used overall instrument figure-of-merit, this article presents simple arguments leading to the surprising conclusion that this is untrue for these constant-wavelength powder diffractometers, provided only that the cylindrical samples used with the banana detector have a height greater than 2.4 times their diameter.

Keywords: **neutron powder diffraction**; **constant-wavelength powder diffractometers**; **detector configuration**.

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Other factors

- Count-rate / saturation
- Known / proven technology?
- Pixel size
- Sample geometry / shadowing
- Performance variation
- Static or moveable?
- Restricted geometry
- Detector stability v time v T
- Maintenance / replacement
- In vacuum?
- Unit £

Figure of Merit

What to use in the figure of merit?

- Flux at sample position
- Total count-rate on detector
- Divergence profile
- Brilliance transfer
- Resolution of a particular diffraction peak(s) at detector
- Number of unwanted neutrons
- Combinations

- Effects of sample volume / geometry
- Detector layout / varying resolution

McStas optimisation

What might be optimised in McStas?

- Detector layout in plane
- Detector coverage out of plane
- Sample size / geometry
- M-coatings of a complex guide
- Cost v performance of a guide
- Divergence acceptance / transport
- Chopper positioning / performance
- Maximising good:bad neutron transport
- Optimal detector resolution / pixel size vs sample geometry vs beam transport
- Etc…

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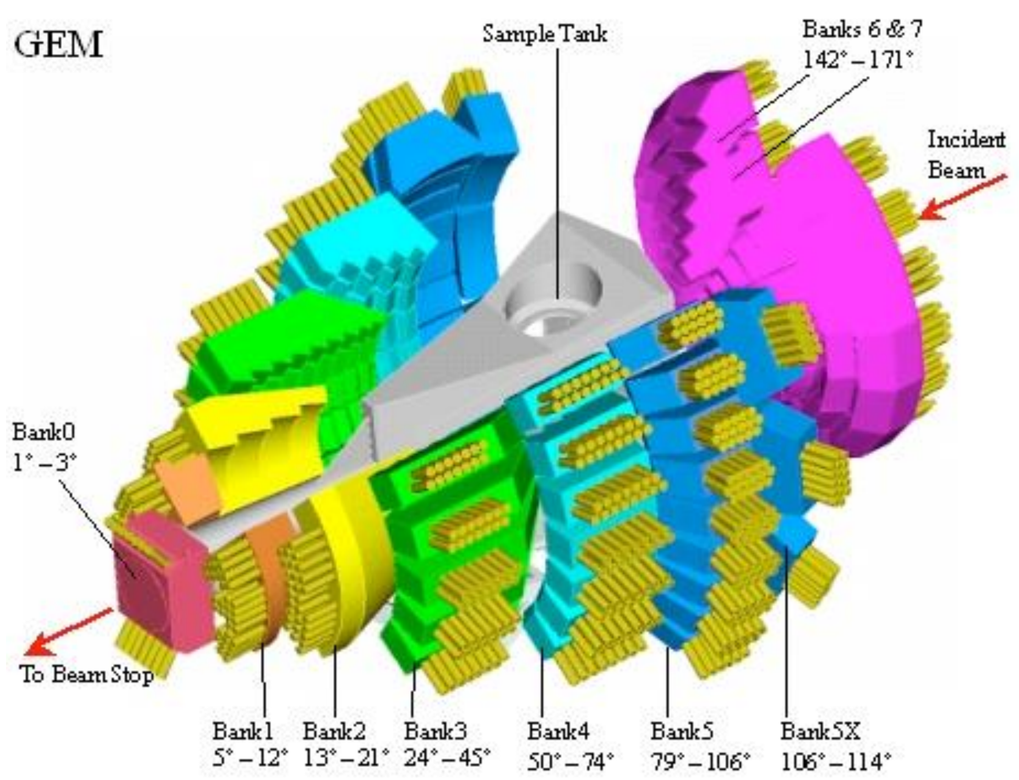
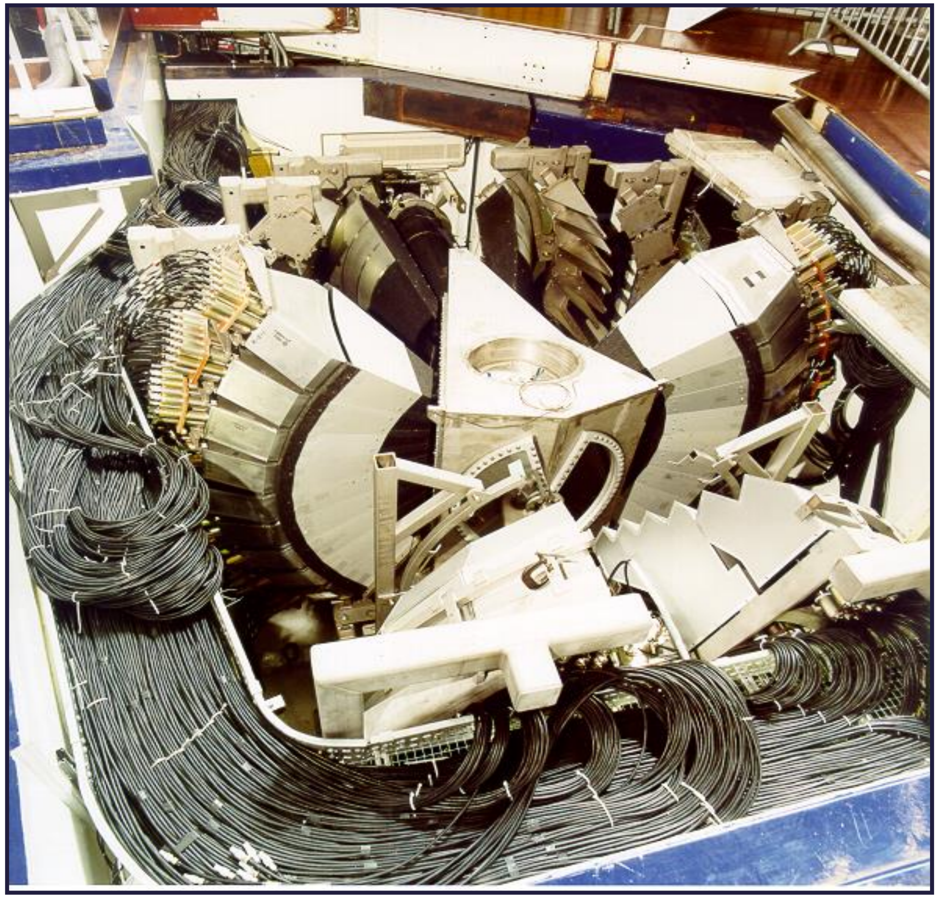
Final thoughts

