



A cold chopper spectrometer for the ESS

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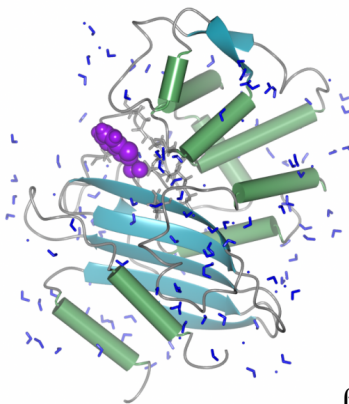
**Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II)
Technische Universität München**

Soft matter materials are dominating in

- Gas oil industry
- Pharmaceutical applications
- Food industry

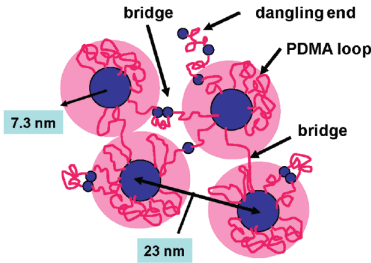
Biological activity is closely linked to proton dynamics in the sytem, e.g. :

- Hydration shell dynamics
- Conformational changes
- Hydrogen bond network

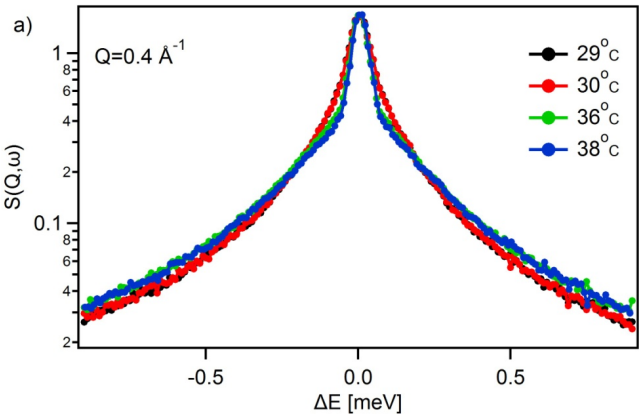


β -lactamase

Stimuli – Responsive Polymers



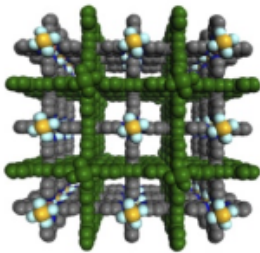
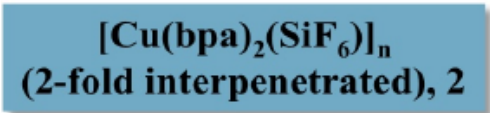
M.-T. Popescu et al. Marcomolecules 45 (2012) 3523



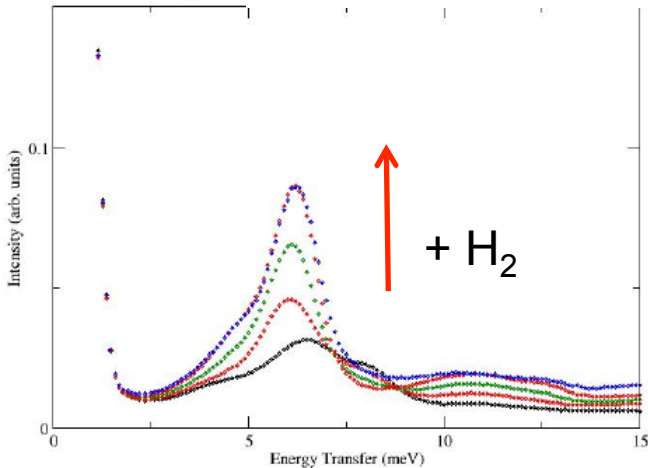
M. Philipp et al. , E13 – TUM (2013)

- Materials development
- Energy materials
 - H₂ storage (adsorption / absorption)
 - Ionic liquids for batteries
- ...

