A Liquids Reflectometer at the Spallation Neutron Source

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Spallation Neutron Source

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Outline

I. **Neutrons and Contrast**

II. **A Reflectometer, Deconstructed**

III. **Performance and Challenges**

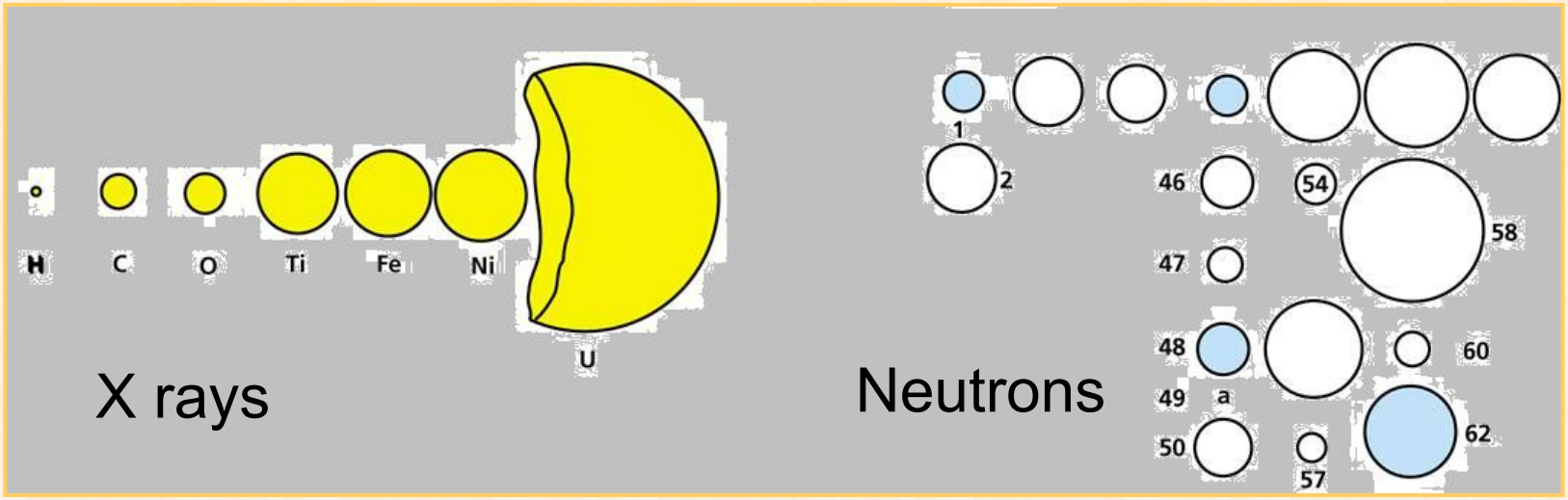
I. Neutrons and Contrast

Neutrons scatter from nuclei,

X rays see electrons
Neutrons see nuclei

=>

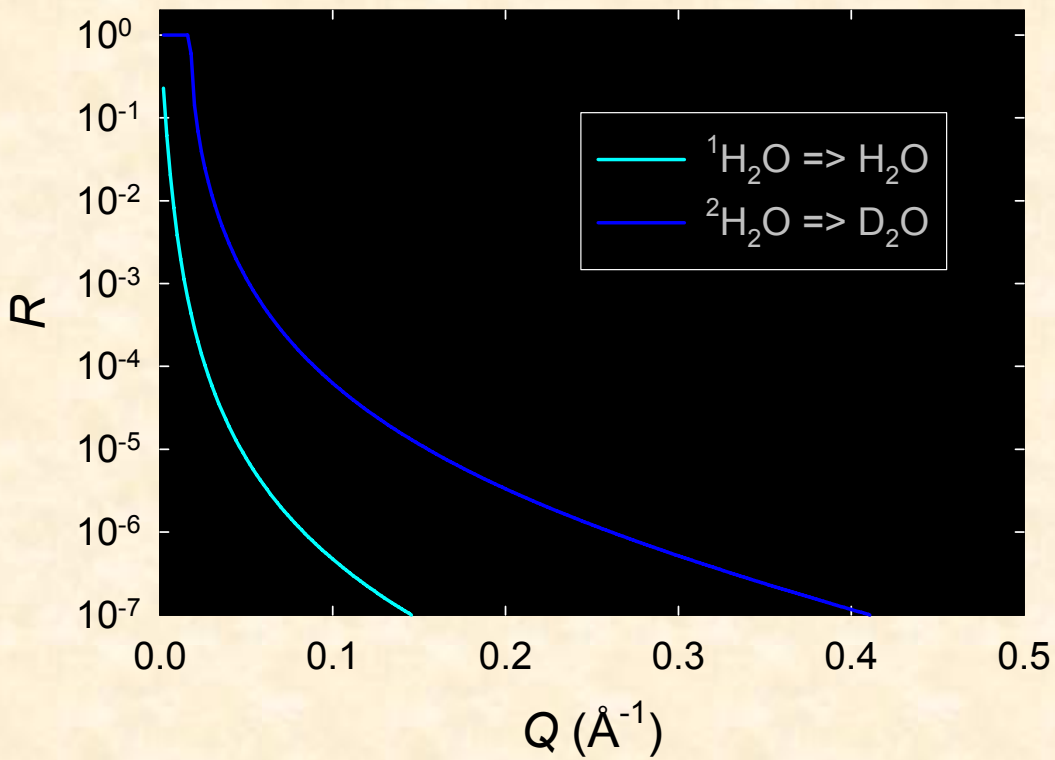
Isotopic substitution



H C O Ti Fe Ni U

Radii of balls = *b* = scattering amplitude

so we can use isotopic substitution to enhance contrast.