Instrument design v reality: GEM





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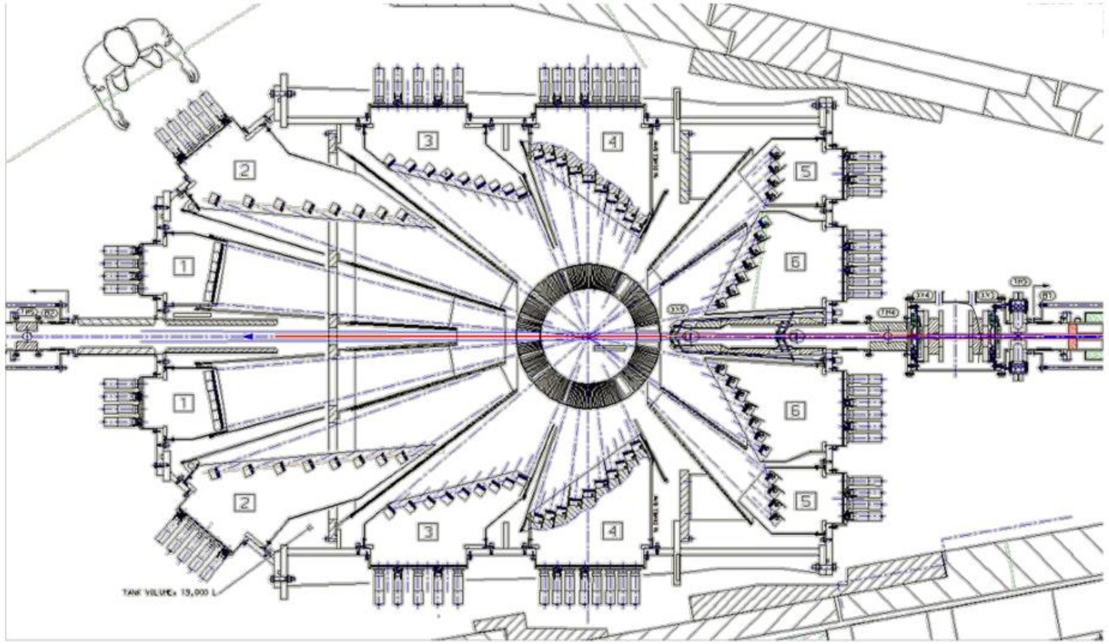
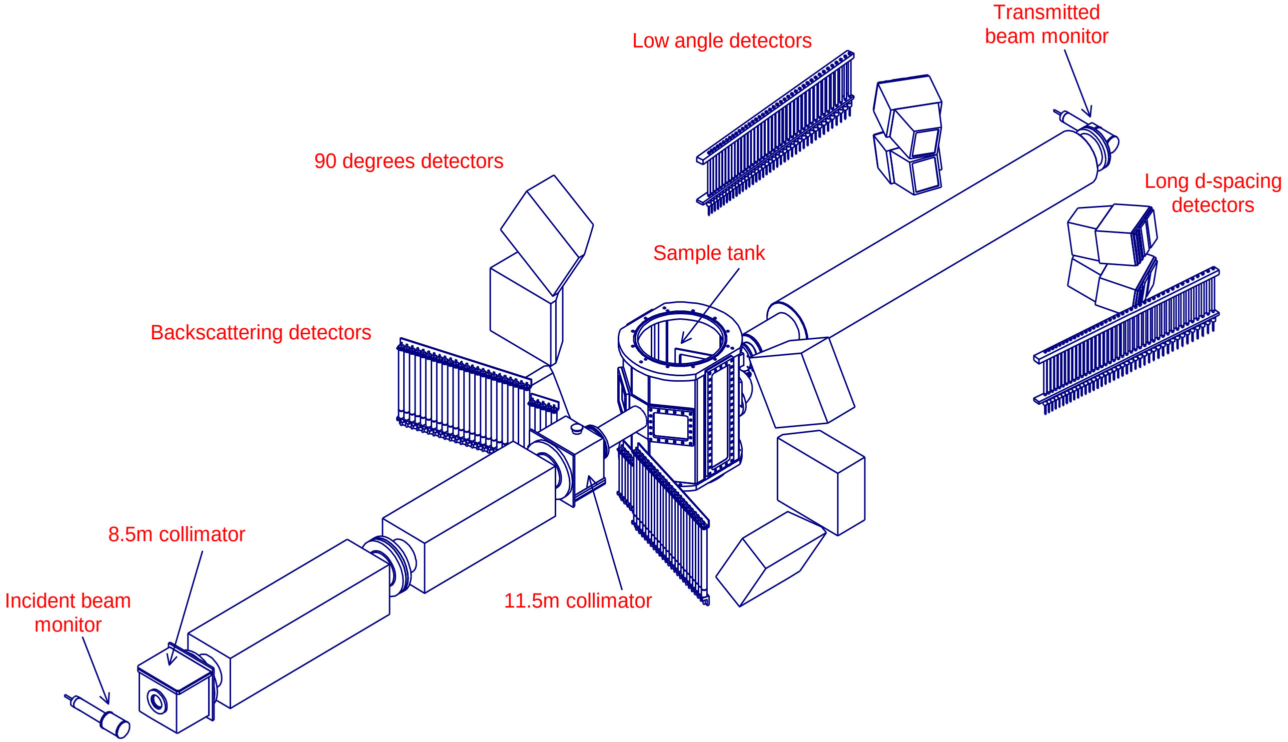
Initially constructed in the late 1990s this powder/liquids diffractometer hybrid changed the way TOF diffraction instruments were designed and built