H₂ adsorption in MOFs

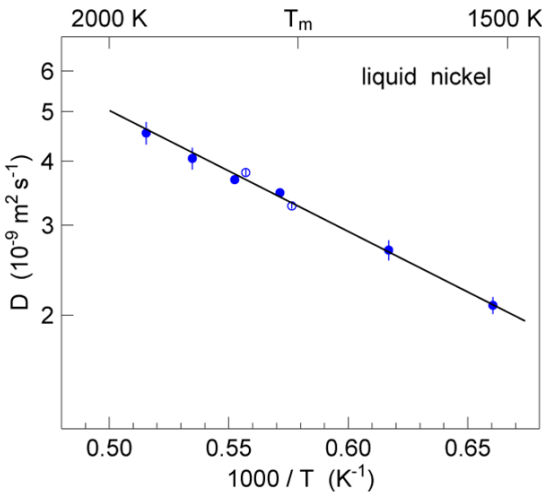


BET surface 735 m² /g
Pore diameter: 3.5 x 3.5 Å



J. Eckert et al University of South Florida (2013)

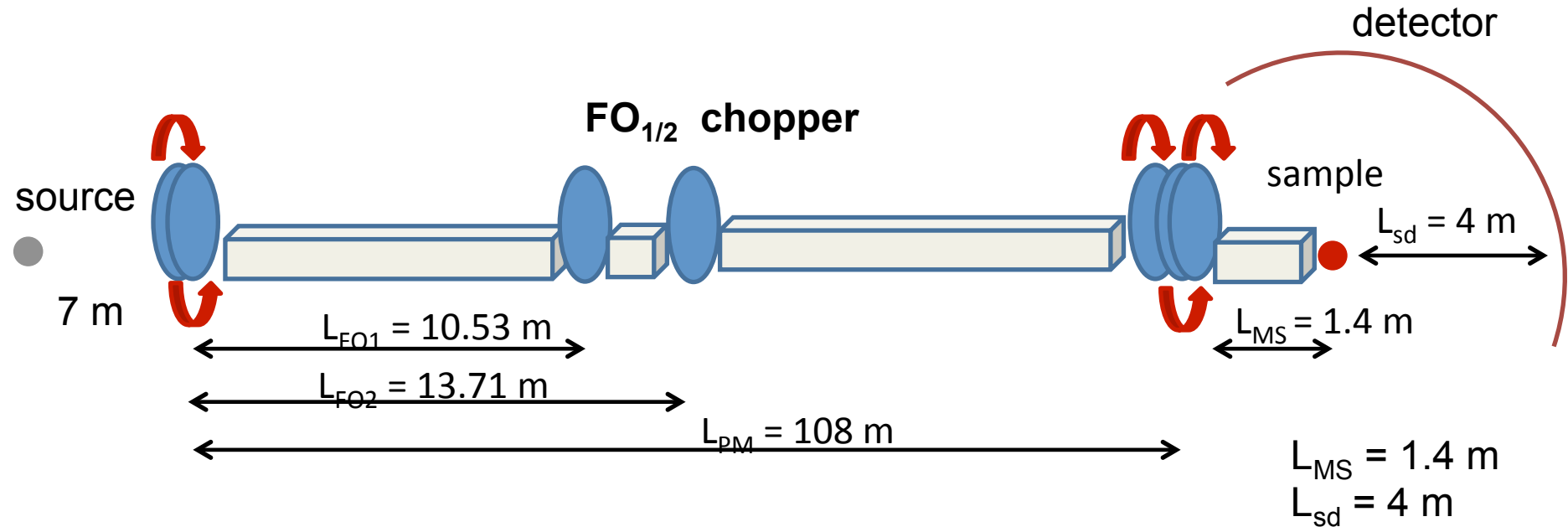
Diffusion coefficients in liquid metals



Meyer, Stüber, Holland-Moritz, Heinen, Unruh, Phys. Rev. B 77 (2008) 092201

- Disordered Materials
 - Rich dynamic landscape
 - Dynamics governs functionality
 - Trend to increasing complexity to approach more realistic scenarios
- 
- Small sample sizes and dedicated sample environment
 - Time resolved measurements
 - Pump-probe experiments / secondary characterisation online (NMR, Raman,...)

- Flexible to high energy resolution
100 μeV @ 5 Å
5 μeV @ 9 Å
- Large Q- ω space
- Multi-energy mode
- Clean resolution function
- Excellent signal to noise ratio
- Medium Q resolution
- Extended / focused beam size