$$Q = 4\pi \sin\alpha / \lambda$$

$$n \approx 1 - (b/v)\lambda^2/2\pi$$

λ := wavelength

b/v := scatt. density

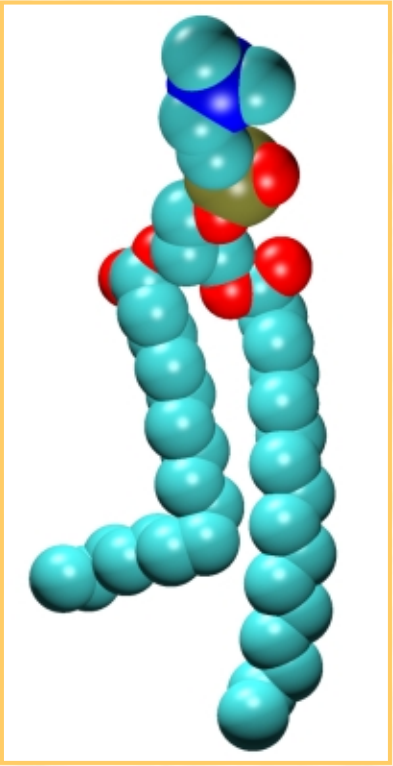
n_{H2O}= 1.00000197

n_{D2O}= 0.99997771

$(b/v)_{H2O}$= -0.56×10^{-6} Å^{-2}

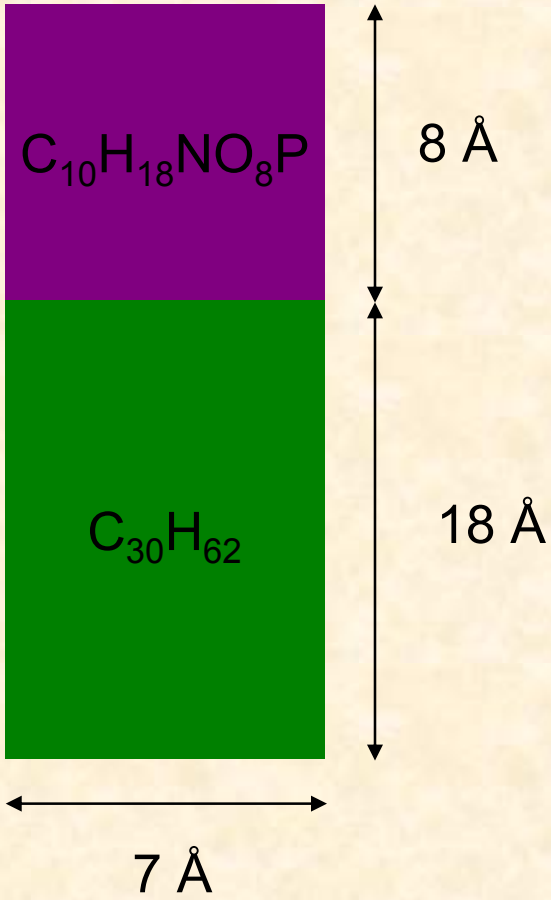
$(b/v)_{D2O}$= 6.34×10^{-6} Å^{-2}

Reflectivity is a low spatial resolution probe



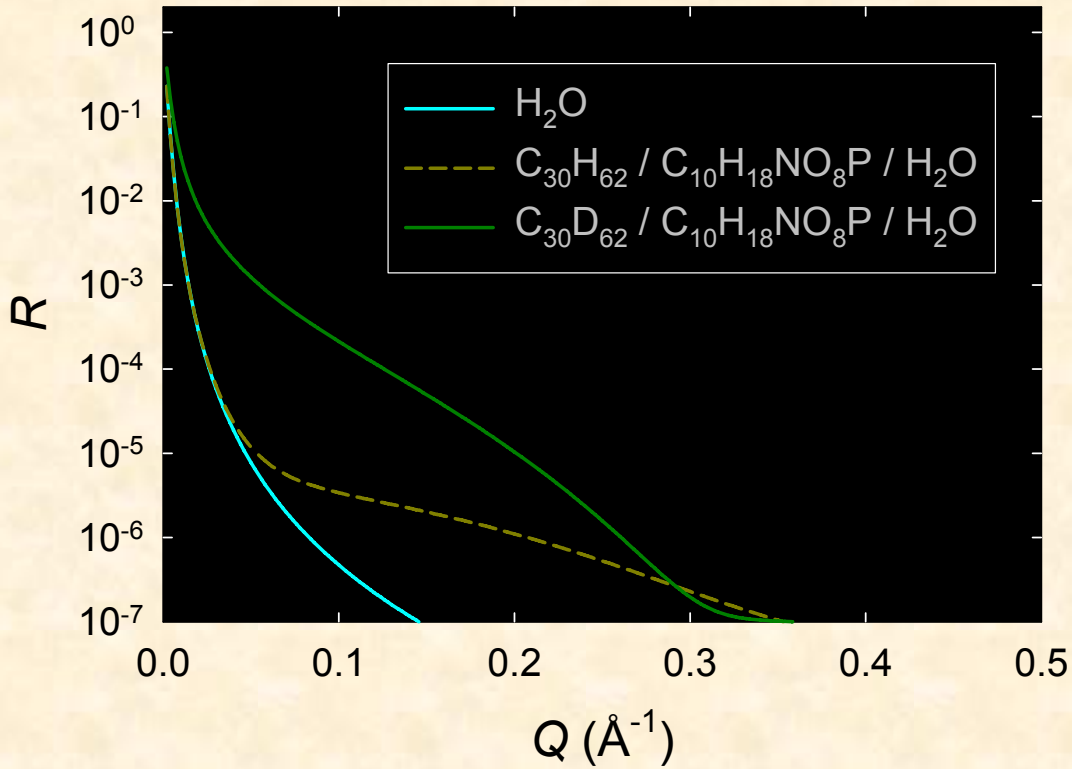
dipalmitoyl phosphatidylcholine (DPPC)

