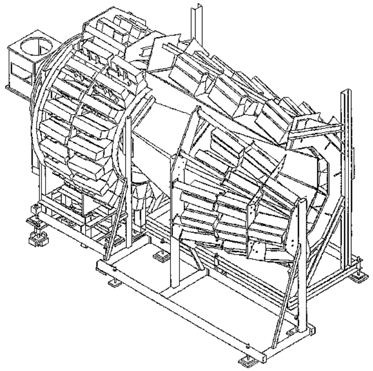
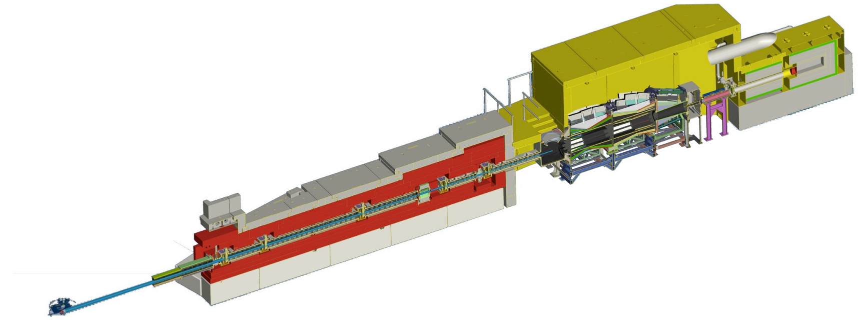
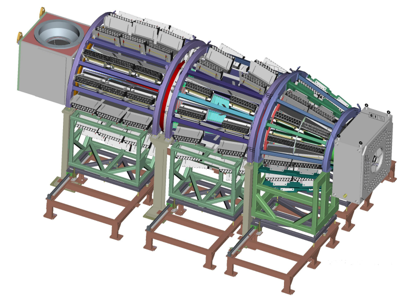




Light Element Optimized Disordered Materials Diffractometers on Spallation Neutron Sources



Daniel Bowron

2nd ISIS-CSNS workshop
PDF and Total Scattering Methods
7th – 9th November 2016

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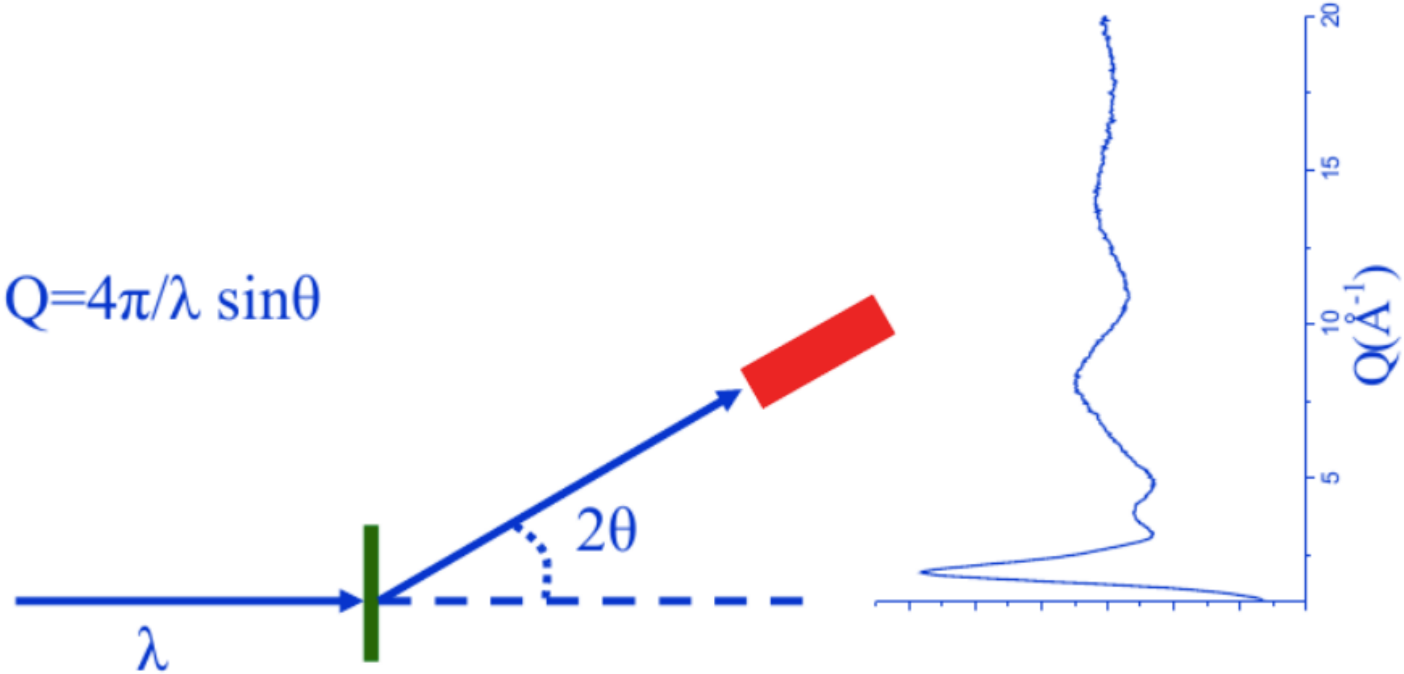
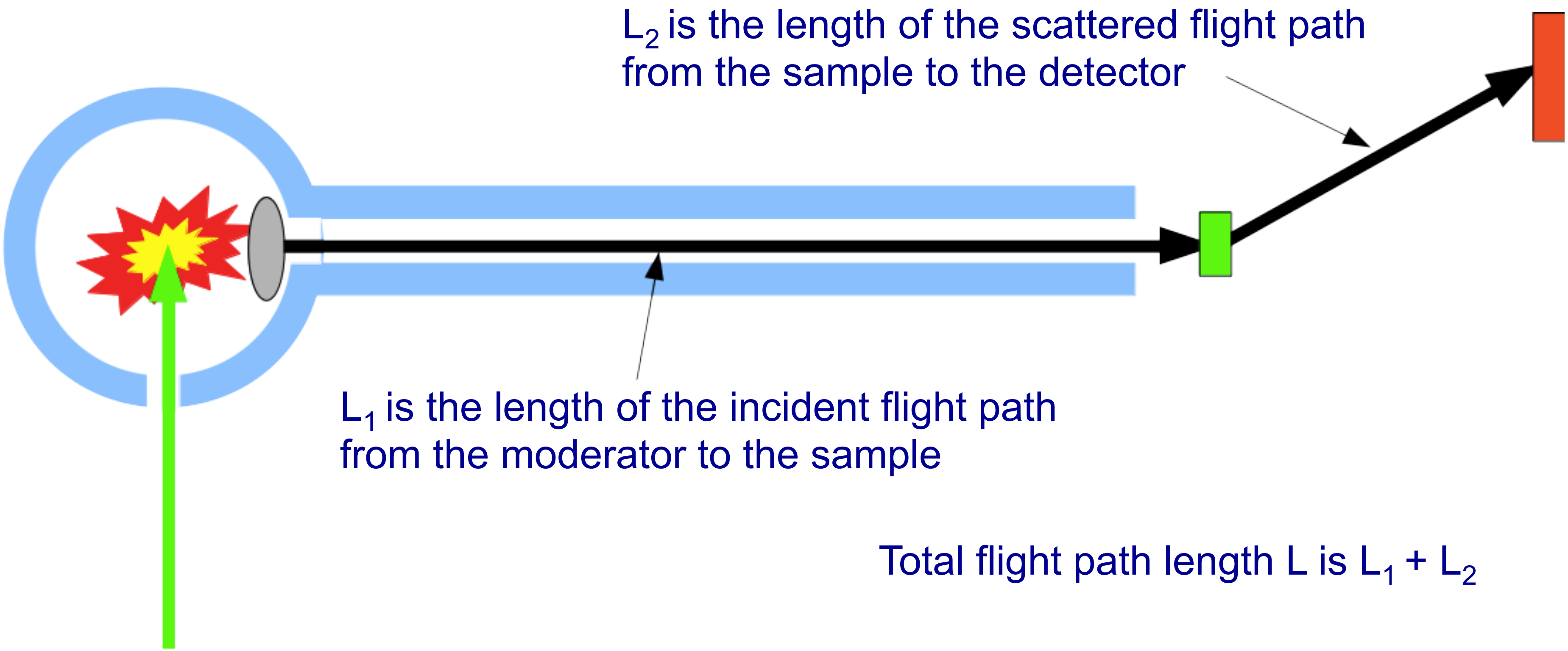
Schematic of a neutron scattering measurement



Time-of-Flight Neutron Scattering



Total flight path length L is $L_1 + L_2$

The time of flight (TOF) is the time in μs taken for a neutron to travel 1m (μs m^{-1})

The time of arrival at the detector, t_0 , is the TOF (μs m^{-1}) multiplied by the total flight path (m)

Time of flight neutron scattering: Some useful relationships

Time of arrival

$$t_0 = \mathrm{TOF}\,.\,L$$

$$t_0 = 252.77\,\lambda\,L$$

Neutron wavelength

$$\lambda = 0.0039562.\mathrm{TOF} = 0.0039562.\frac{t_0}{L}$$

Neutron velocity

$$v = \frac{10^6}{\mathrm{TOF}}$$

Neutron wave vector

$$k = \frac{2\pi}{\lambda} = \frac{1588.2}{\mathrm{TOF}}$$

Neutron energy

$$E = \frac{81.807}{\lambda^2}$$

$$v\left[m\,s^{-1}\right]\,,\,t_0\left[\mu s\right]\,,\mathrm{TOF}\left[\mu s\,m^{-1}\right]\,,\,L\,[m]\,,\,\lambda\left[\text{Å}\right],\;k\left[\text{Å}^{-1}\right]\,,\,E\,[\mathrm{meV}]$$

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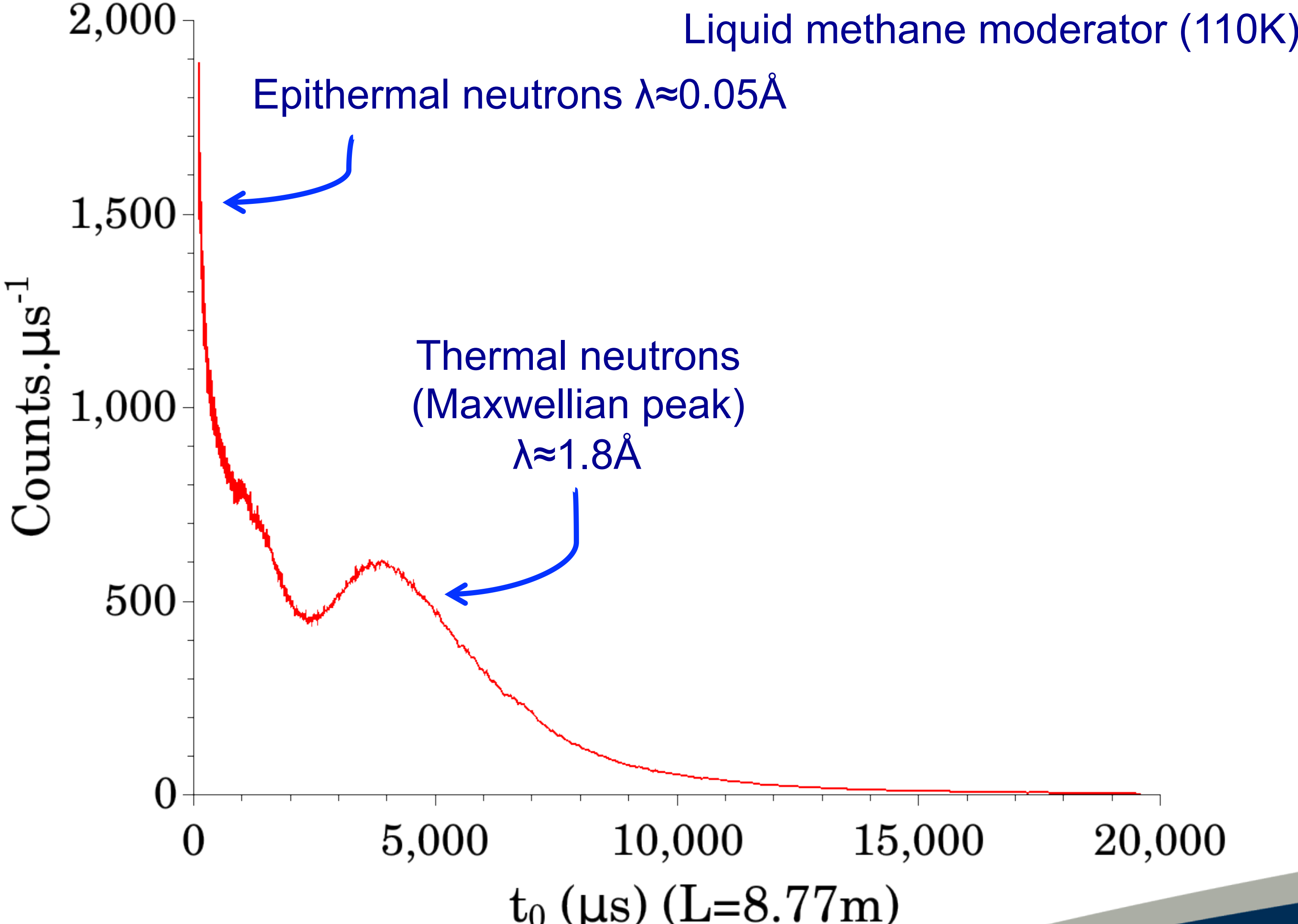
Time of flight neutron scattering

Wavelength	Energy	Time of arrival (L=10m)	Speed
20Å	0.205 meV	50554 μs	197.8 ms^{-1}
10Å	0.818 meV	25277 μs	395.6 ms^{-1}
5Å	3.273 meV	12638.5 μs	791.2 ms^{-1}
4Å	5.113 meV	10110.8 μs	989.0 ms^{-1}
3Å	9.090 meV	7583.1 μs	1319 ms^{-1}
2Å	20.452 meV	5055.4 μs	1978 ms^{-1}
1Å	81.807 meV	2527.7 μs	3956 ms^{-1}
0.5Å	327.228 meV	1263.9 μs	7912 ms^{-1}
0.25Å	1.309 eV	631.9 μs	15825 ms^{-1}
0.1Å	8.181 eV	252.8 μs	39557 ms^{-1}
0.05Å	32.723 eV	126.4 μs	79114 ms^{-1}

Time-of-flight neutron scattering: spectral profile



Time-of-flight neutron scattering: spectrum parameterization

$$\Phi_{\mathrm{Epithermal}}(E) = \frac{\Phi_0}{E^A} \qquad \Phi_{\mathrm{Maxwellian}}(E) = J\frac{E}{T^2}\exp\left\{\frac{-E}{T}\right\}$$

$$\Phi_{\mathrm{Total}}(E) = \Phi_{\mathrm{Maxwellian}} + \Delta(E)\Phi_{\mathrm{Epithermal}}$$

$$\Delta(E) = \frac{1}{\left[1+\exp\left\{\frac{W_1}{\sqrt{E}} - W_2\right\}\right]}$$

$$\Phi(\lambda) = \Phi(E)\left(\frac{\delta E}{\delta\lambda}\right) = 2\Phi(E)\left(\frac{E}{\lambda}\right)$$

Time-of-flight neutron scattering: spectrum parameterization

Methane moderator

$$\Phi_0\,(\text{at }750\text{MeV})\rightarrow 2.7\left[10^{10}n(\text{eVsr}100\text{cm}^2\mu\text{As})^{-1}\right]$$

Proton beam energy

Typical moderator view

$$A\rightarrow 0.92$$

$$J\rightarrow 5.7\left[10^{10}n(\text{sr}100\text{cm}^2\mu\text{As})^{-1}\right]$$