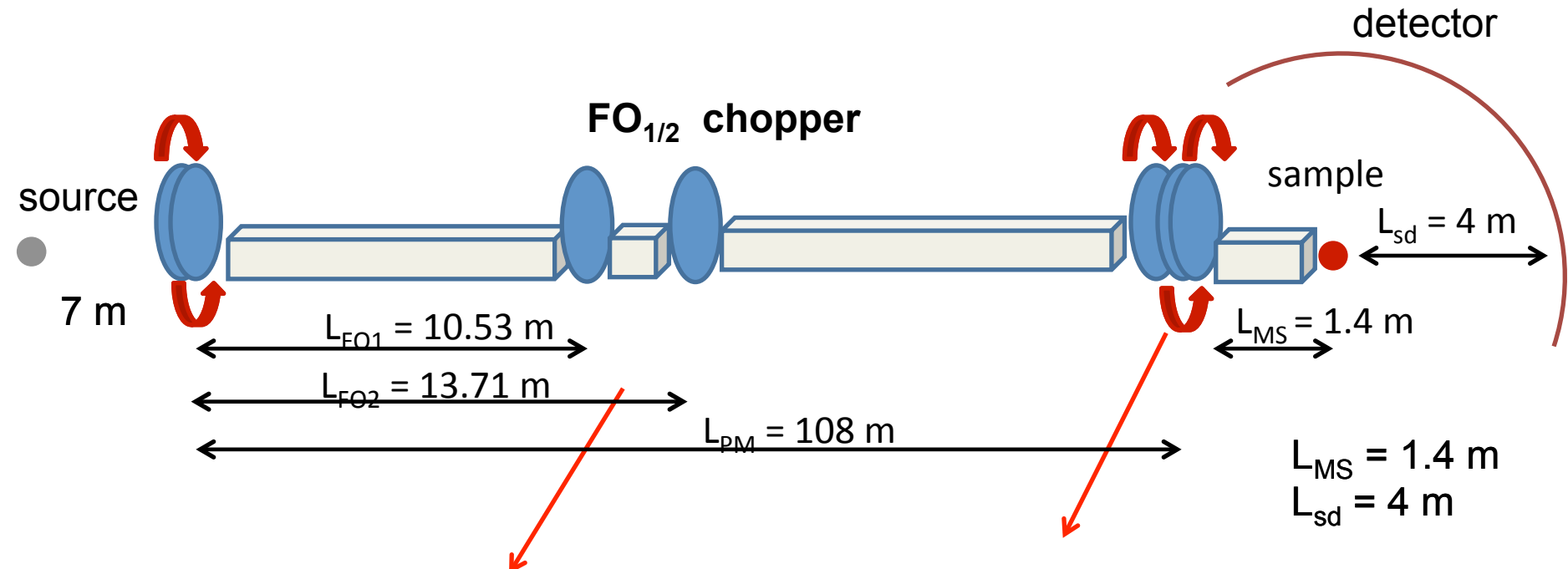


Pulse shaping

Counter-rotating chopper pair
14 - 100 Hz

Monochromating

Counter-rotating chopper pair
140 - 400 Hz

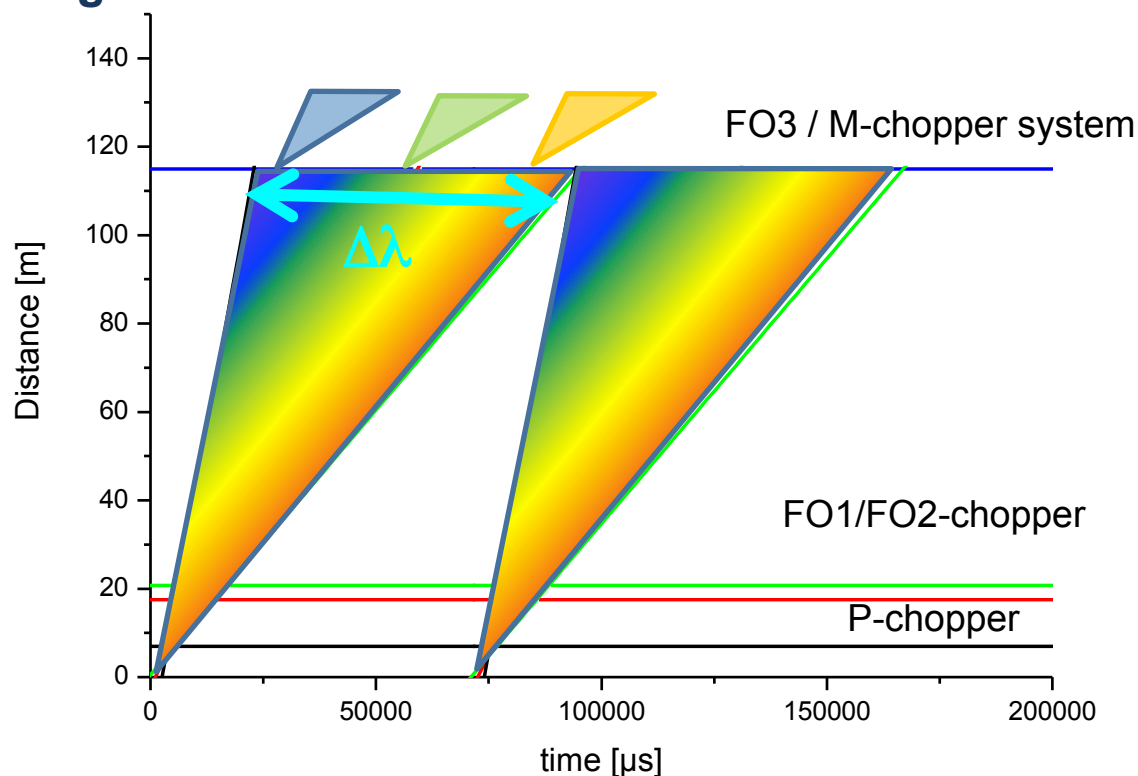


Frame overlap chopper to prevent overlap of subsequent source pulses

Frame overlap chopper to chose between

- Single pulse option $(n_2 - 1) \times 14 \text{ Hz}$
- Multi-Energy Mode (Rate Repetition Multiplication (RRM), 1 – N_2 pulses

Time-distance Diagramm