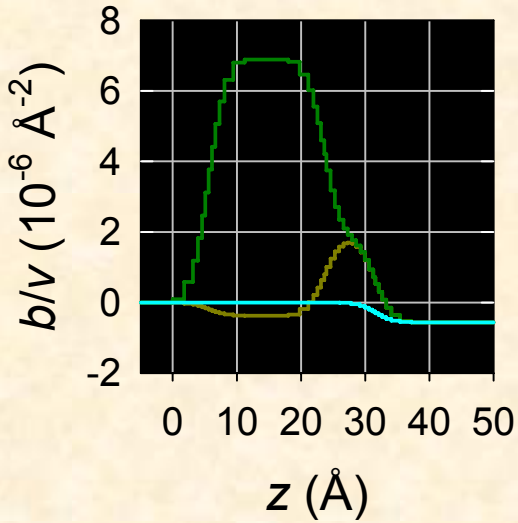
=>



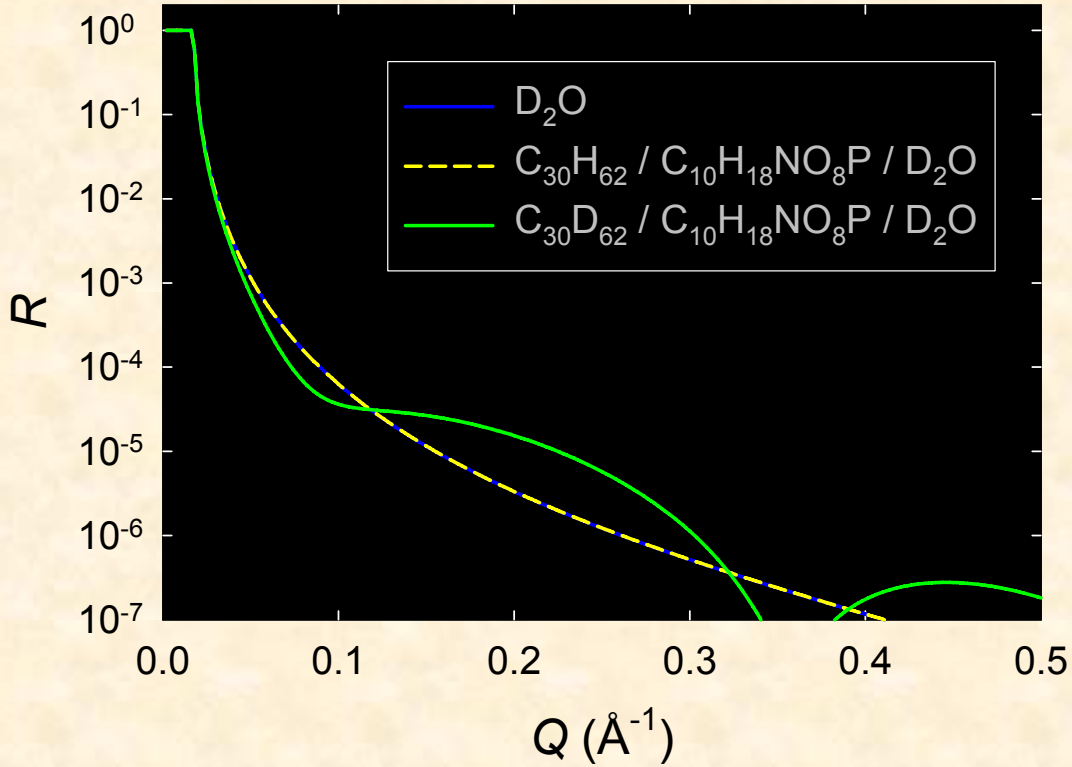
Phospholipids for physicists

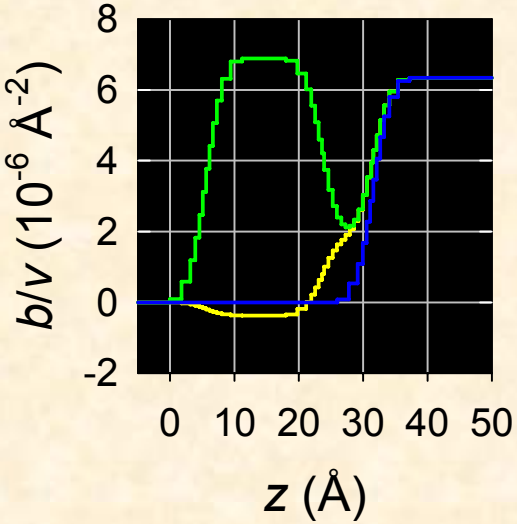
Langmuir film – DPPC / H_2O



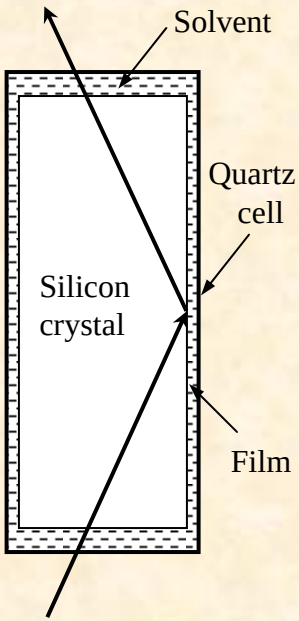


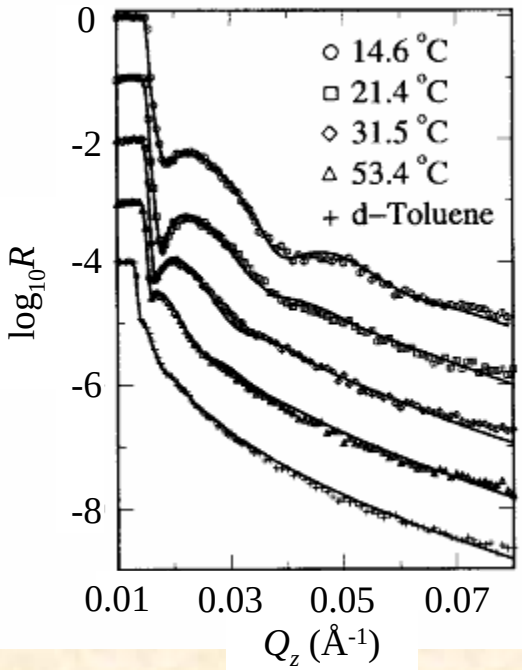
Langmuir film – DPPC / D_2O

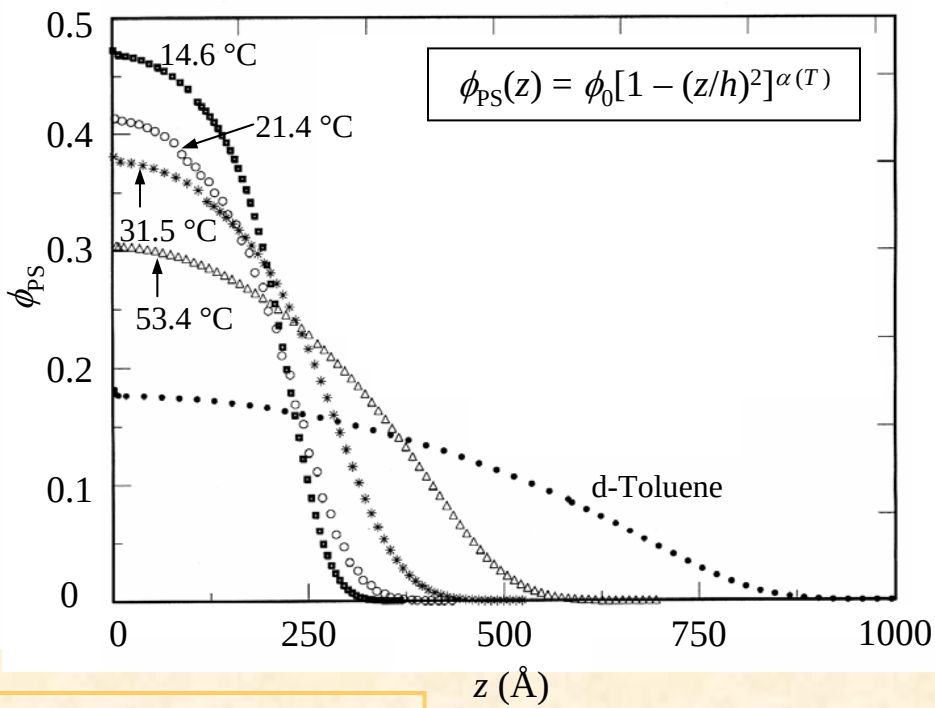