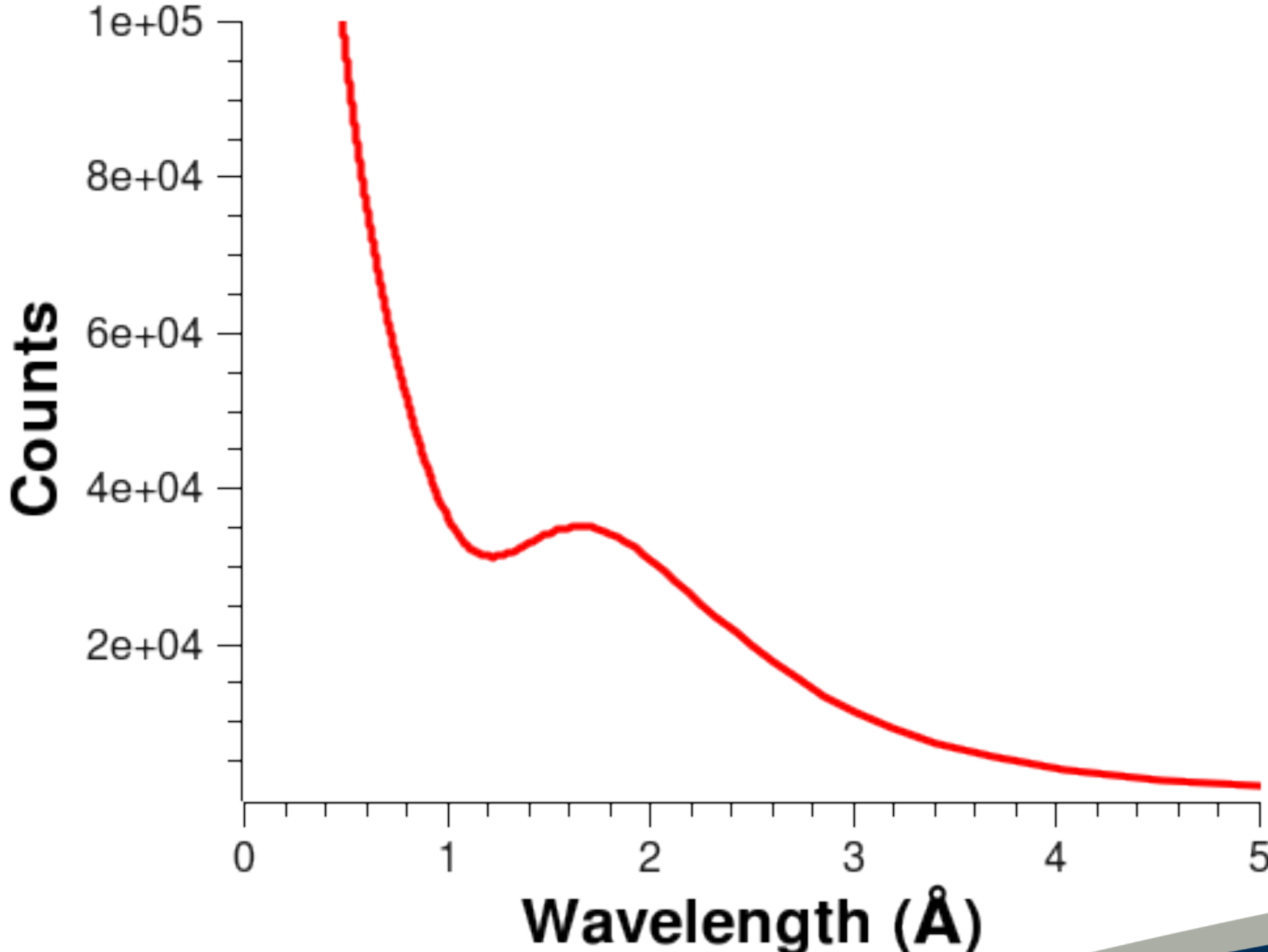
$$T\,(\text{eV})\rightarrow 0.011$$

$$W_1\,(\text{eV})^{\frac{1}{2}}\rightarrow 1.7$$

$$W_2\rightarrow 7.0$$

Time-of-flight neutron scattering: spectrum parameterization

Methane moderator



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Light element optimized diffractometers
SANDALS type

Utilise:

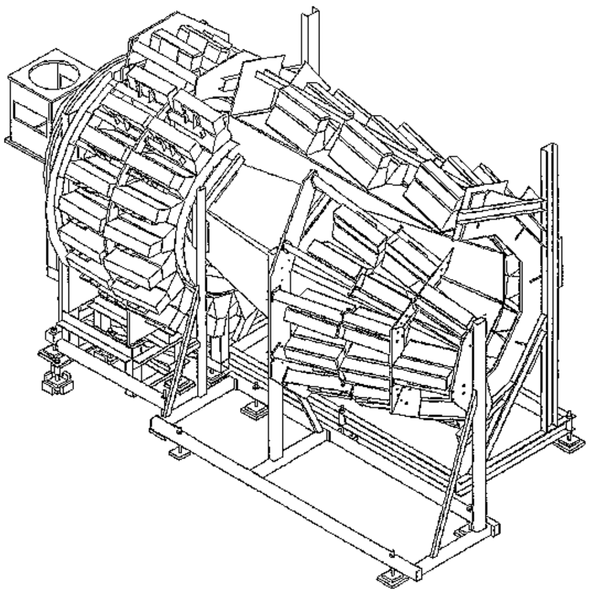
(1) relatively small forward scattering angles: 1º to 40º

(2) high energy neutrons $0.05Å \le \lambda \le 5.0Å$

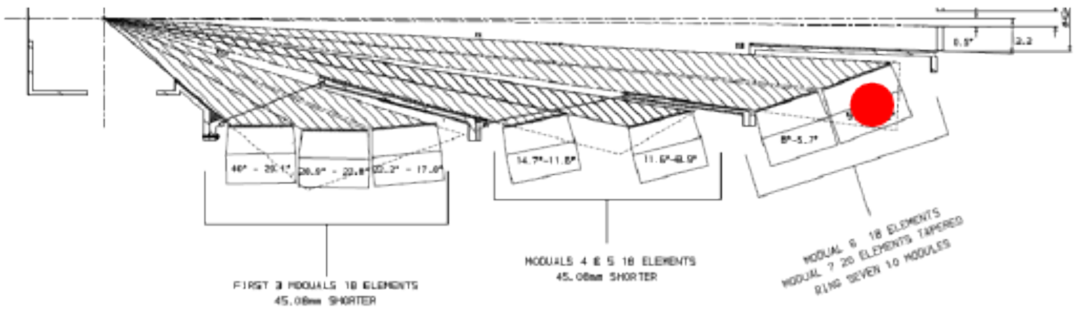
(3) wide accessible Q-range $0.1Å^{-1} \le Q \le 50Å^{-1}$

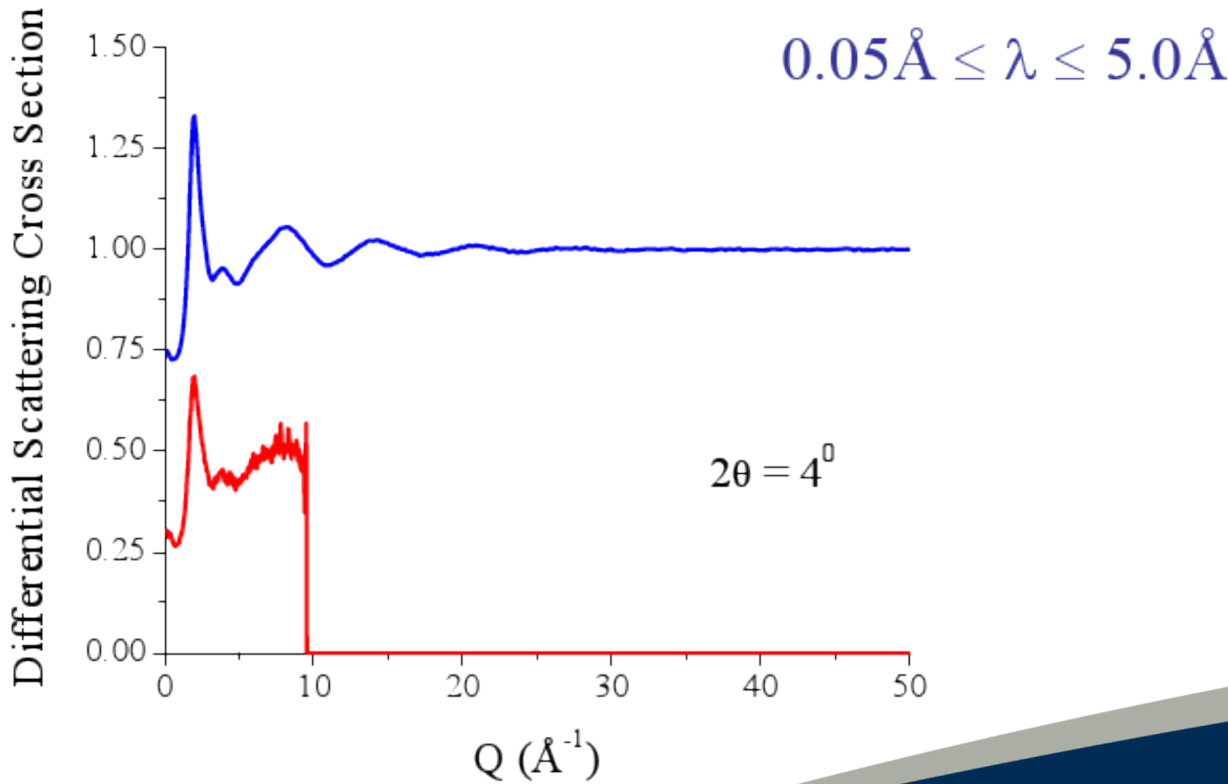
(4) flat plate sample geometry

(5) moderate resolution $\Delta Q/Q \approx 2\%$

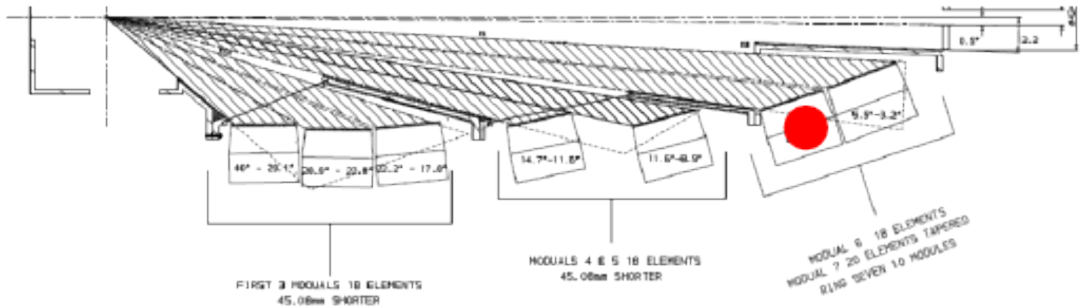


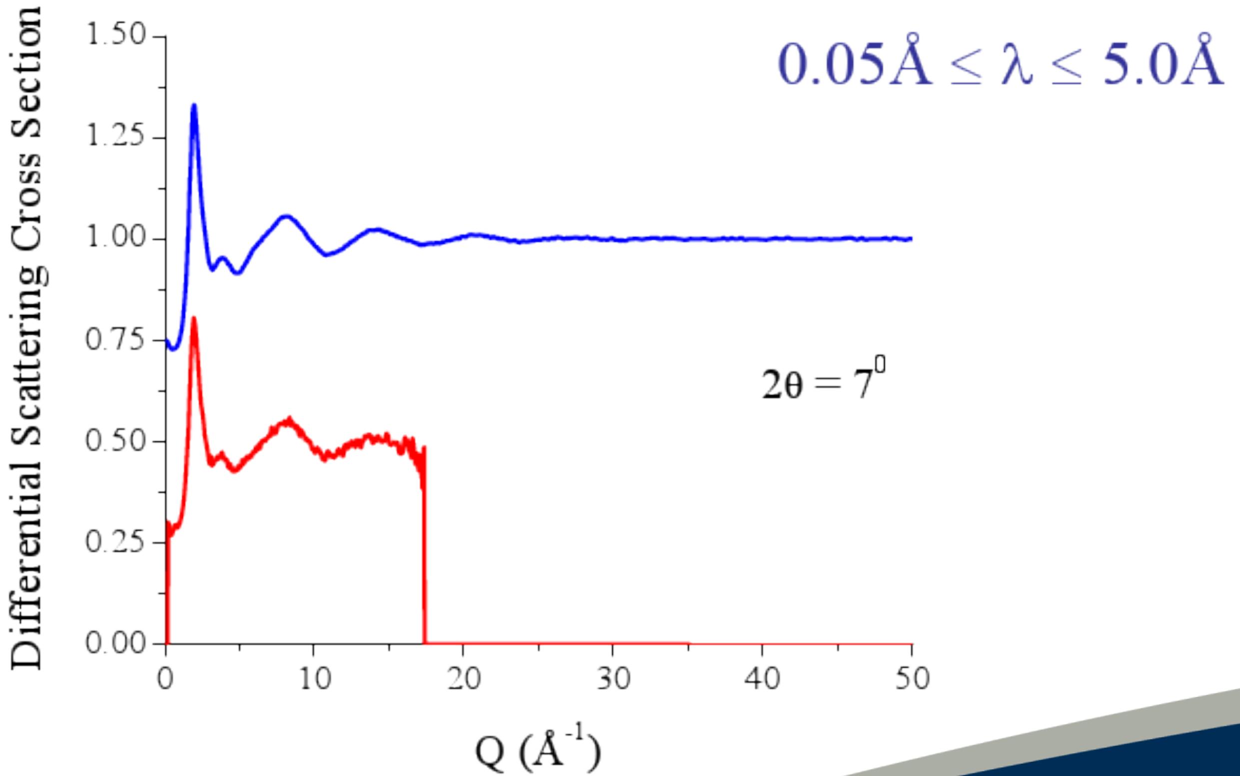
Distribution of Q-ranges across the detector banks