Instrument design: Polaris rebuild v 2006





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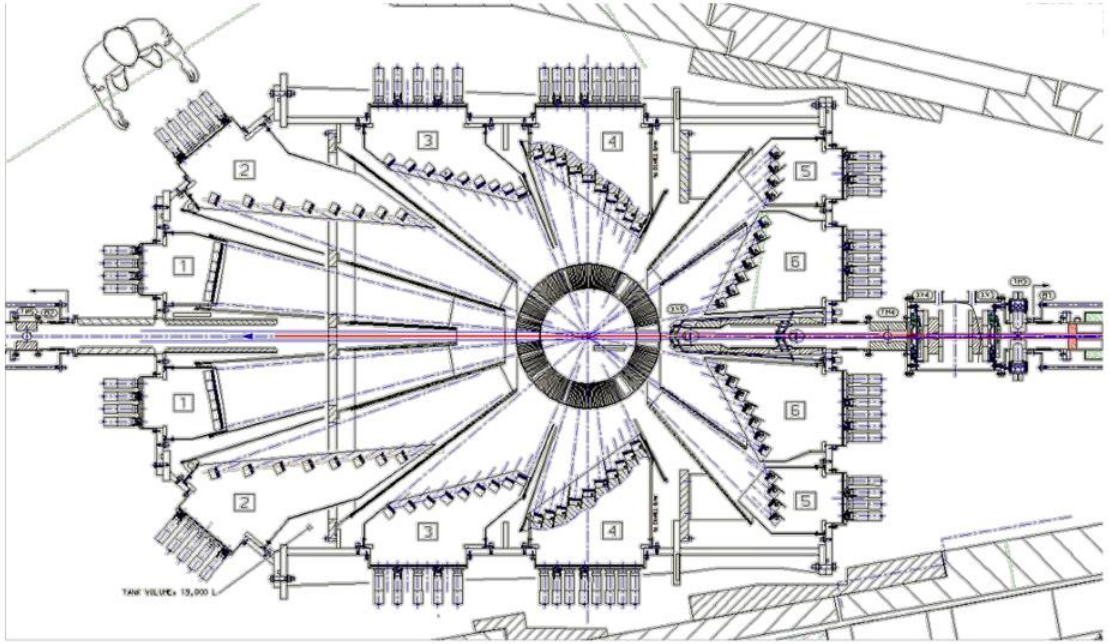
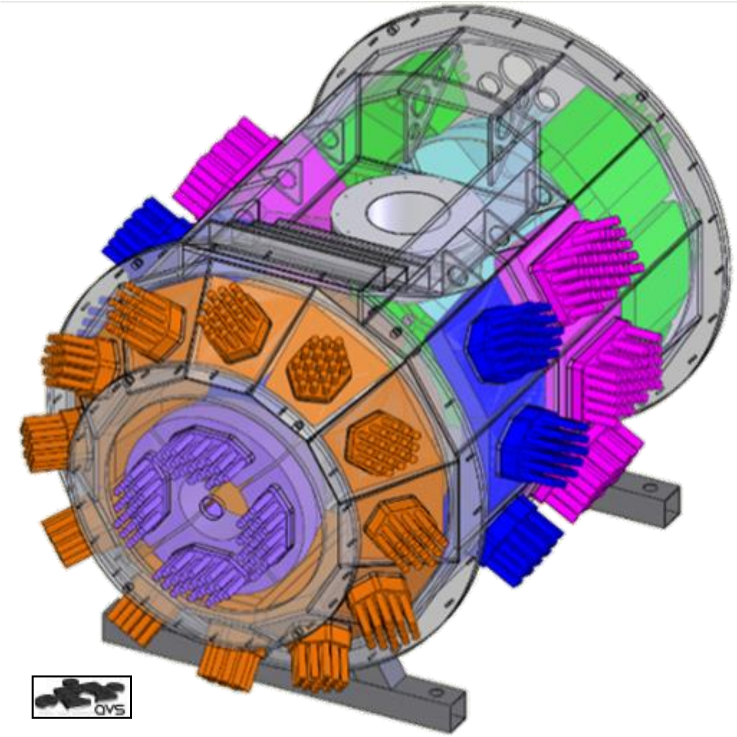
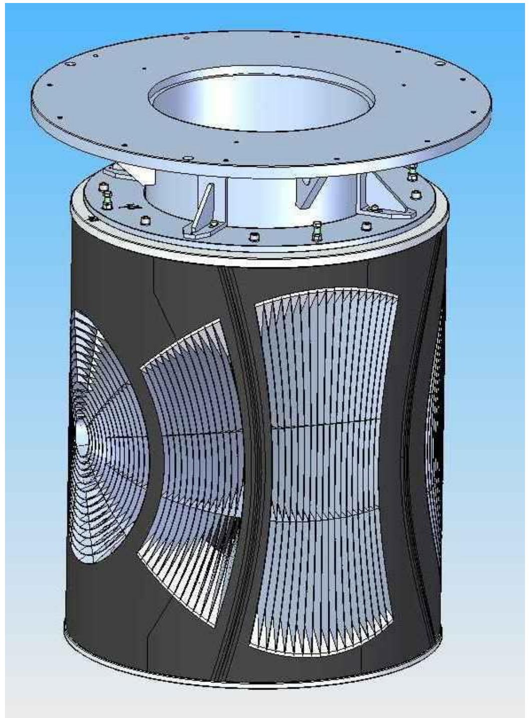
Instrument design: Polaris