Neutrons weakly absorbed, so we can use exotic environments



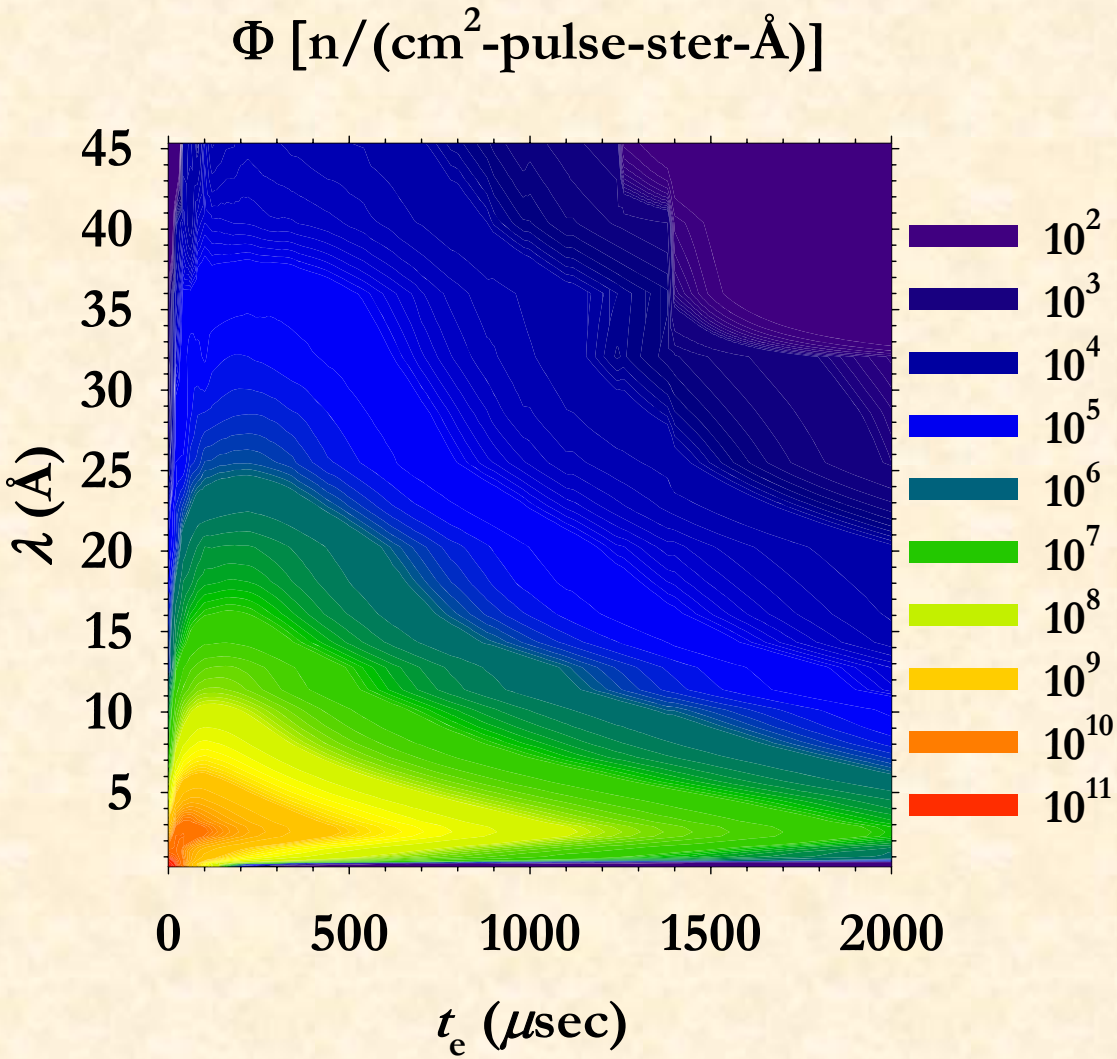




[Karim, et al., Phys. Rev. Lett. 73, 3407 (1994)]

II. Reflectometer, Deconstructed

Neutron source spectrum



<u>Characteristics</u>

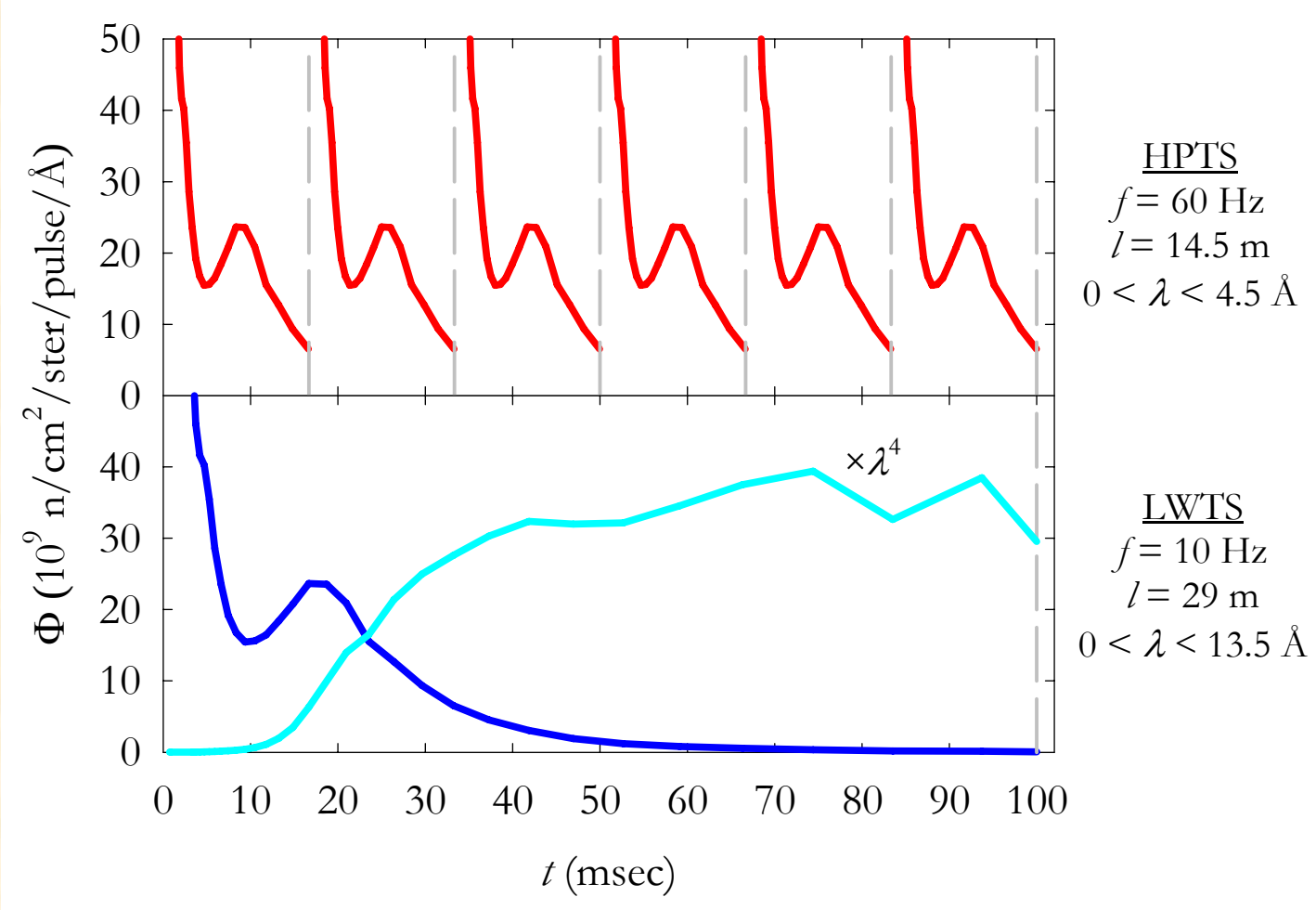
- 2 MW power level
- Coupled H_2 moderator
- Proton frequency 60 Hz