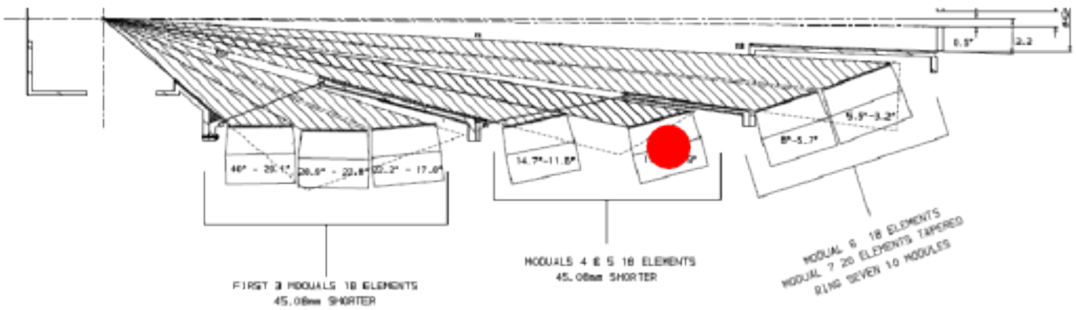


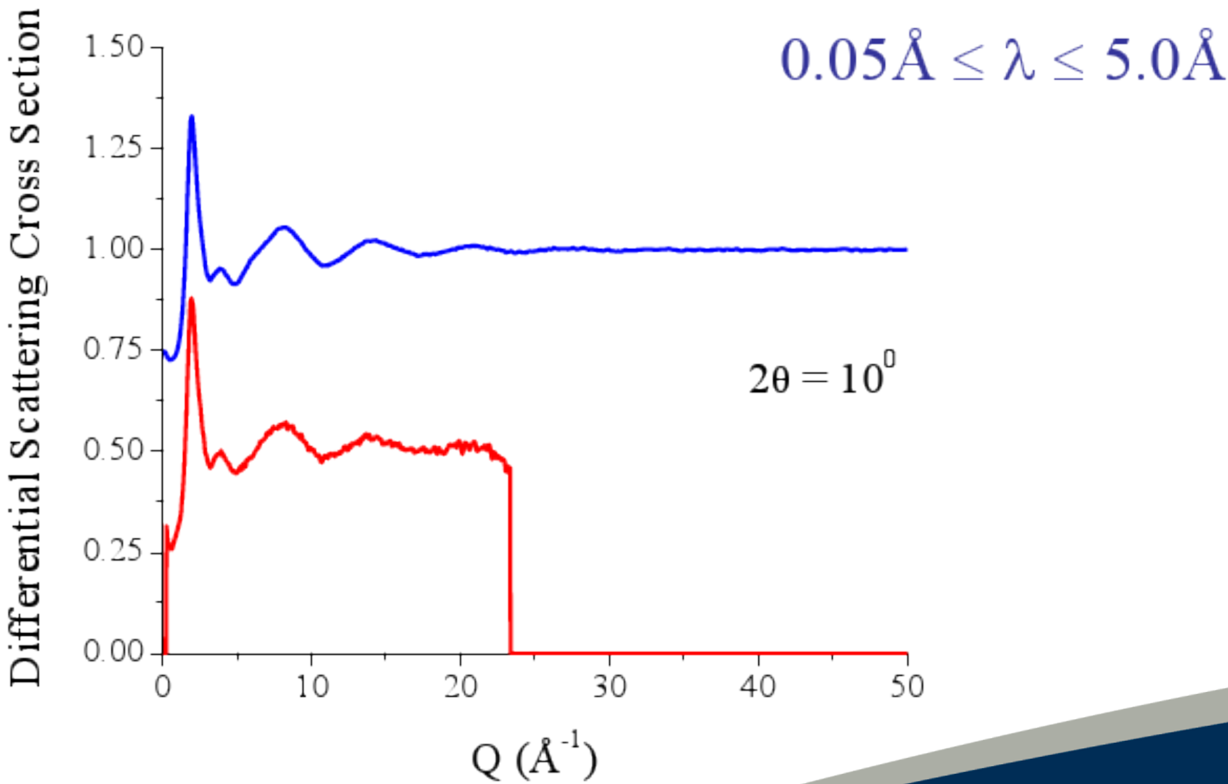
Distribution of Q-ranges across the detector banks



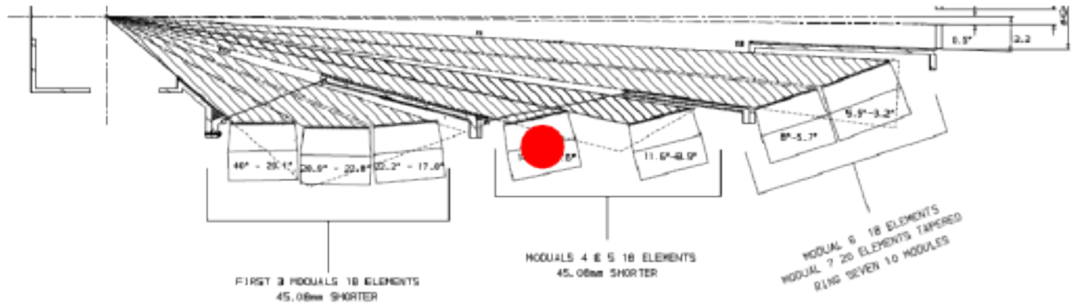


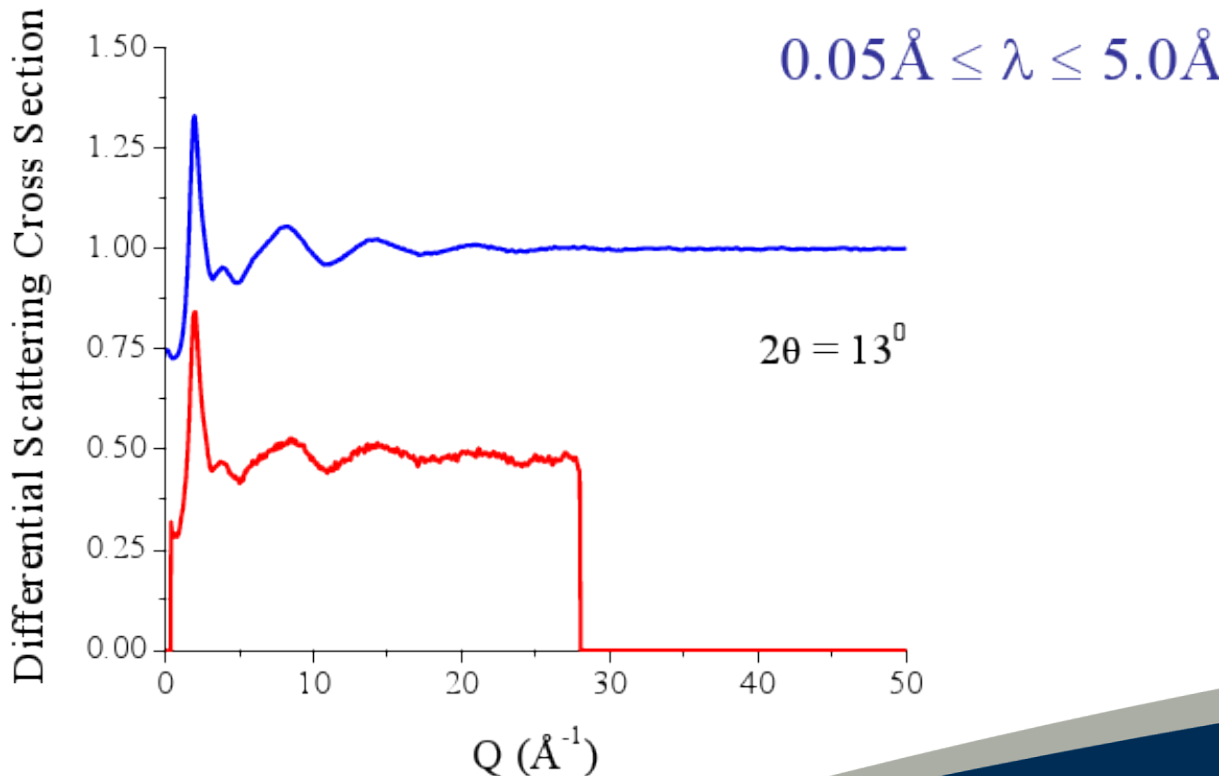
Distribution of Q-ranges across the detector banks



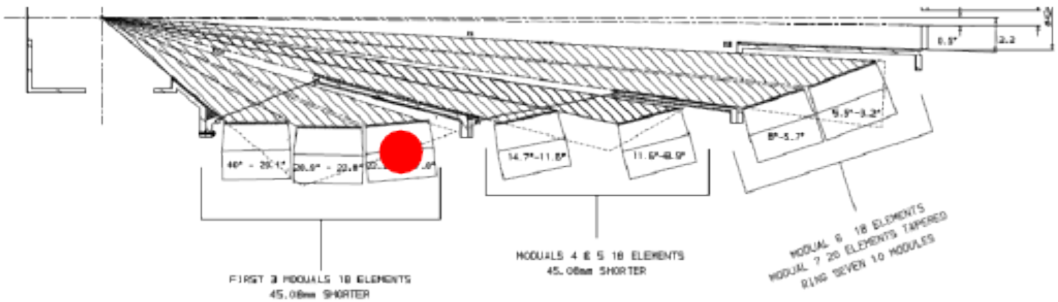


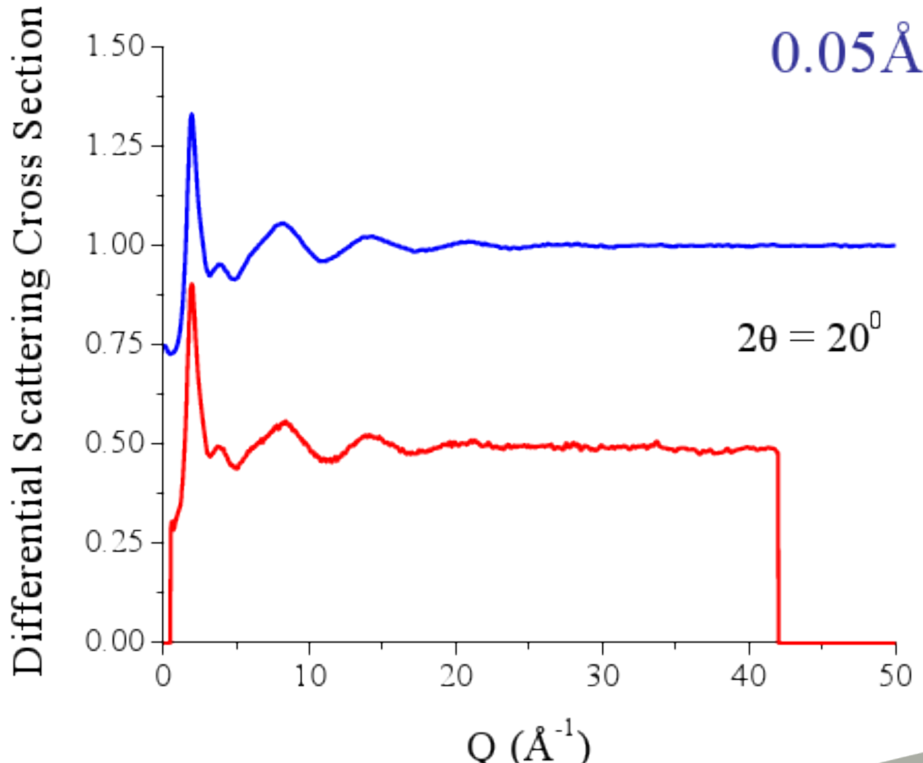
Distribution of Q-ranges across the detector banks





Distribution of Q-ranges across the detector banks





$0.05Å \leq \lambda \leq 5.0Å$

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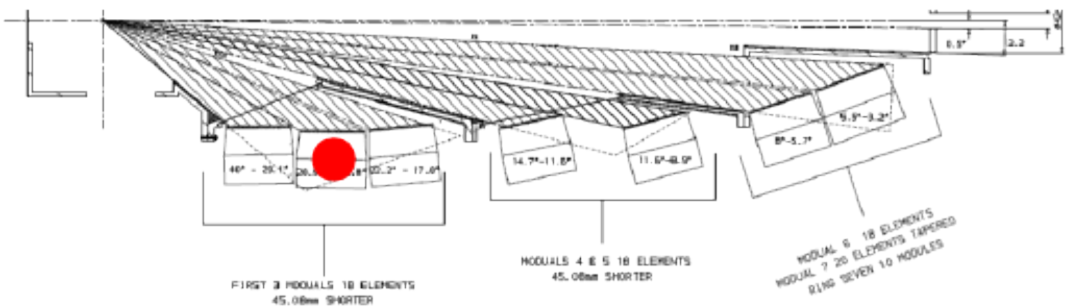
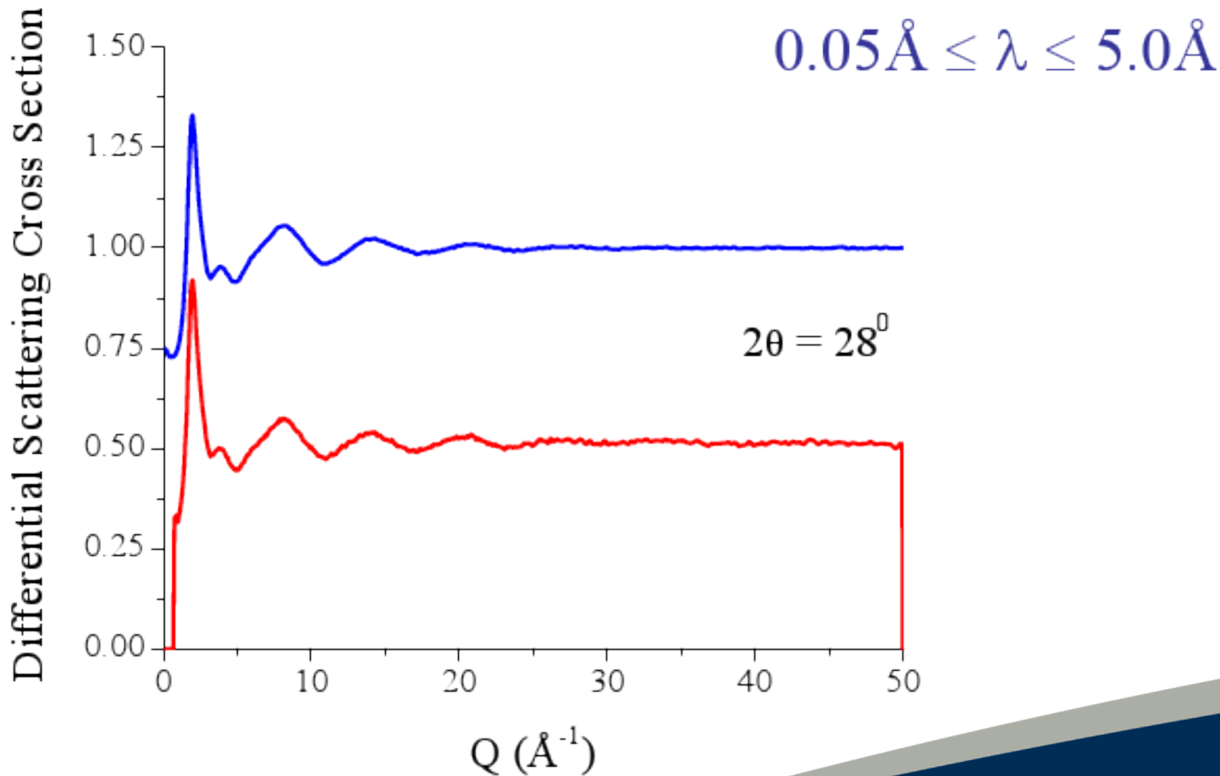
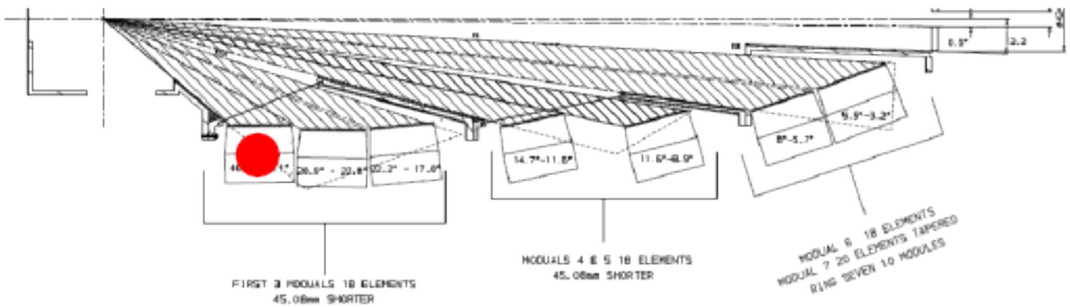
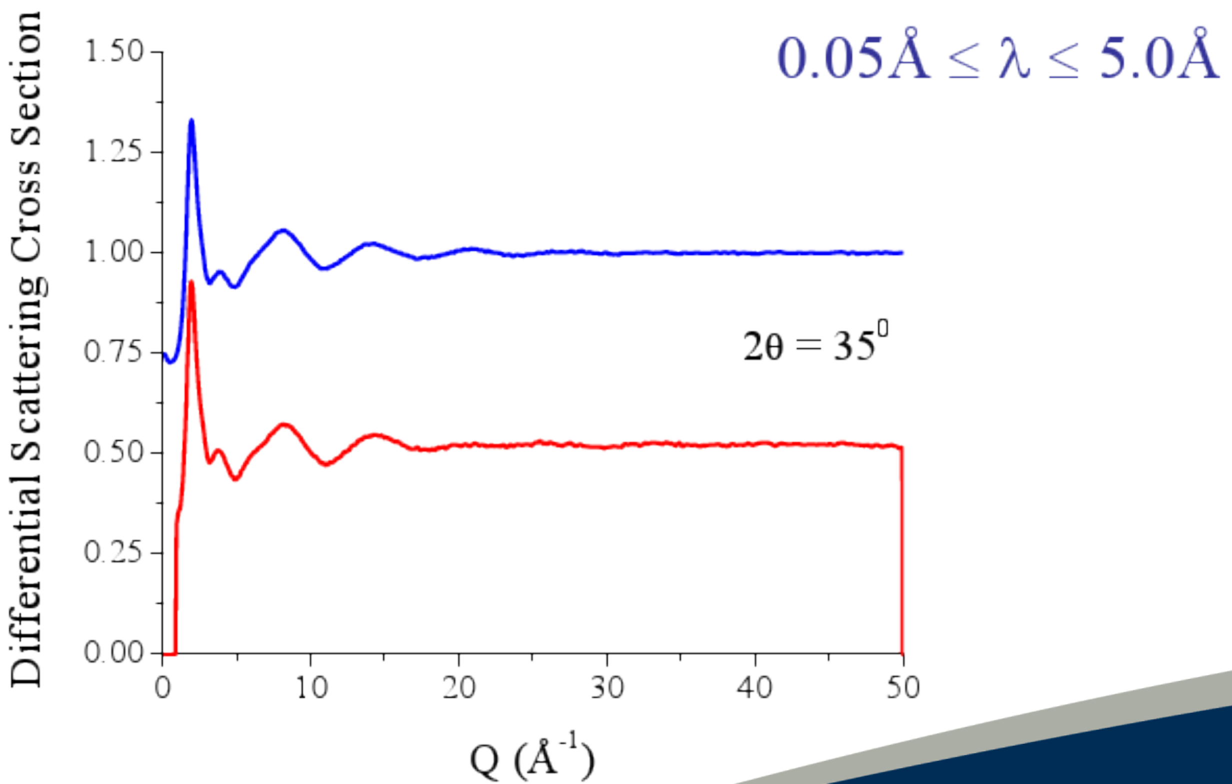
Distribution of Q-ranges across the detector banks