N_1	N_2	ΔE (FWHM) 2 Å [μ eV] ($\Delta L = 10 / 20$ mm)	ΔE (FWHM) 5 Å [μ eV] ($\Delta L = 10 / 20$ mm)	ΔE (FWHM) 9 Å [μ eV] ($\Delta L = 10 / 20$ mm)	$\Delta\lambda$ [Å]
2	10	1469 / 1485	95 / 99	16.7 / 18.9	2.6
4	20	736 / 757	49 / 56	9.4 / 13	2.14
6	28	509 / 546	36 / 45	7.5 / 11.5	1.96

Use of FO3 chopper:

$$FO2 = (R-1)/R * N_2$$

1 – N_2 pulses pro source frame

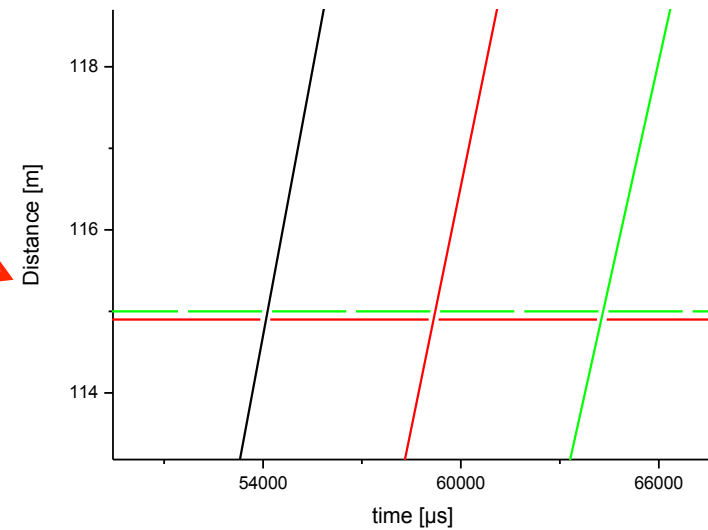
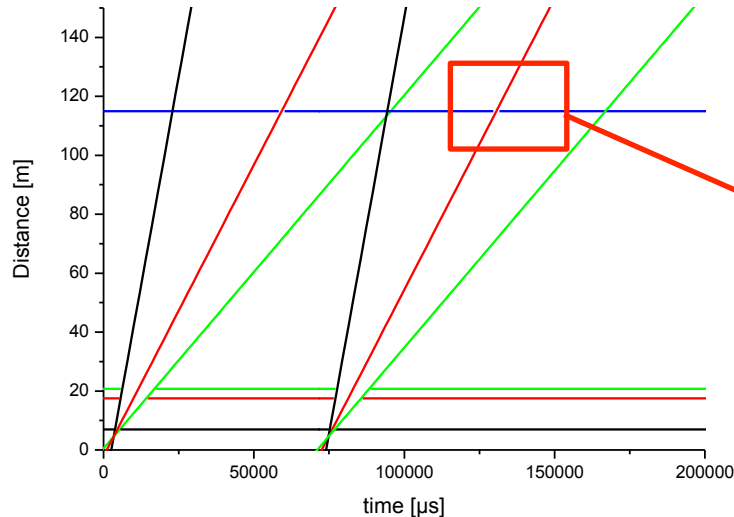