Neutrons emitted as gas, piped to instruments

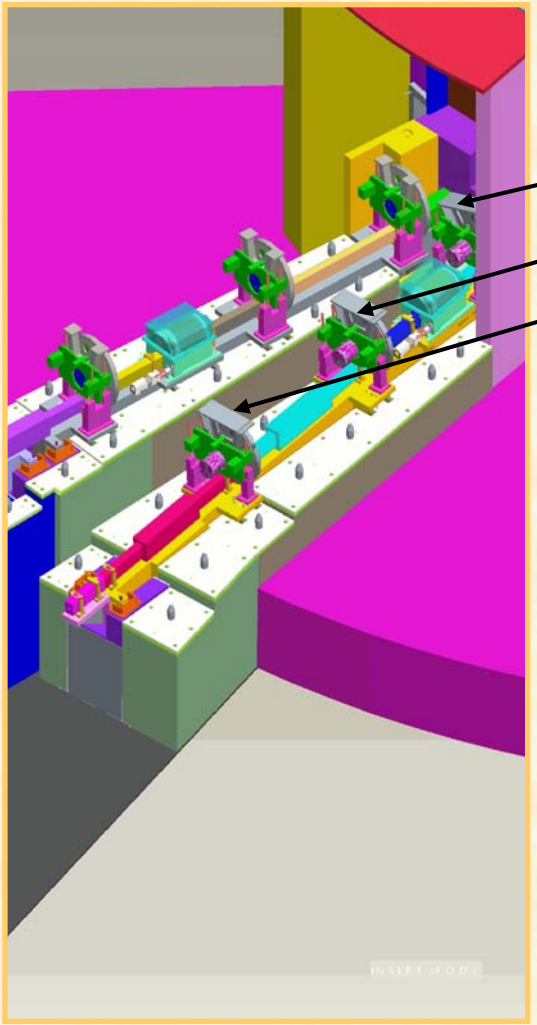
Time-of-flight

$t - t_e = (m_n/h)\, L\, \lambda$

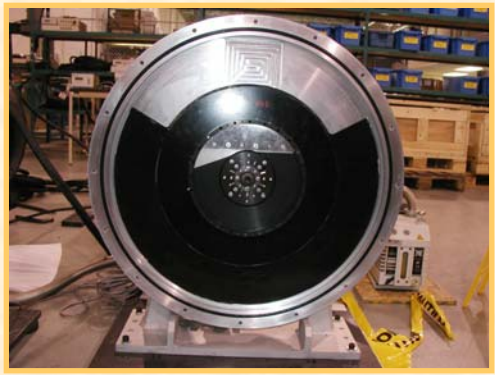
Bandwidth comparison

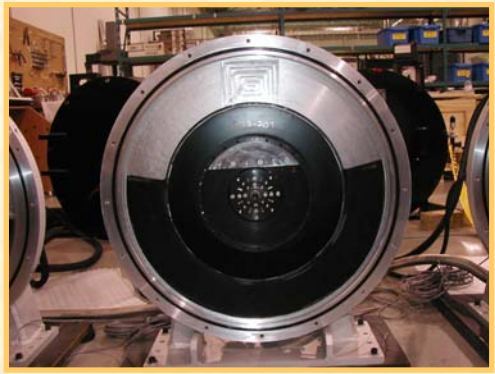


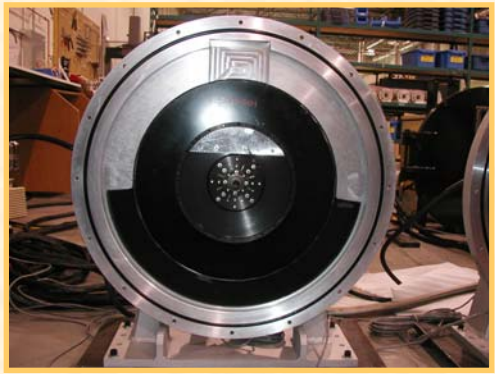
Bandwidth choppers



Choppers
1
2
3

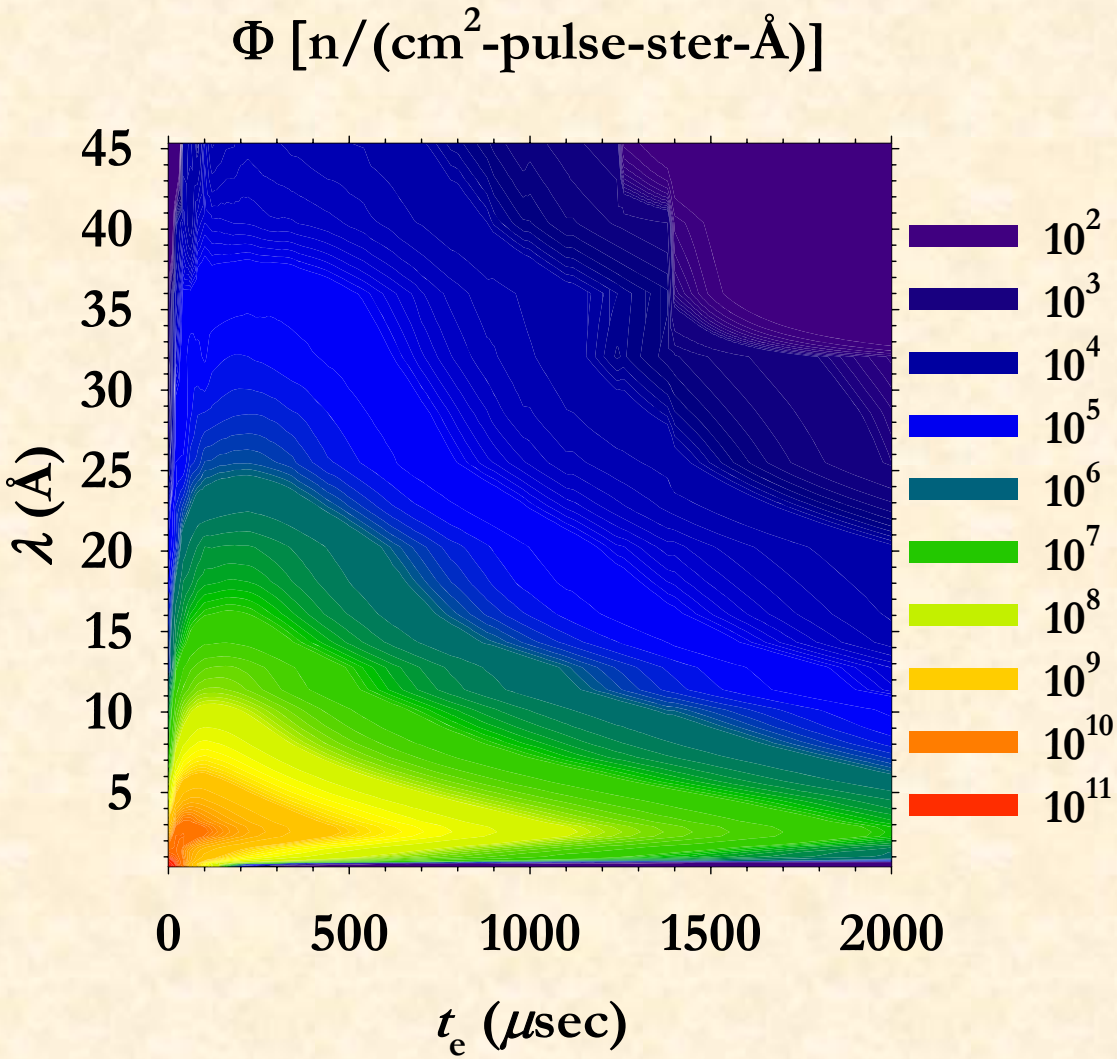






Installed