Distribution of Q-ranges across the detector banks





Real-space resolution of a total scattering measurement

$$F(Q) = \rho_0 \int_0^\infty 4\pi r^2 g(r) \frac{\sin Qr}{Qr} dr \qquad g(r) = \frac{1}{(2\pi)^3 \rho_0} \int_0^\infty 4\pi Q^2 F(Q) \frac{\sin Qr}{Qr} dQ$$

$$g(r) = \frac{1}{(2\pi)^3 \rho_0} \int_0^{Q_{max}} 4\pi Q^2 F(Q) \frac{\sin Qr}{Qr} dQ$$

$$Q = \frac{4\pi}{\lambda} \sin\theta$$

A typical fixed wavelength measurement $2\theta = 130° \ \lambda = 0.5A \rightarrow Q_{max} = 22.8A^{-1}$

A typical pulsed source measurement $2\theta = 40° \ \lambda = 0.05A \rightarrow Q_{max} = 86A^{-1}$

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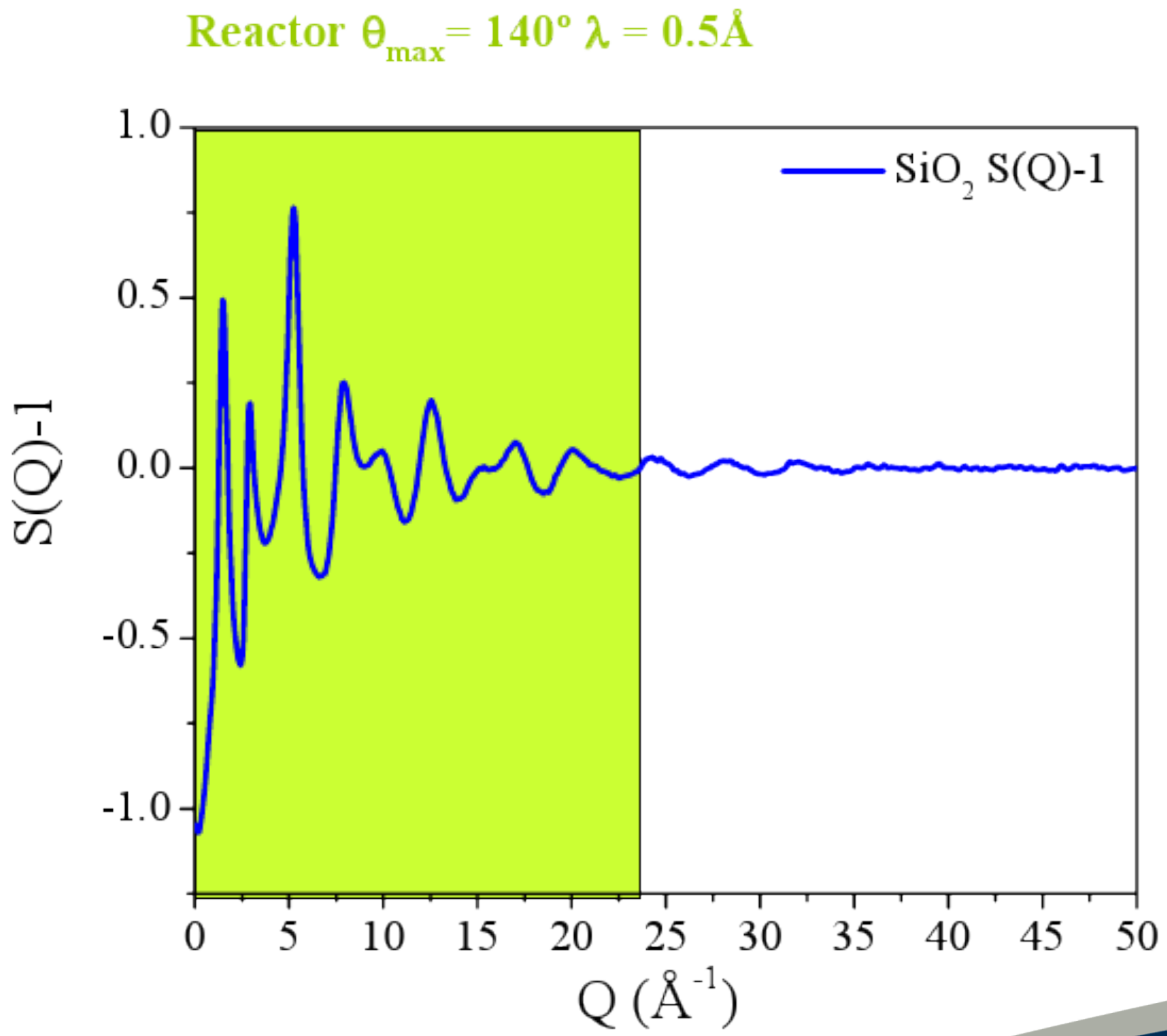
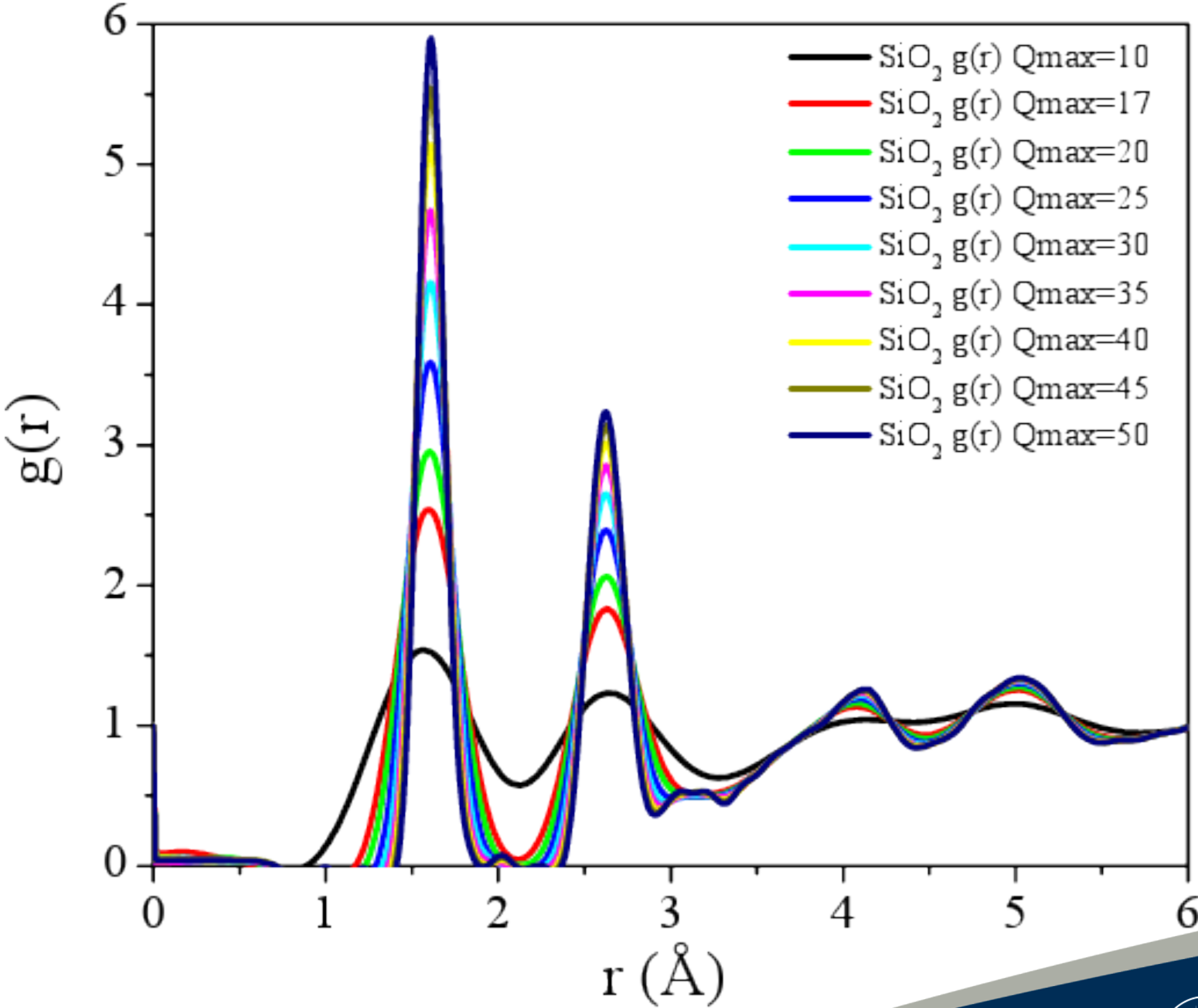
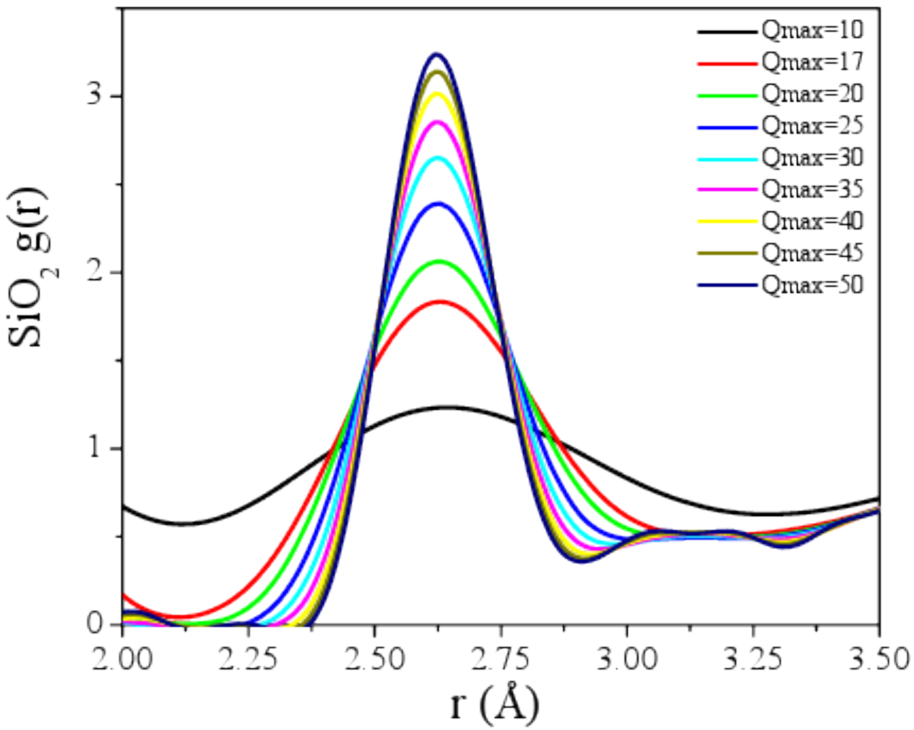
Real-space resolution of a total scattering measurement