Wavelength band

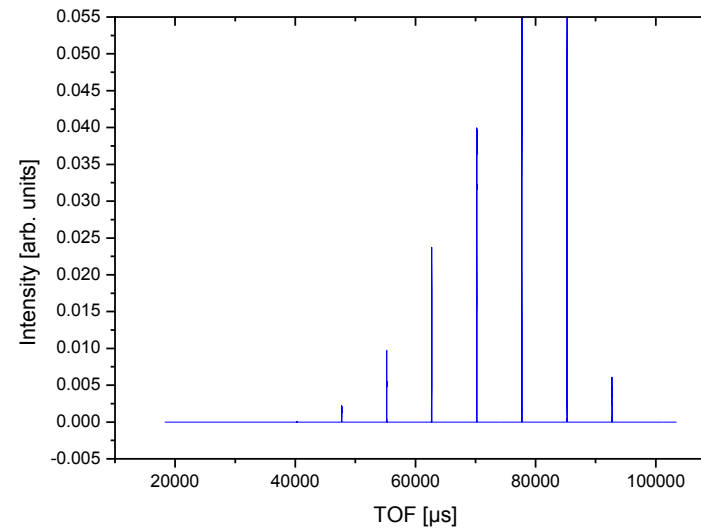
$$N_1 = 2: \Delta\lambda = 2.6 \text{ \AA}$$

$$N_1 = 4: \Delta\lambda = 2.14 \text{ \AA}$$

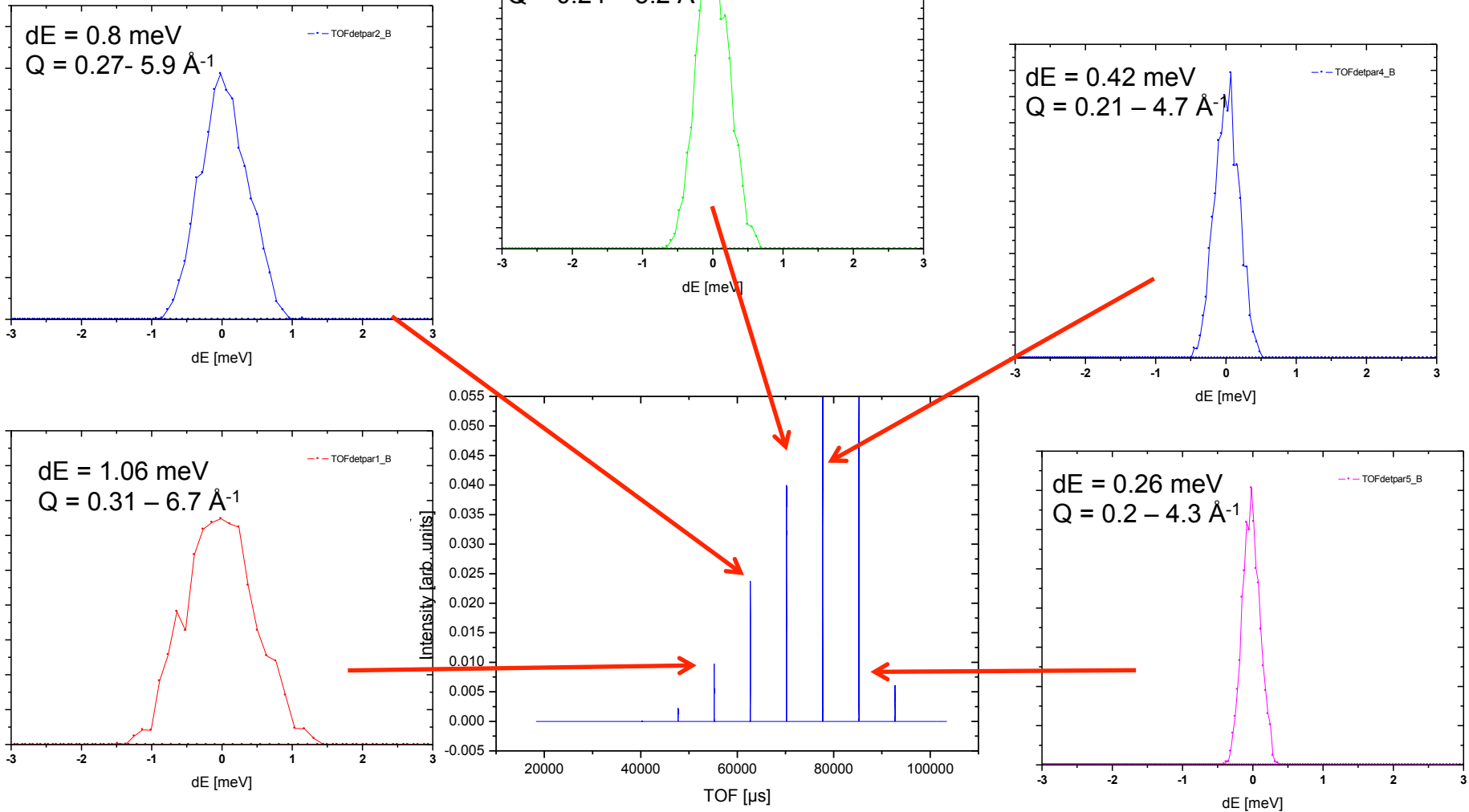
$$N_1 = 6: \Delta\lambda = 1.96 \text{ \AA}$$