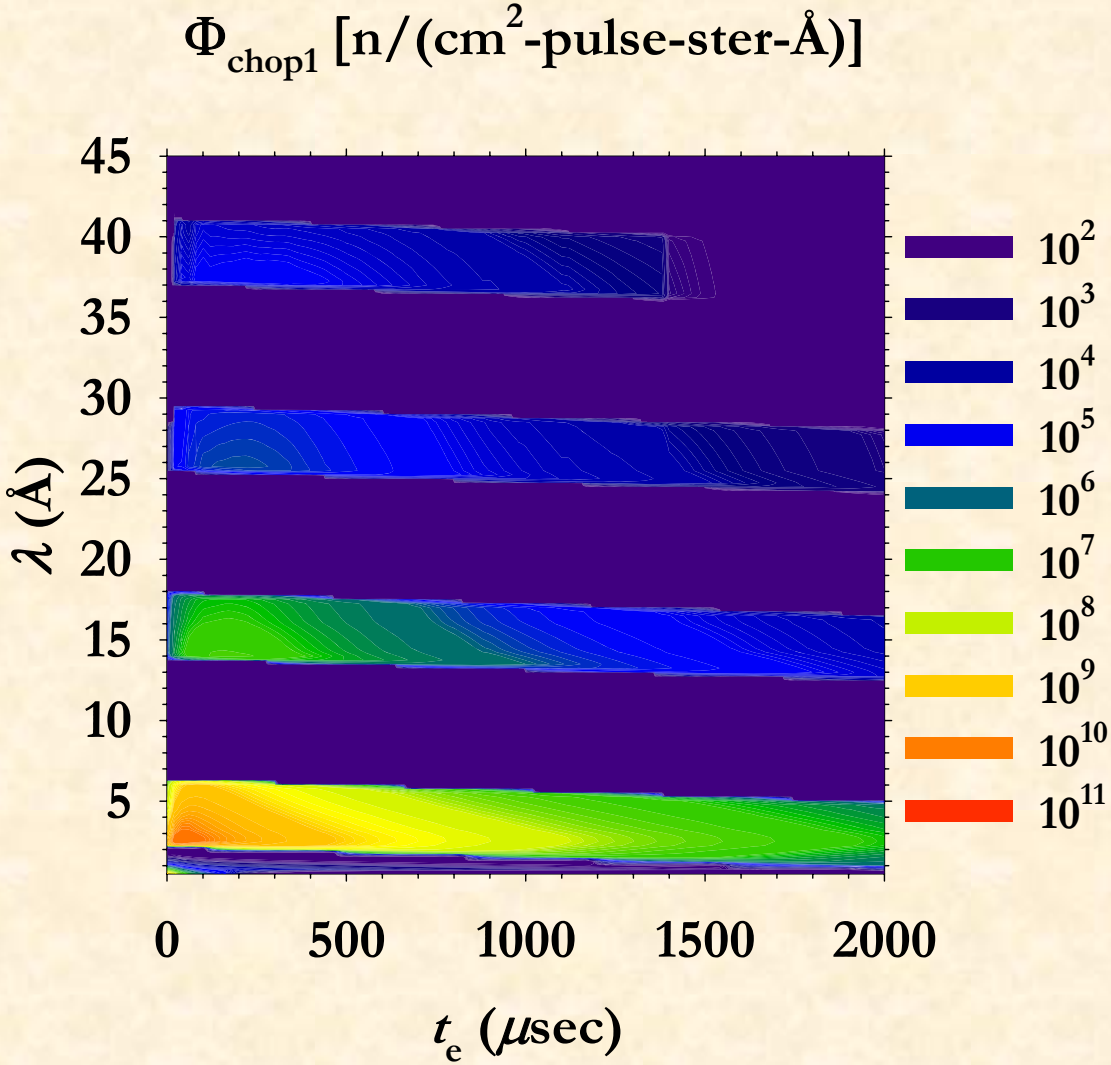
Function of bandwidth choppers



Characteristics

- 2 MW power level
- Coupled H_2 moderator
- Proton frequency 60 Hz
- No choppers

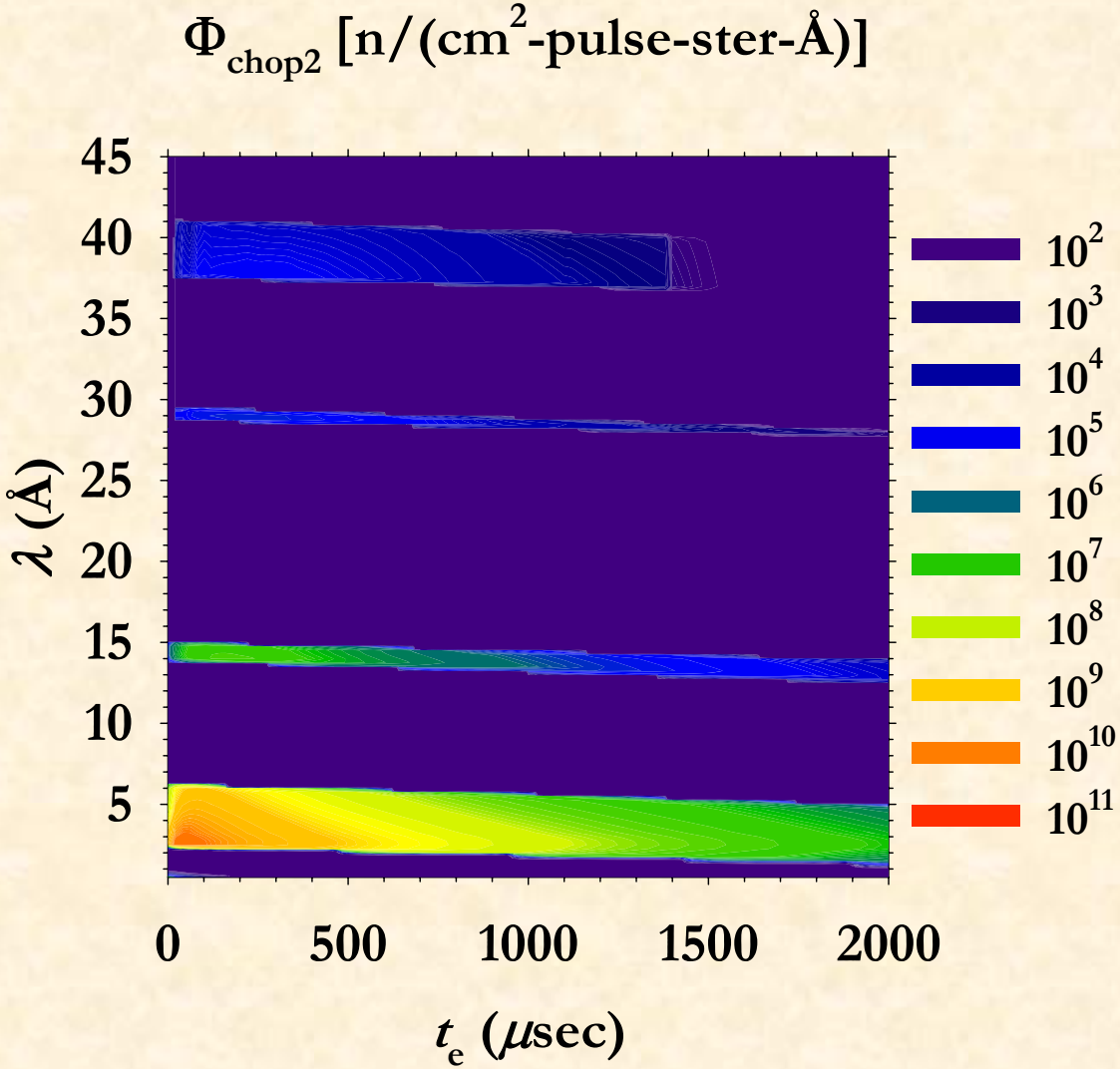
Function of bandwidth choppers



Characteristics

- 2 MW power level
- Coupled H_2 moderator
- Proton frequency 60 Hz
- Select 2.5 Å < λ < 6 Å
  - First chopper