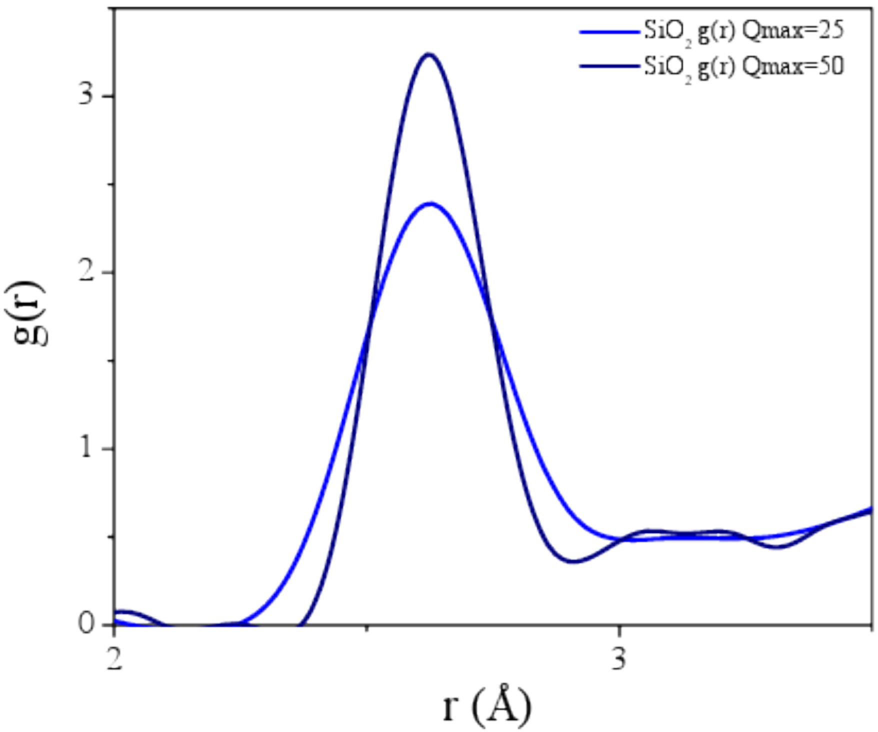


Real-space resolution of a total scattering measurement



Real-space resolution of a total scattering measurement





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Q resolution of a total scattering measurement

$$Q = \frac{4\pi}{\lambda}\sin\theta$$

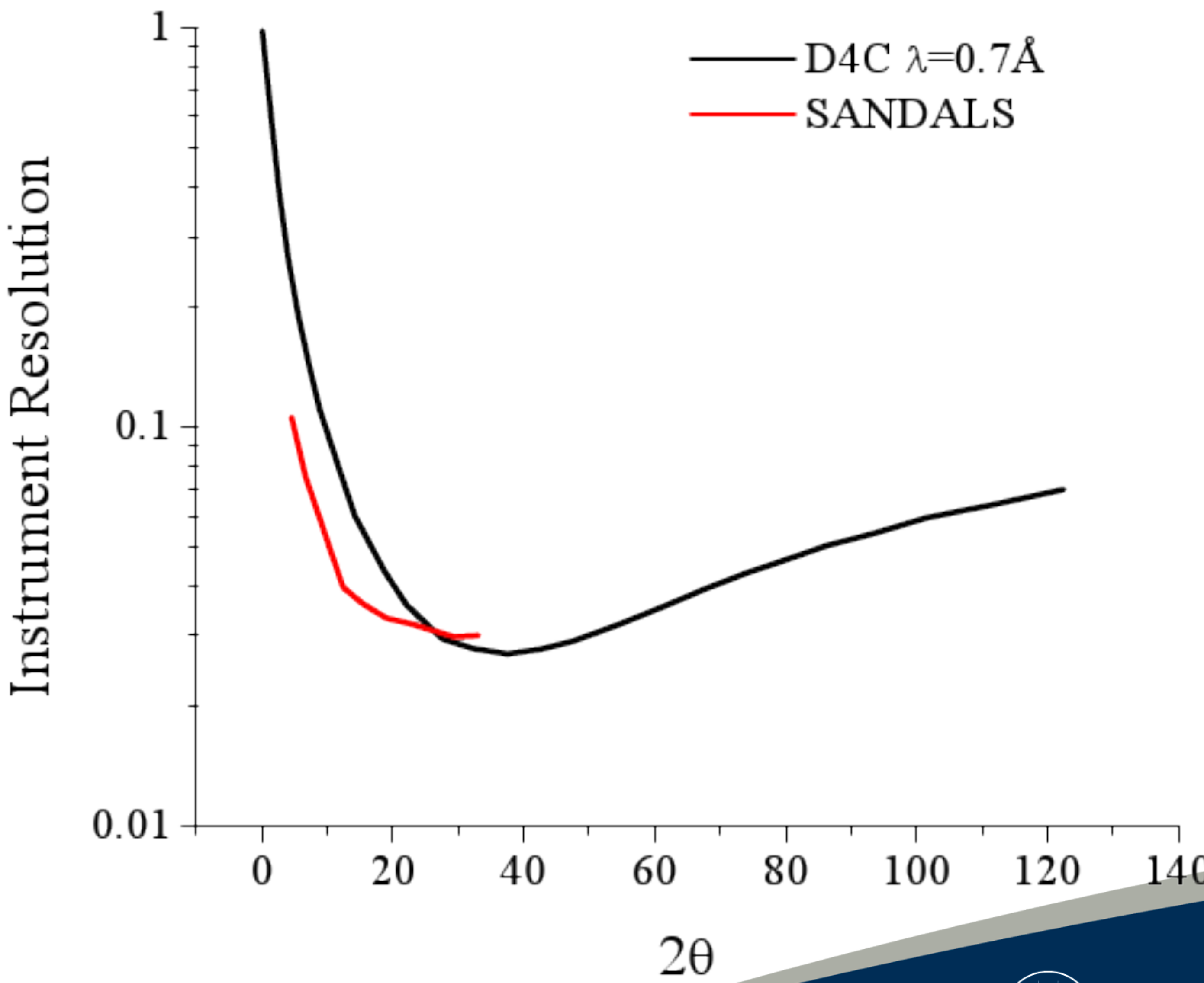
$$\Delta Q = \left(\frac{\delta Q}{\delta\theta}\right)\Delta\theta + \left(\frac{\delta Q}{\delta\lambda}\right)\Delta\lambda$$

$$\Delta Q = Q[\cot\theta\Delta\theta + \Delta\lambda/\lambda]$$

Under the conditions that the wavelengths of the scattered neutrons are measured by time of flight with detectors at fixed scattering angle 2θ, it can be shown that the resolution ΔQ/Q of the TOF neutron diffractometer is roughly constant as a function of TOF.

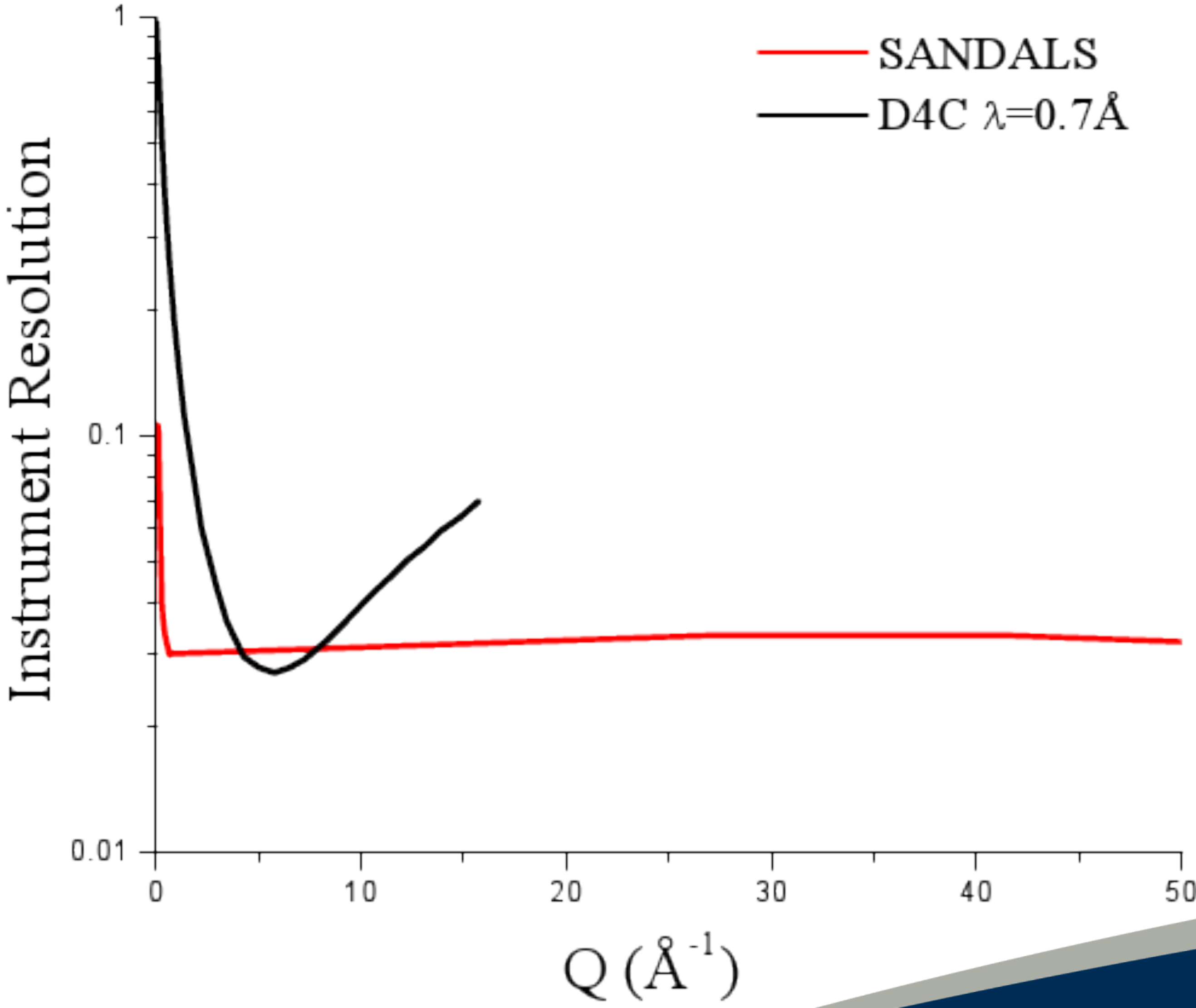
Q resolution of a total scattering measurement

$\Delta\theta/\theta$



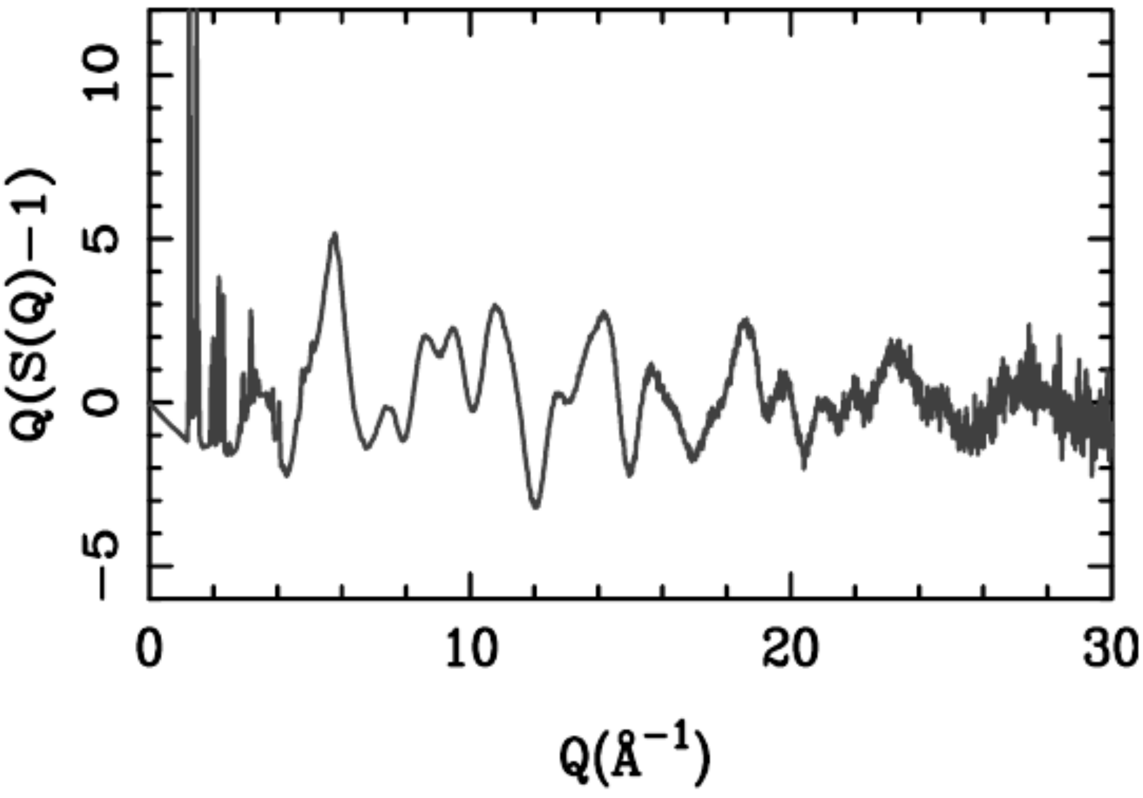
Q resolution of a total scattering measurement

ΔQ / Q



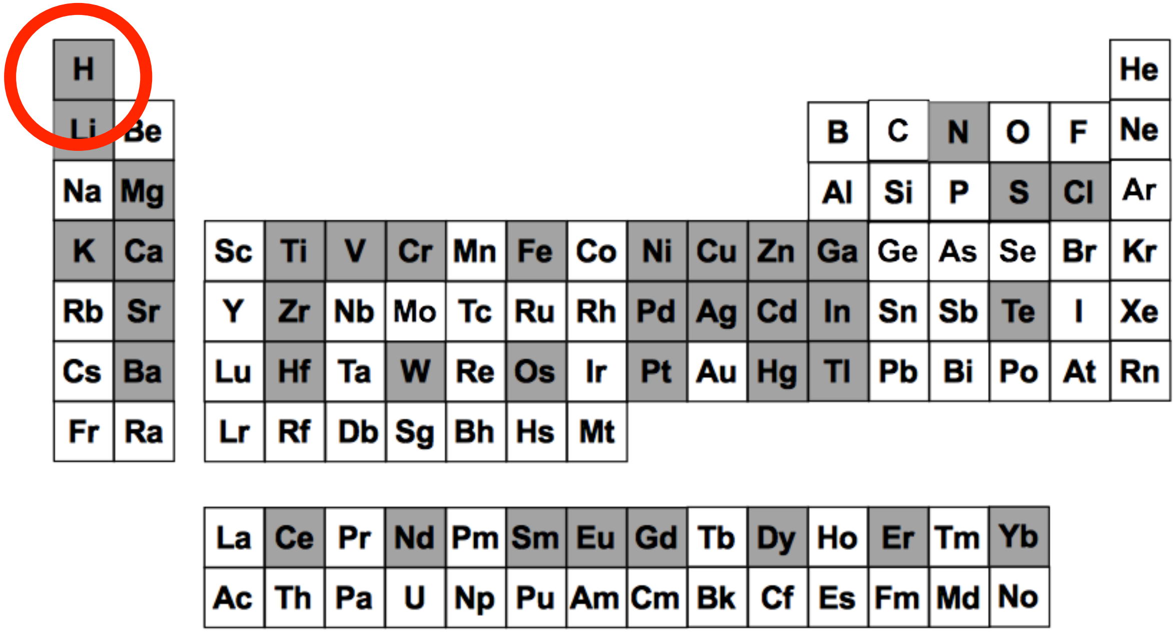
Q-resolution is particularly important for total scattering studies

In total scattering studies it is important to accurate measure both the sharp Bragg and the diffuse scattering components.