$N_1 = 4$, $N_2 = 20$, Ratio 2
 $\lambda = 1.51 - 2.98 \text{ \AA}$



$N_1 = 4, N_2 = 20, \text{Ratio } 2$
 $\lambda = 1.51 - 2.98 \text{ \AA}$

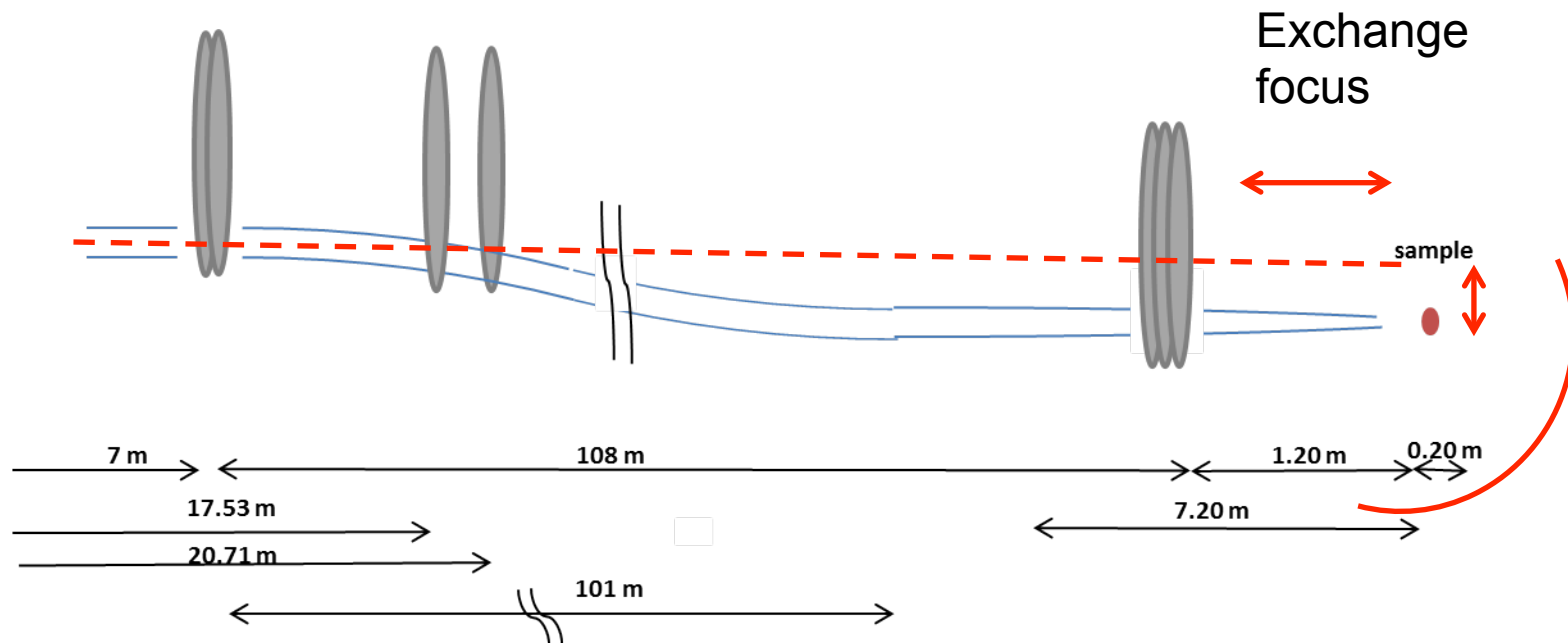


- Avoid direct line of sight
- Standard option: 20 x 40 mm²
- Focus option: 10 x 10 mm²

in collaboration with:

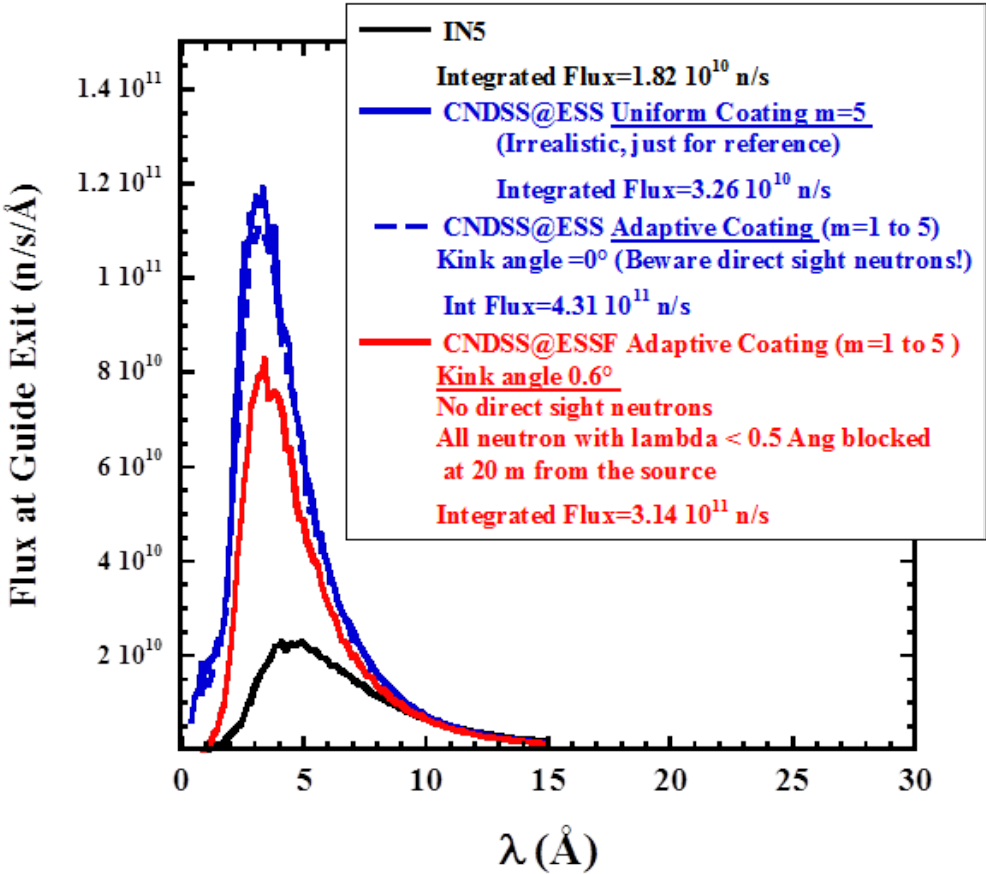
*J.-M. Zanotti, S. Longeville, Ch. Alba-Simionsco
LLB, France*

S – Bender Guide vs kinked elliptic guide



Cold Neutron Disk Chopper Spectrometer at ESS Flux at guide Exit (McStas Simulations)

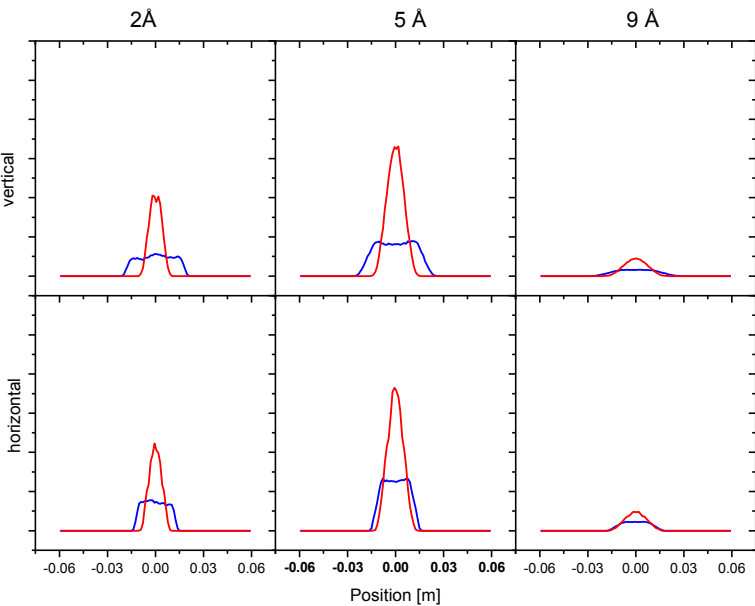
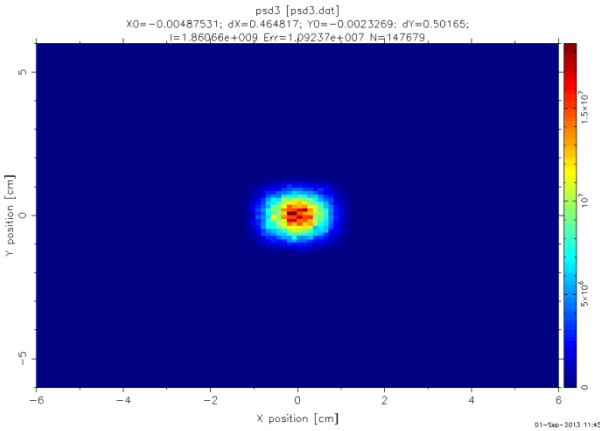
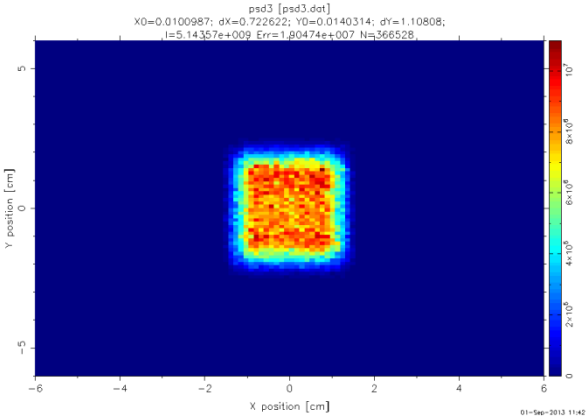
NB: For CNDSS@ESS: Hor. & Vert. elliptic guide