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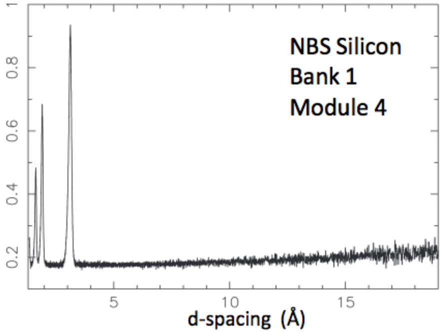
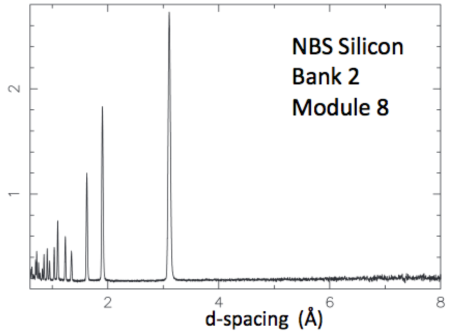
Instrument reality: Polaris

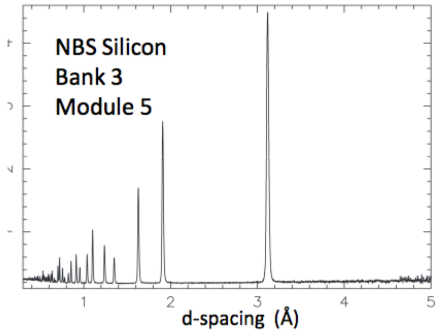


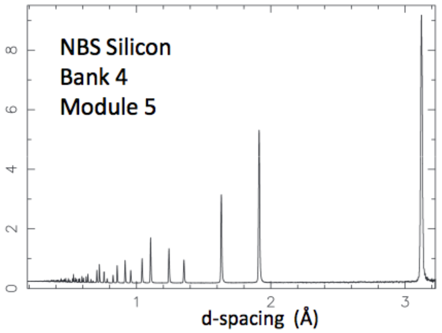


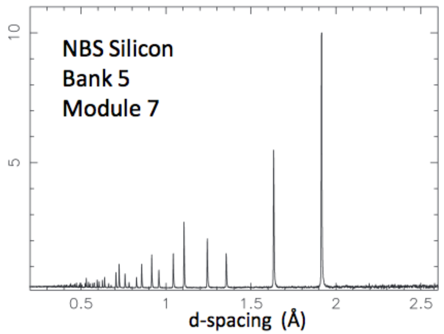

Instrument performance: Polaris

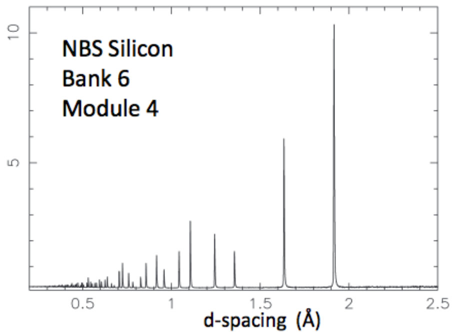


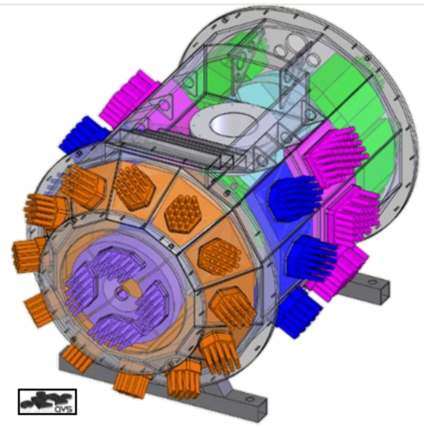












Bank 1 – cyan
Bank 2 – green
Bank 3 – pink
Bank 4 – blue
Bank 5 – orange
Bank 6 - purple

- Increased count rate ×3 at high scattering angle to >20 for low angle banks
- Resolution improvement e.g. bank 5 and 6 of 3×10^{-3} cf. 5×10^{-3}
- Improvement in data at high Q

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Questions?