Th. Proffen, S. J. L. Billinge, T. Egami and D. Louca, Z. Kristallogr. **218** (2003) 132–143

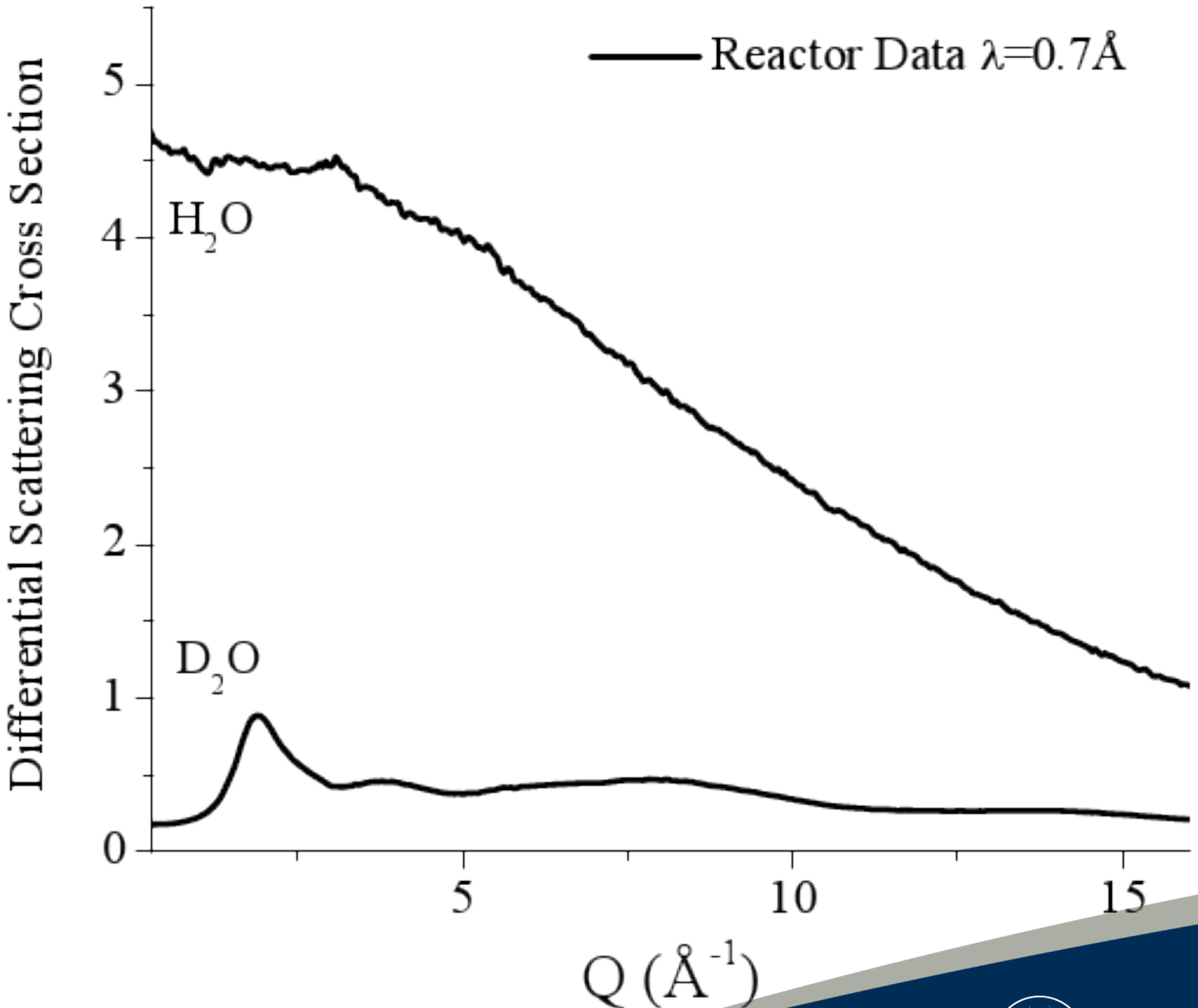
Light element optimized diffractometers SANDALS type



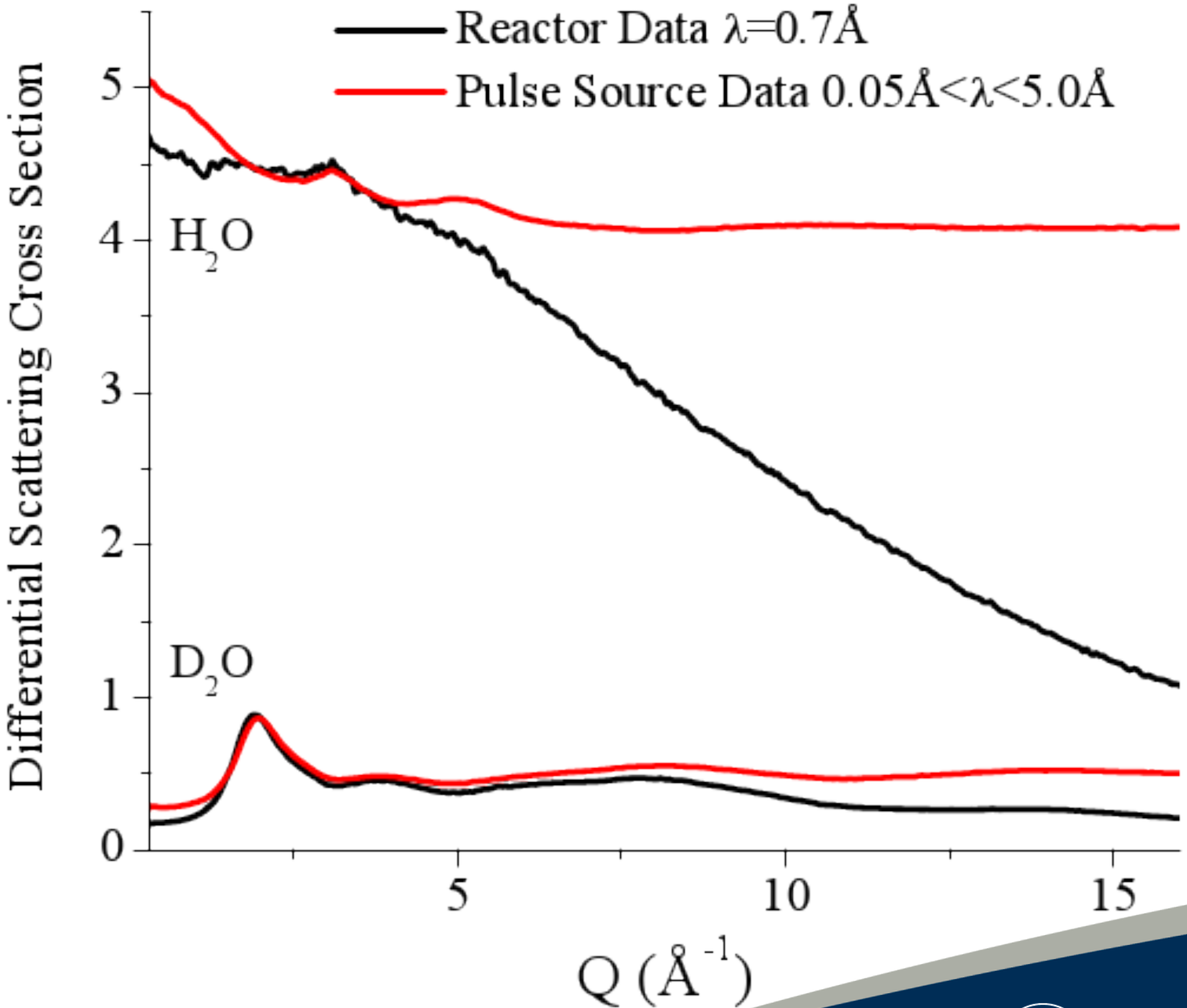
Elements with isotopes that potentially can be used for NDIS ion solvation studies (Δb_c 1fm)

J.E.Enderby, *Chem. Soc. Revs.* 159 (1995)

Inelastic scattering – the challenge for light element neutron diffraction



Inelastic scattering – the challenge for light element neutron diffraction



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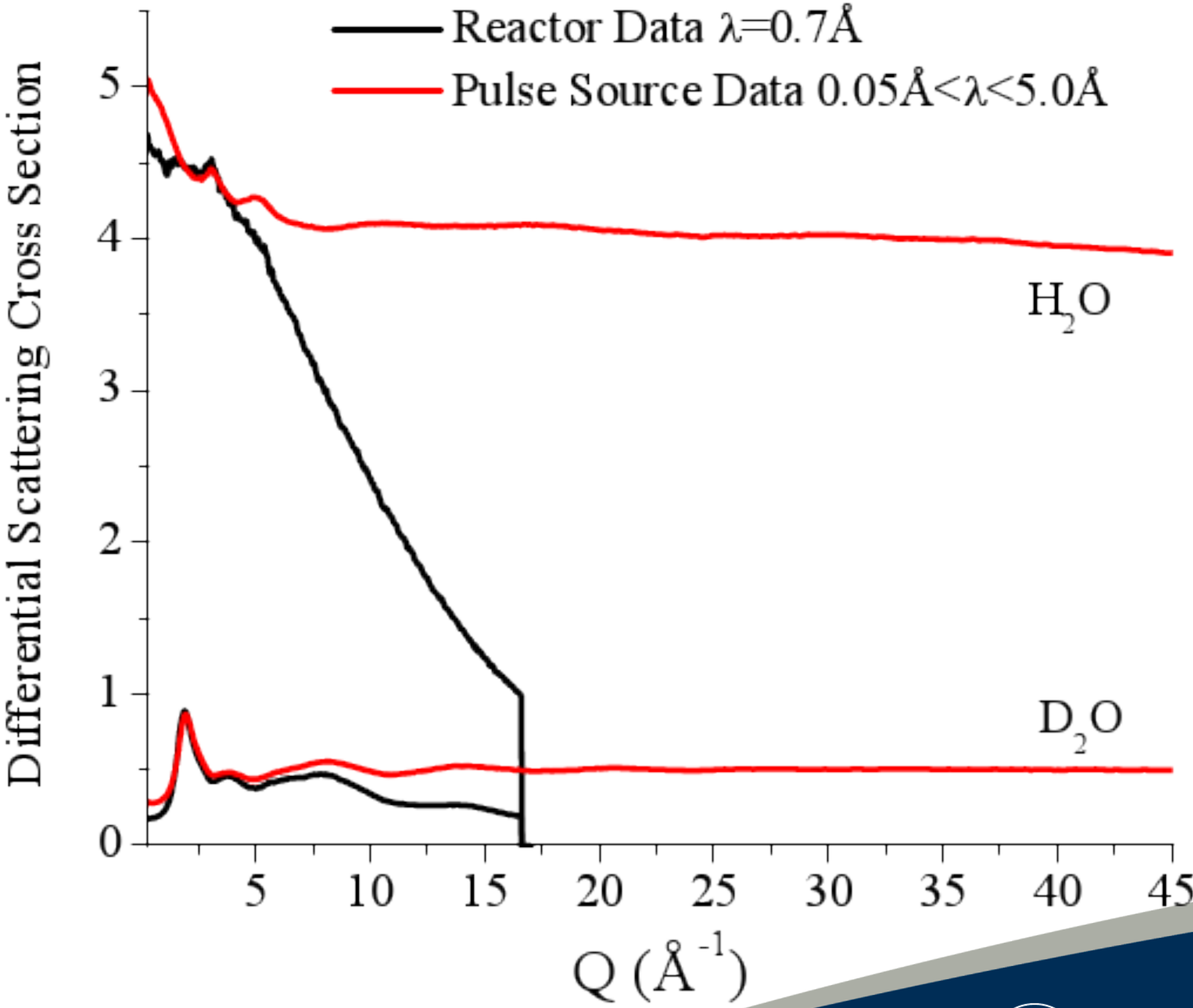
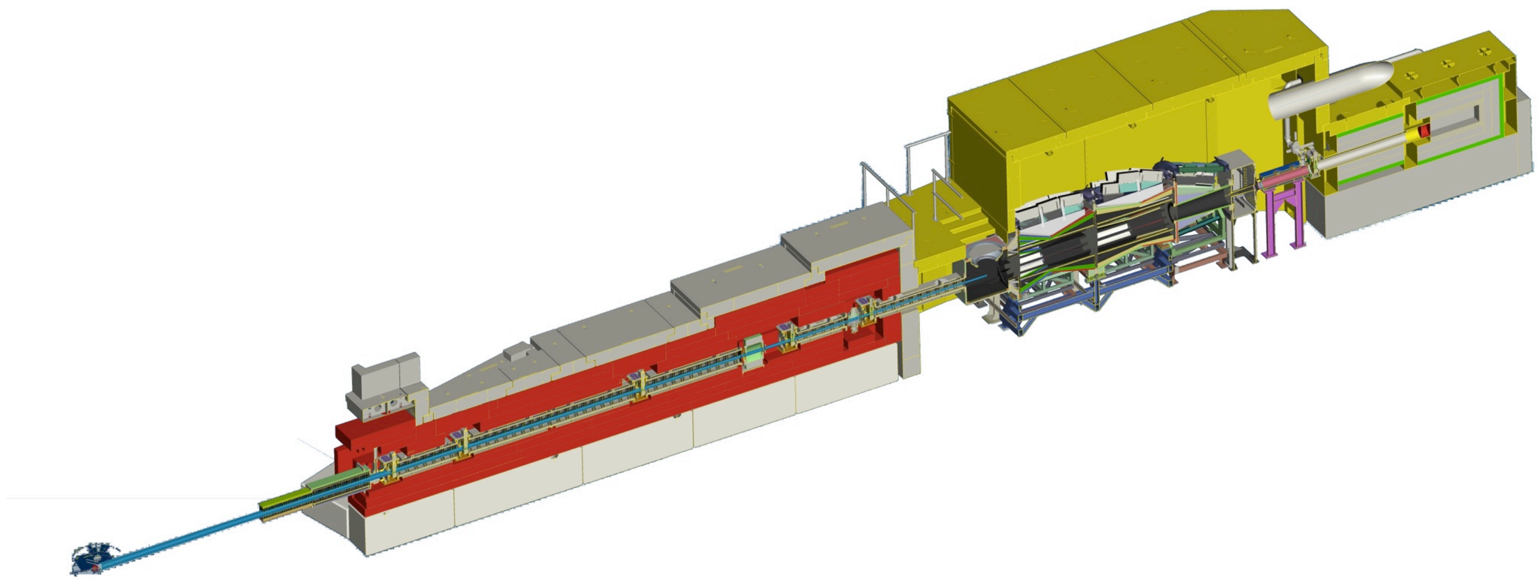
Inelastic scattering – the challenge for light element neutron diffraction



Very wide Q-range diffractometers
NIMROD type



D. T. Bowron, A. K. Soper, K. Jones, S. Ansell, S. Birch, J. Norris,
L. Perrott, D. Riedel, N. J. Rhodes, S. R. Wakefield,
A. Botti, M.-A. Ricci, F. Grazzi, and M. Zoppi
Rev. Sci. Inst. **81** 033905 (2010)