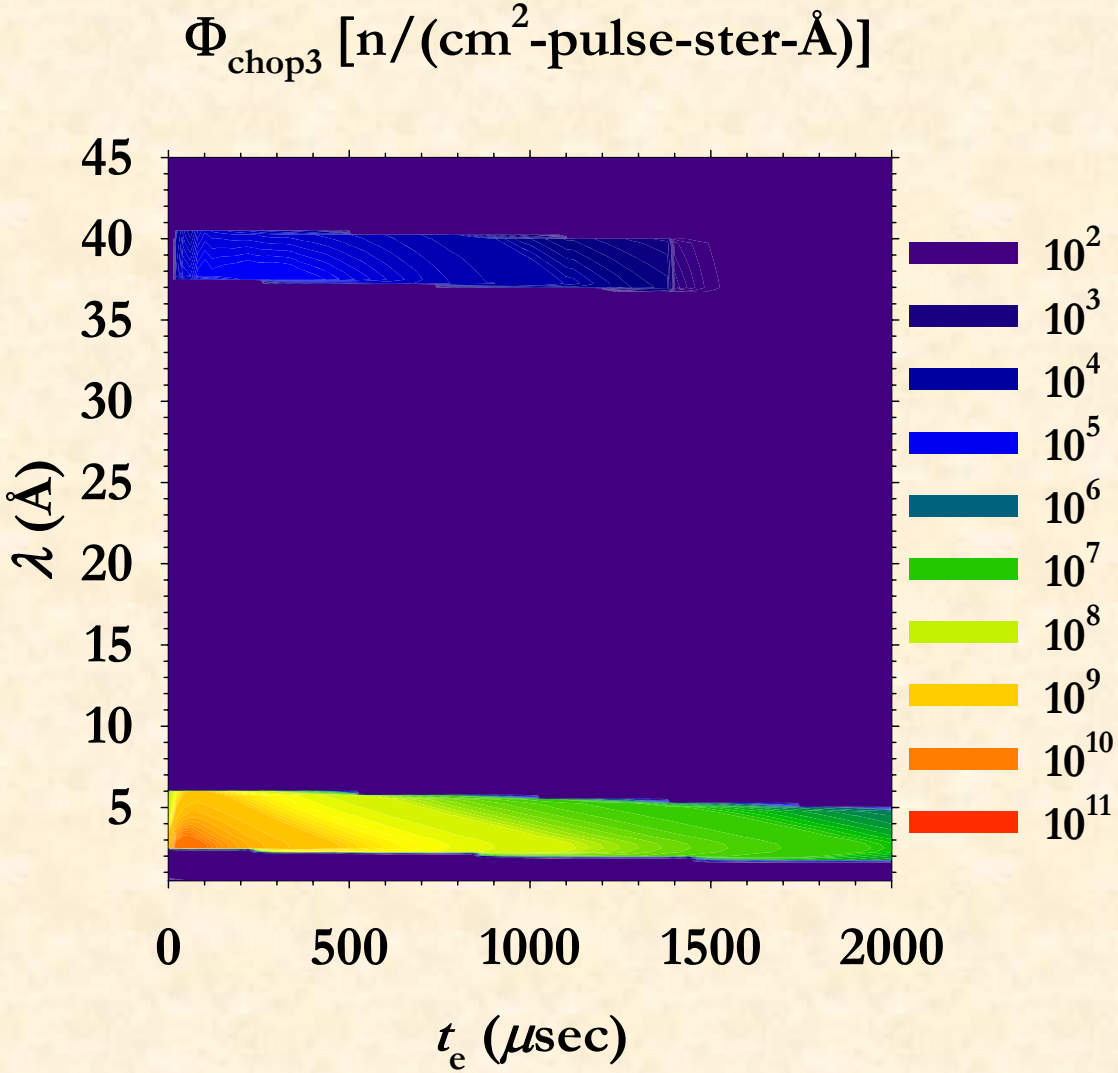
Function of bandwidth choppers



Characteristics

- 2 MW power level
- Coupled H_2 moderator
- Proton frequency 60 Hz
- Select 2.5 Å < λ < 6 Å
  - First chopper
  - Second chopper