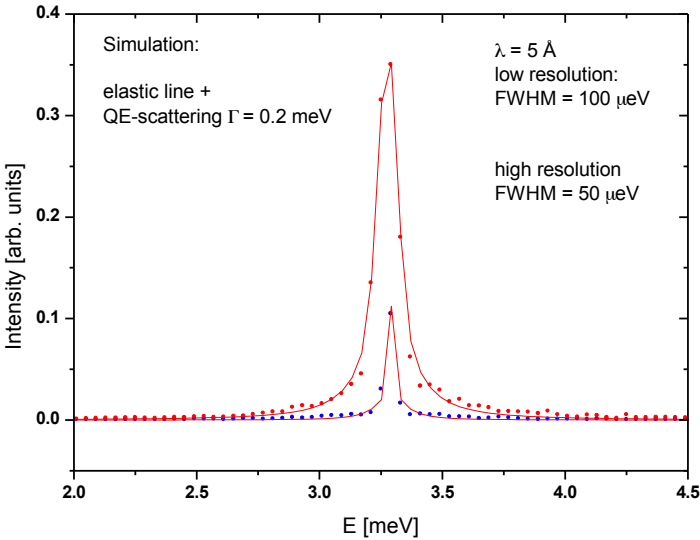
in collaboration with:

*J.-M. Zanotti, S. Longeville,
Ch. Alba-Simionsco LLB, France*

$\lambda = 5 \text{ \AA}$



λ [Å]	Standard [n / (cm ² s Å)]	Focus [n / (cm ² s Å)]
2	9.62 10 ⁸	2.73 10 ⁹
5	1.62 10 ⁹	3.5 10 ⁹
9	3.04 10 ⁸	3.7 10 ⁸



Flux at sample position (Single Energy mode)

λ [Å]	Resolution [μeV]	Standard [n / (cm ² s)]	Focus [n / (cm ² s)]
2	1500	1.05 10 ⁶	2.37 10 ⁶
5	100	1.69 10 ⁶	4.16 10 ⁶
9	20	3.34 10 ⁵	3.84 10 ⁵

Moderator:	cold source
Moderator – sample distance:	116.4 m
Wavelength range:	1.1 – 20 Å
Energy Resolutions: $\Delta E / E =$	0.3 – 3.4% (10 μeV – 112 μeV @ 5Å)
Q-range /Resolution:	@ 2 Å: 0.82 – 5.90 Å ⁻¹ ($\Delta Q = 0.21 – 0.075$ Å ⁻¹) @ 5 Å: 0.32 – 2.36 Å ⁻¹ ($\Delta Q = 0.09 – 0.03$ Å ⁻¹)
Flux at sample @ 5 Å:	standard: $1.6 \cdot 10^9$ neutrons / (s cm ² Å) white beam focus: $3.5 \cdot 10^9$ neutrons / (s cm ² Å) white beam
Beam size at sample:	standard: 40 x 20 mm ² focus: 10 x 10 mm ²
Divergence at sample:	+/- 1 deg
Sample – detector distance:	4 m
Detector technology:	¹⁰ B converter layers
Detector coverage:	-15 – 140 deg

Thank you!