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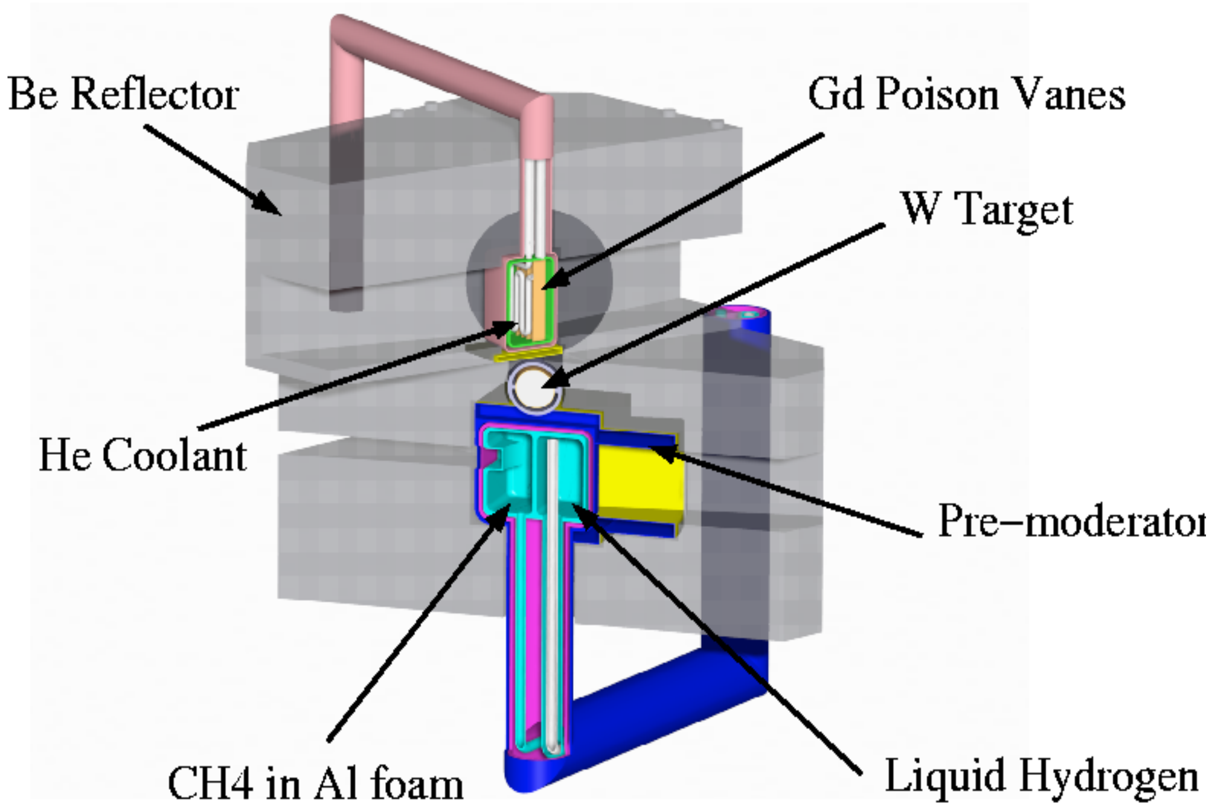
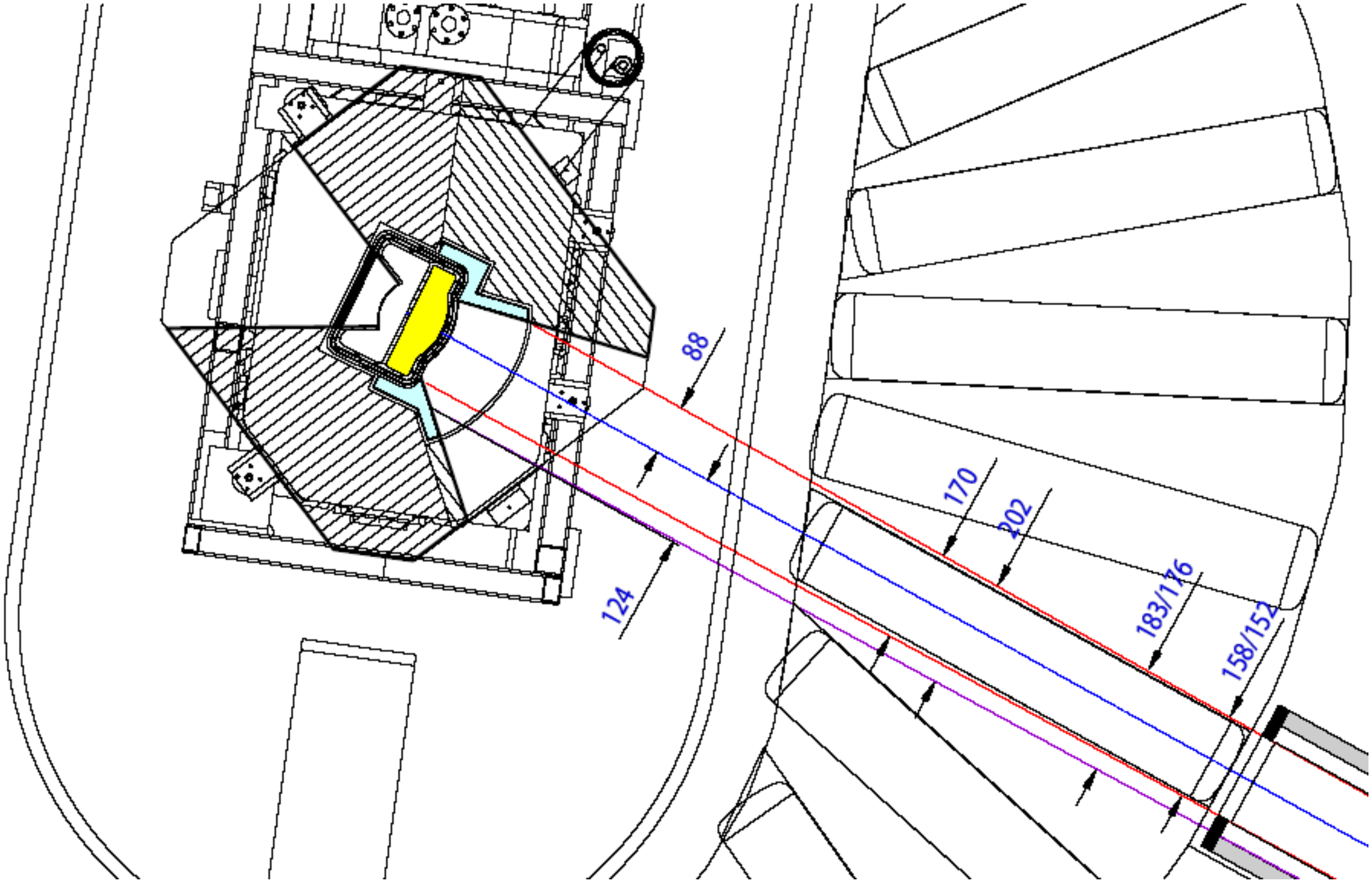
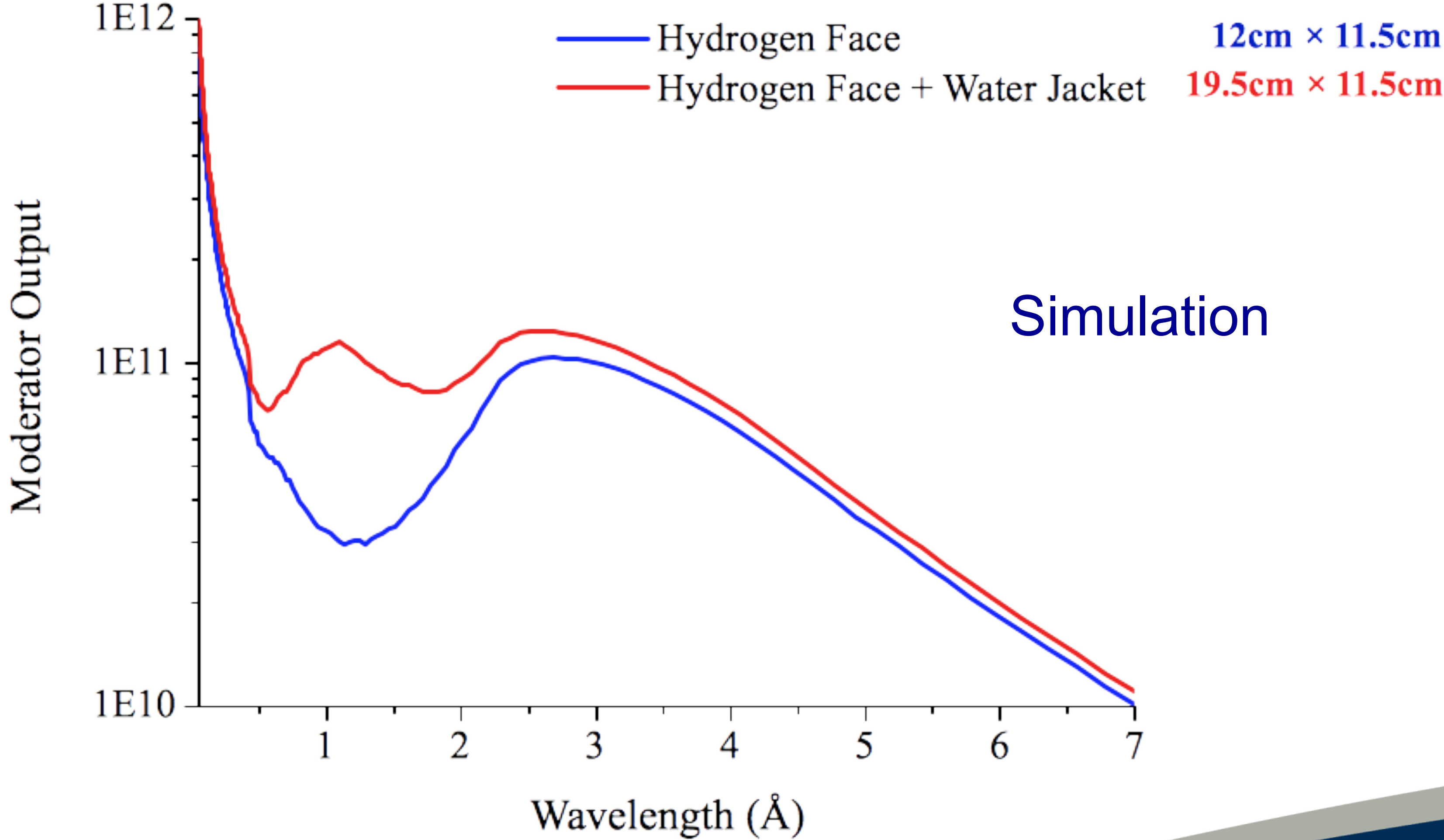
Next generation moderators on ISIS Target Station 2



Combined view of moderator and pre-moderator
High flux across a broad wavelength range



Combined view of moderator and pre-moderator
High flux across a broad wavelength range



Simulation

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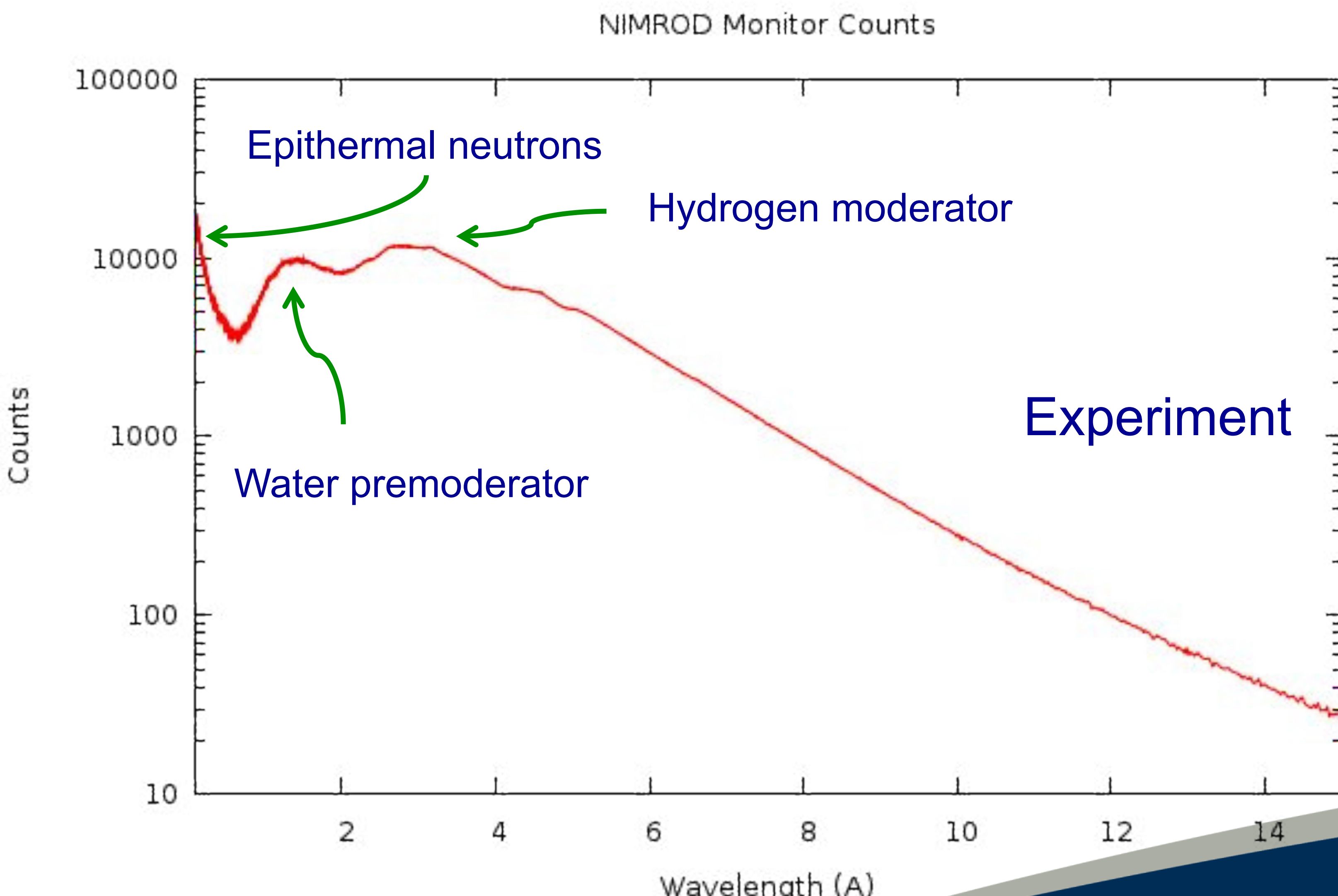
Combined view of moderator and pre-moderator
High flux across a broad wavelength range



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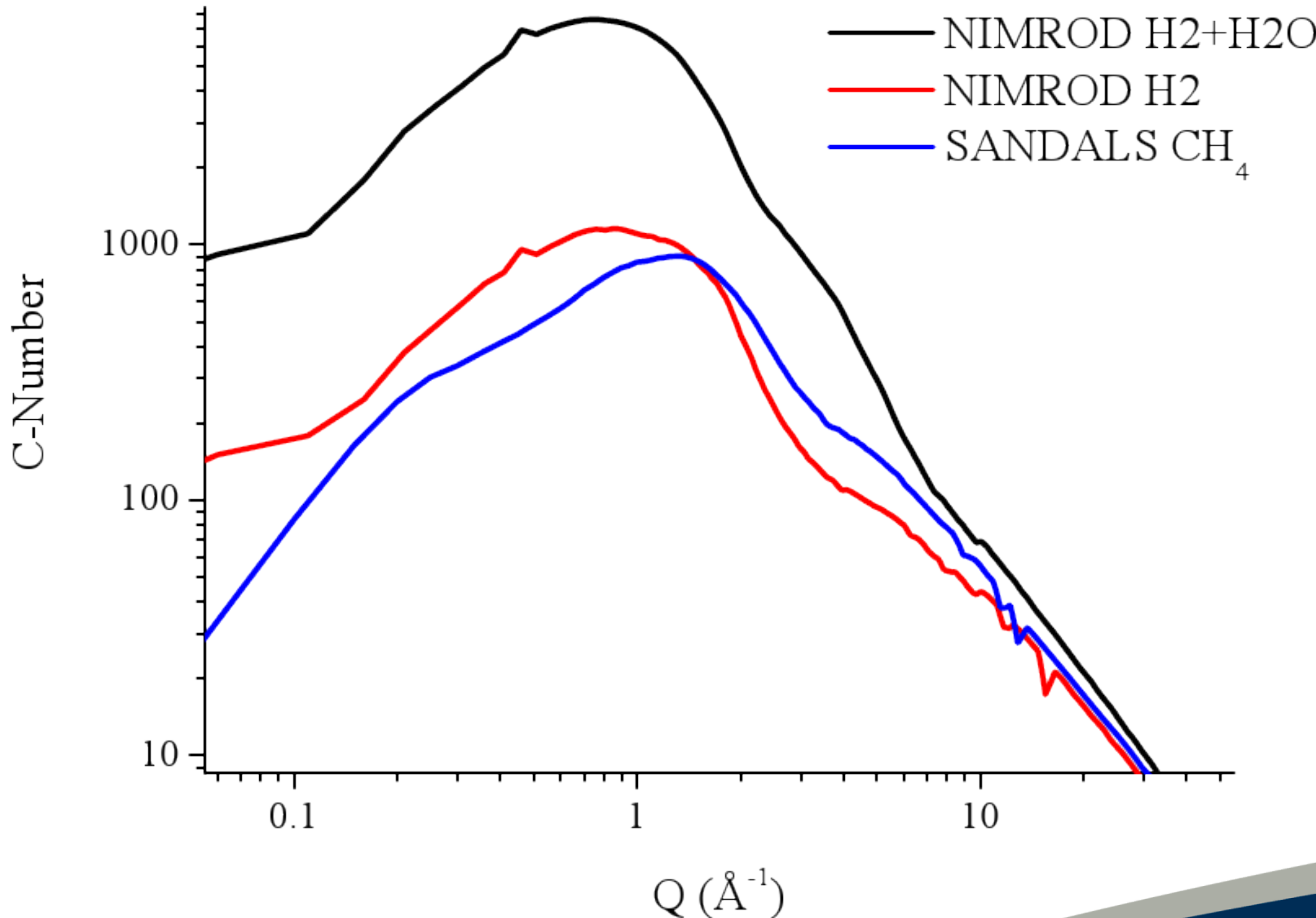
Combined view of moderator and pre-moderator Comparison between SANDALS (TS1) and NIMROD (TS2)



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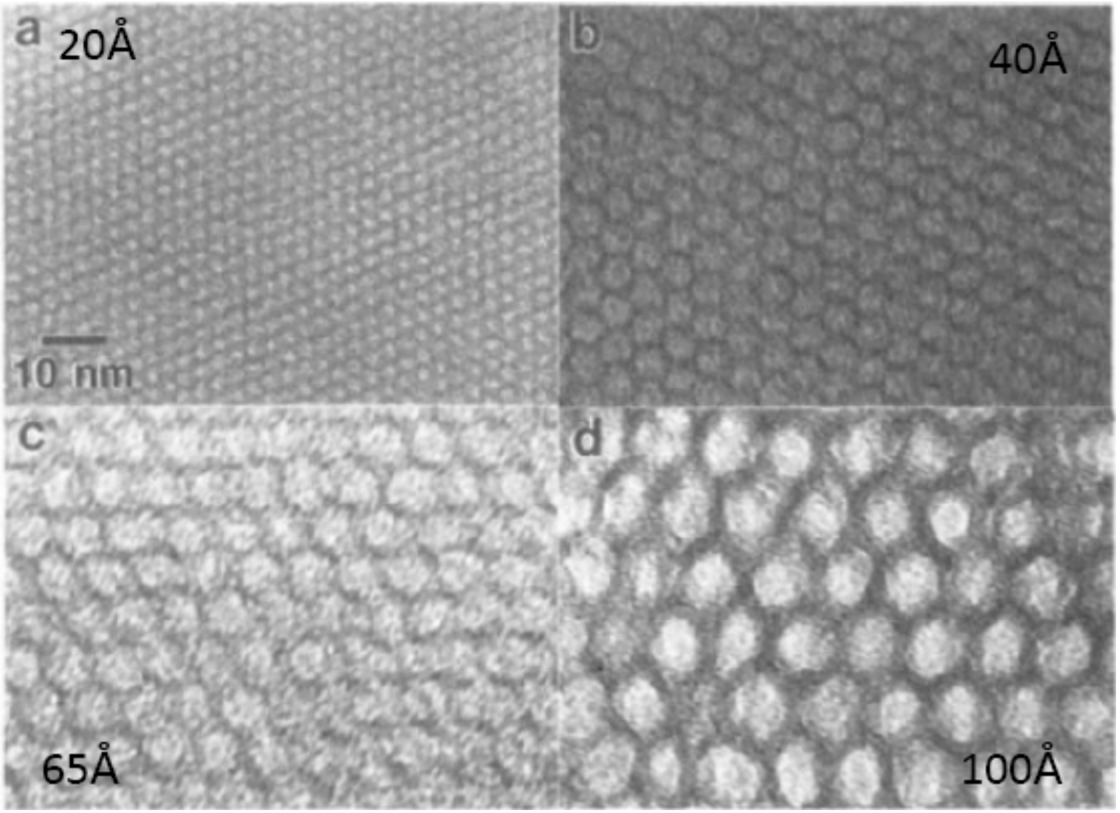
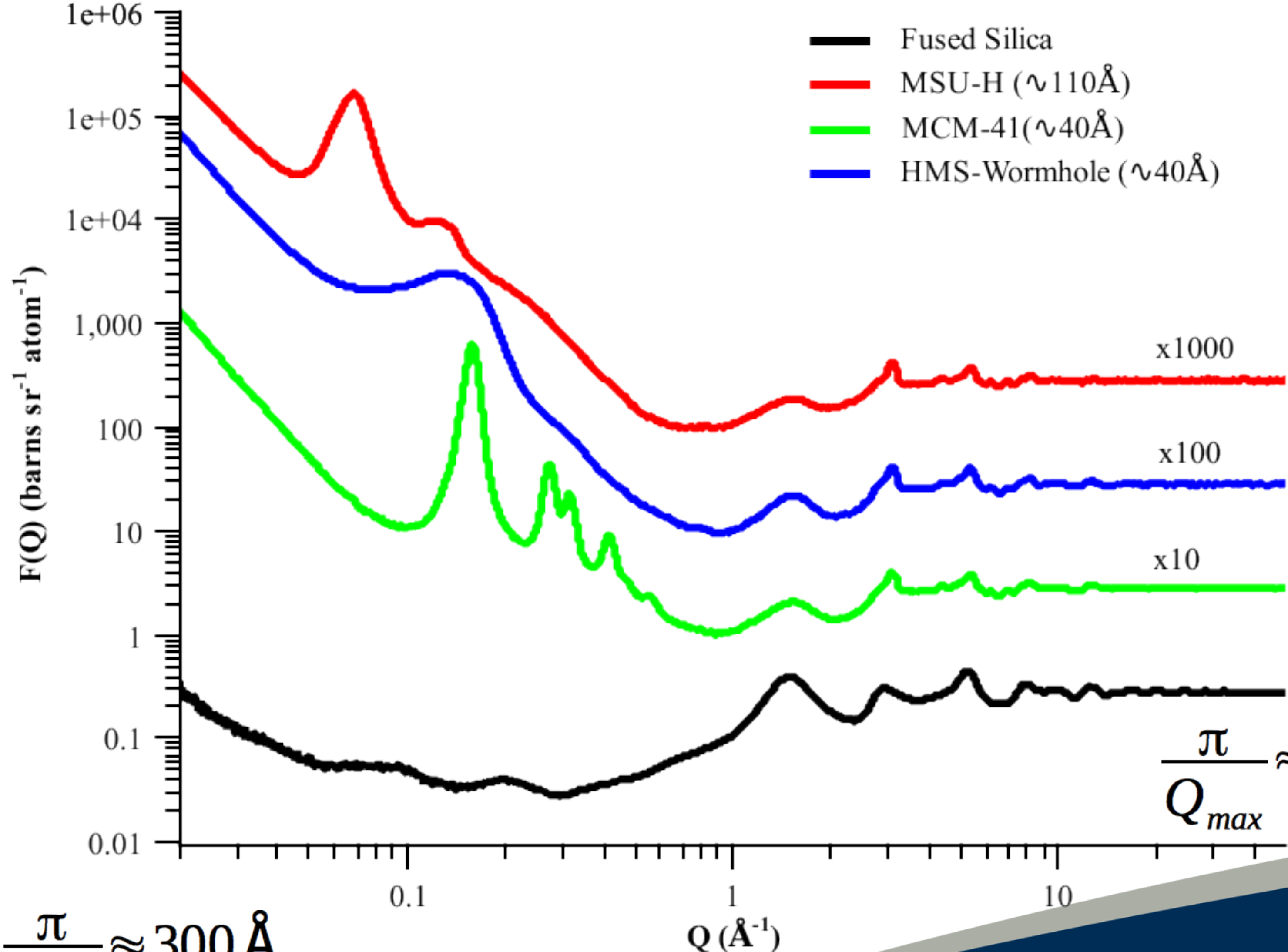
Test of NIMROD performance using mesoporous silicas



C.D.Nunes (University of Lisbon)

Enhanced long wavelength flux translates to good low-Q performance



$$\frac{\pi}{Q_{max}} \approx 0.1\,\text{Å}$$

$$\frac{\pi}{Q_{min}} \approx 300\,\text{Å}$$

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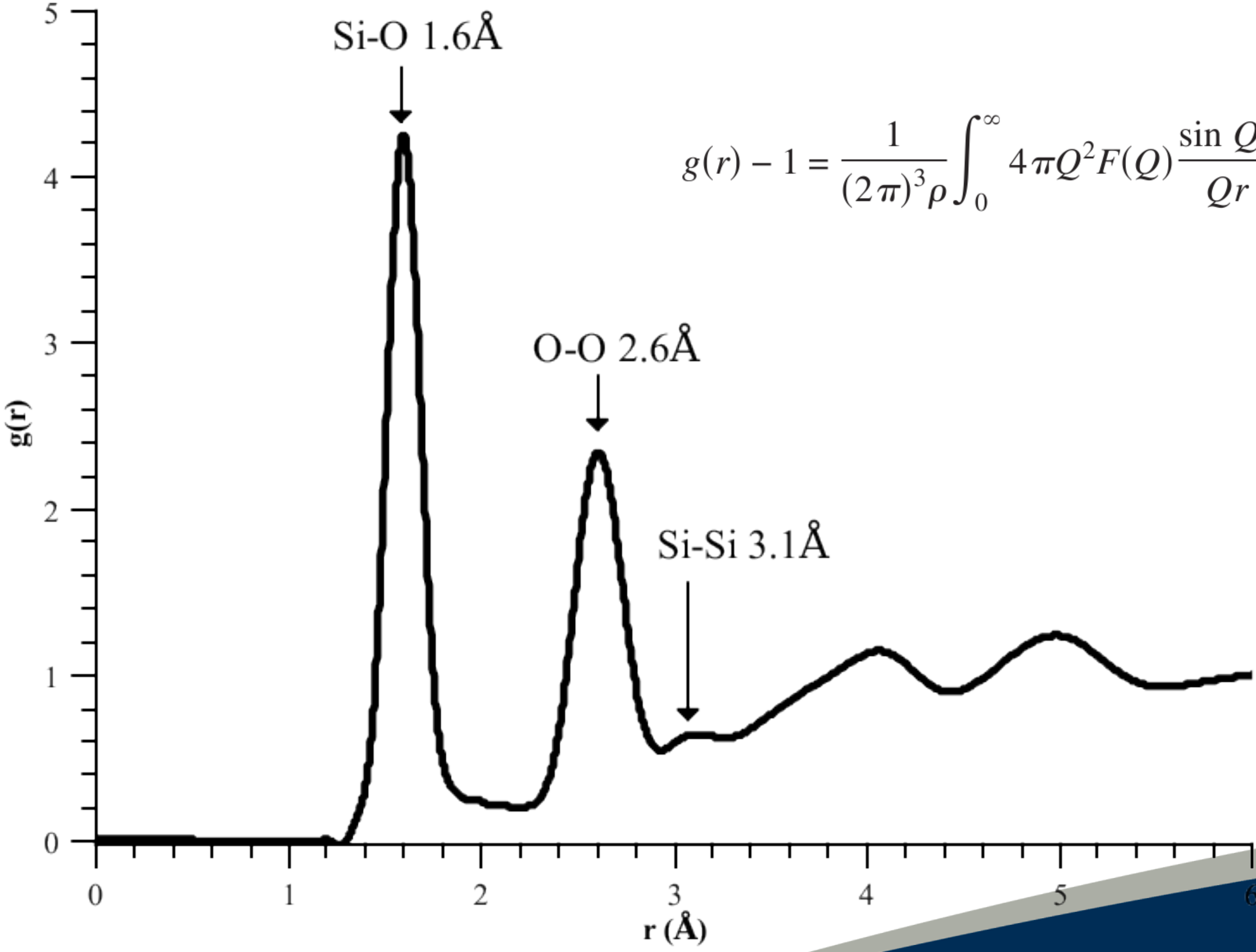
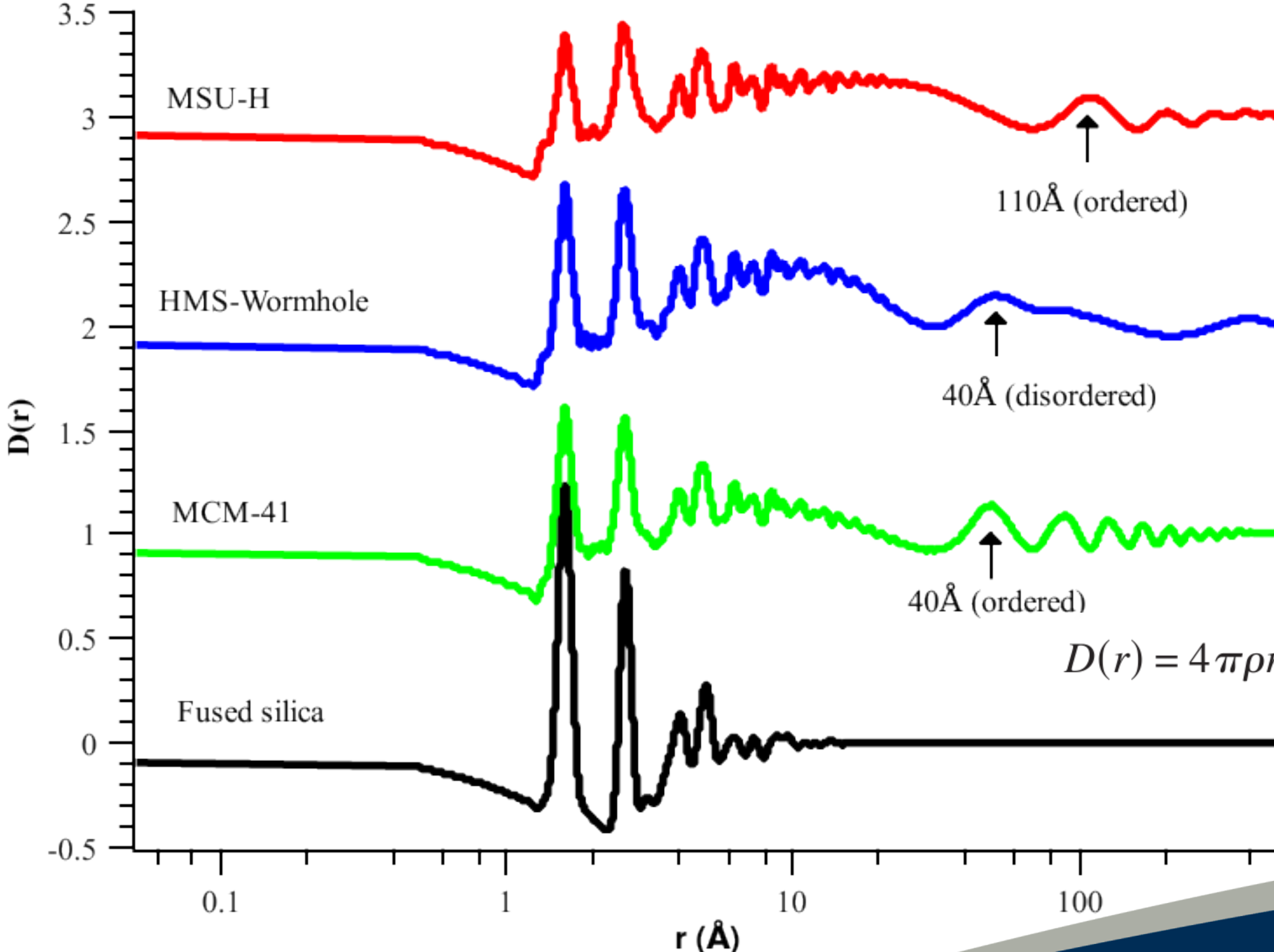
Wide Q-range view of fused silica glass



$$g(r) - 1 = \frac{1}{(2\pi)^3 \rho} \int_0^\infty 4\pi Q^2 F(Q) \frac{\sin Qr}{Qr} dQ.$$

Wide Q-range capability translates to ability to see the nanoscale with atomic resolution



$$D(r) = 4\pi\rho r[g(r) - 1].$$

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Summary:

Light-element optimized disordered materials diffractometers have a very wide range of scientific application

(1)Atomic and molecular liquids and liquid mixtures
(2)Glasses – atomic and molecular
(3)Structured fluids
(4)Polymers and polymer blends
(5)Mesoscale confined fluids
(6)Disordered crystals
(7)....