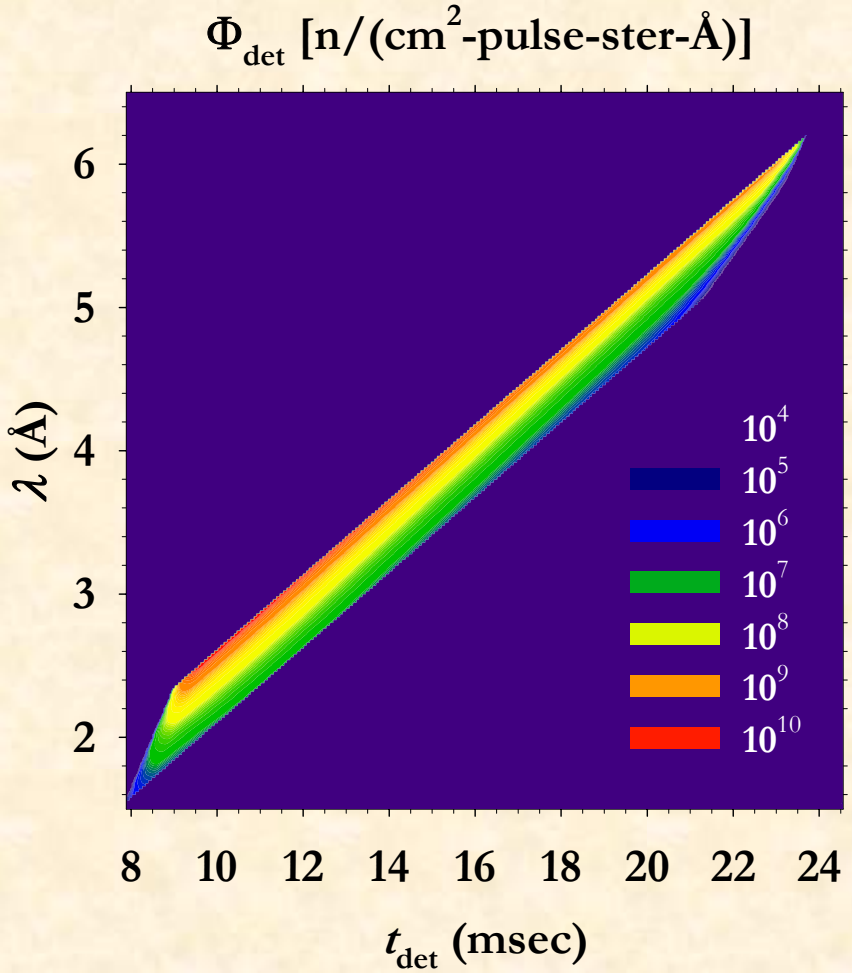
Function of bandwidth choppers



Characteristics

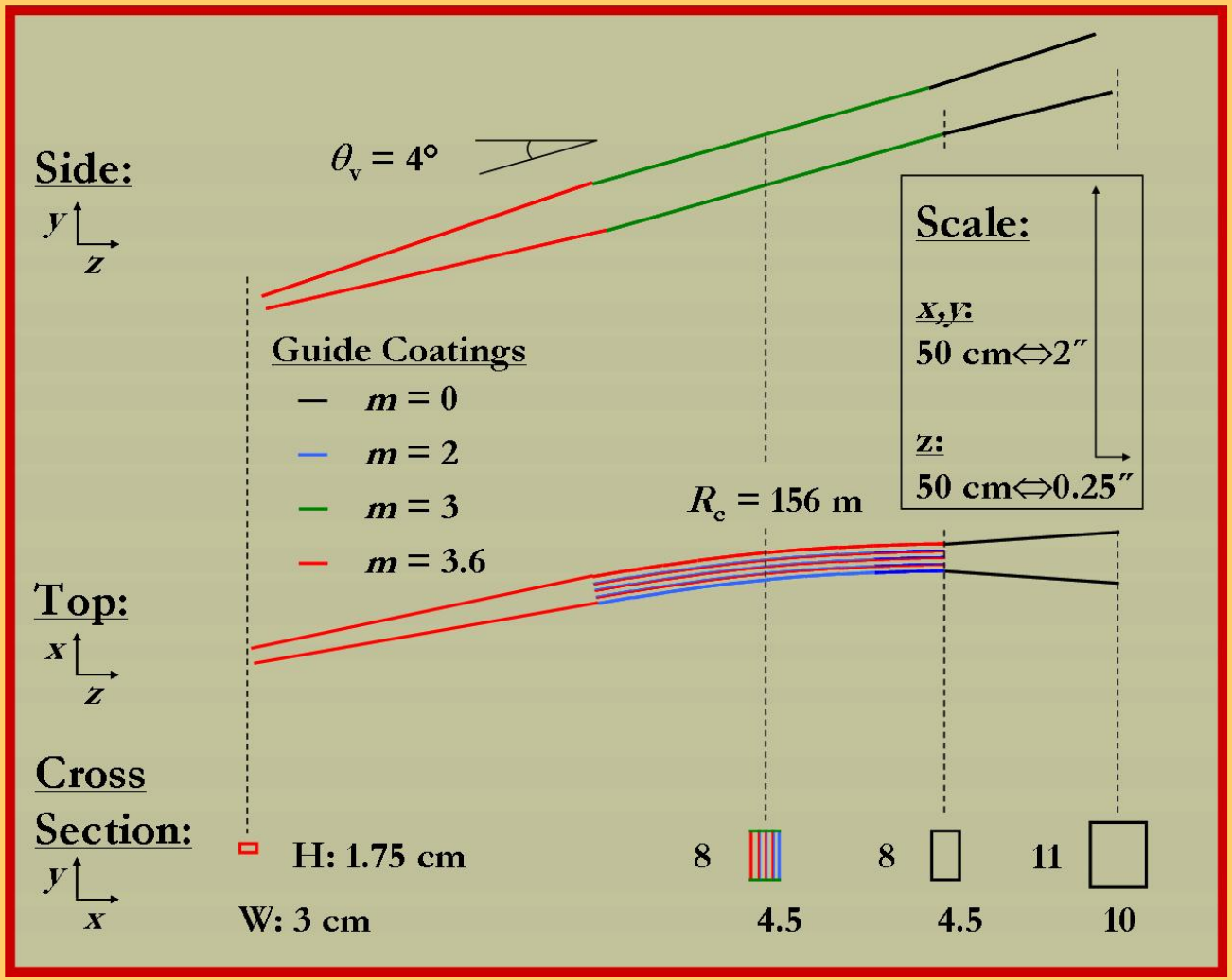
- 2 MW power level
- Coupled H_2 moderator
- Proton frequency 60 Hz
- Select 2.5 Å < λ < 6 Å
  - First chopper
  - Second chopper
  - Third chopper

Wavelength resolution

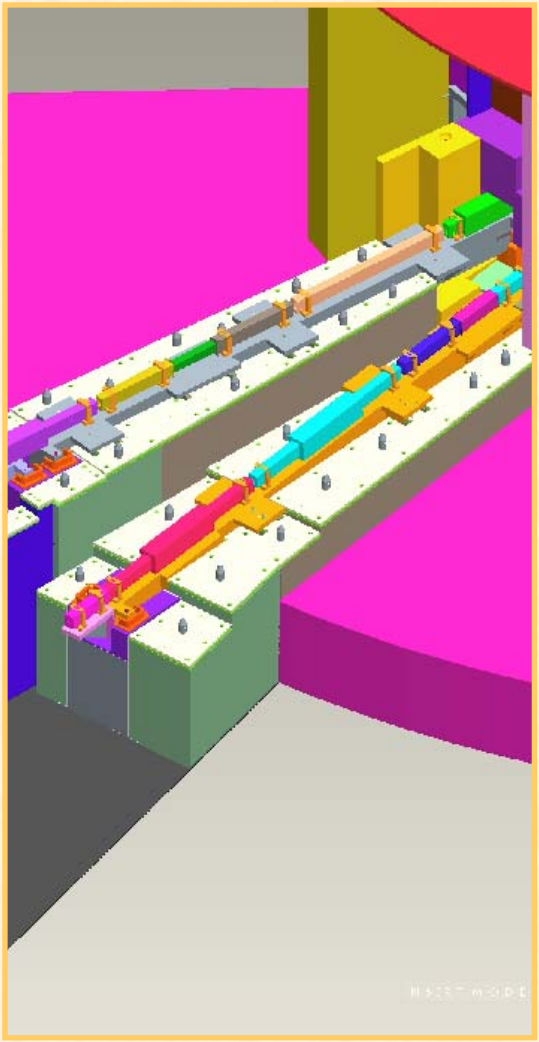


Emission-time distribution and chopper transmission determine wavelength resolution

Guides increase acceptance

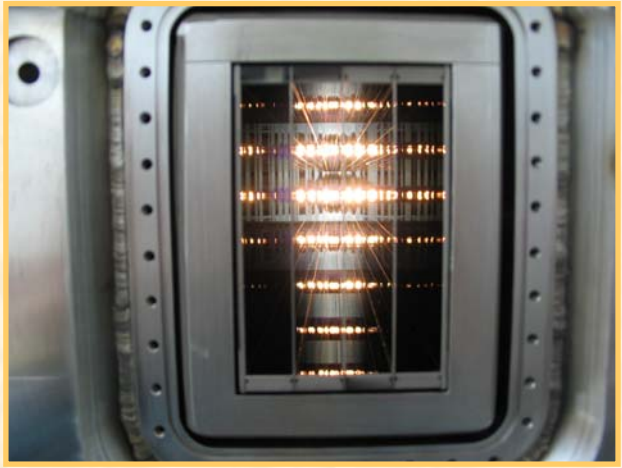


Guide built

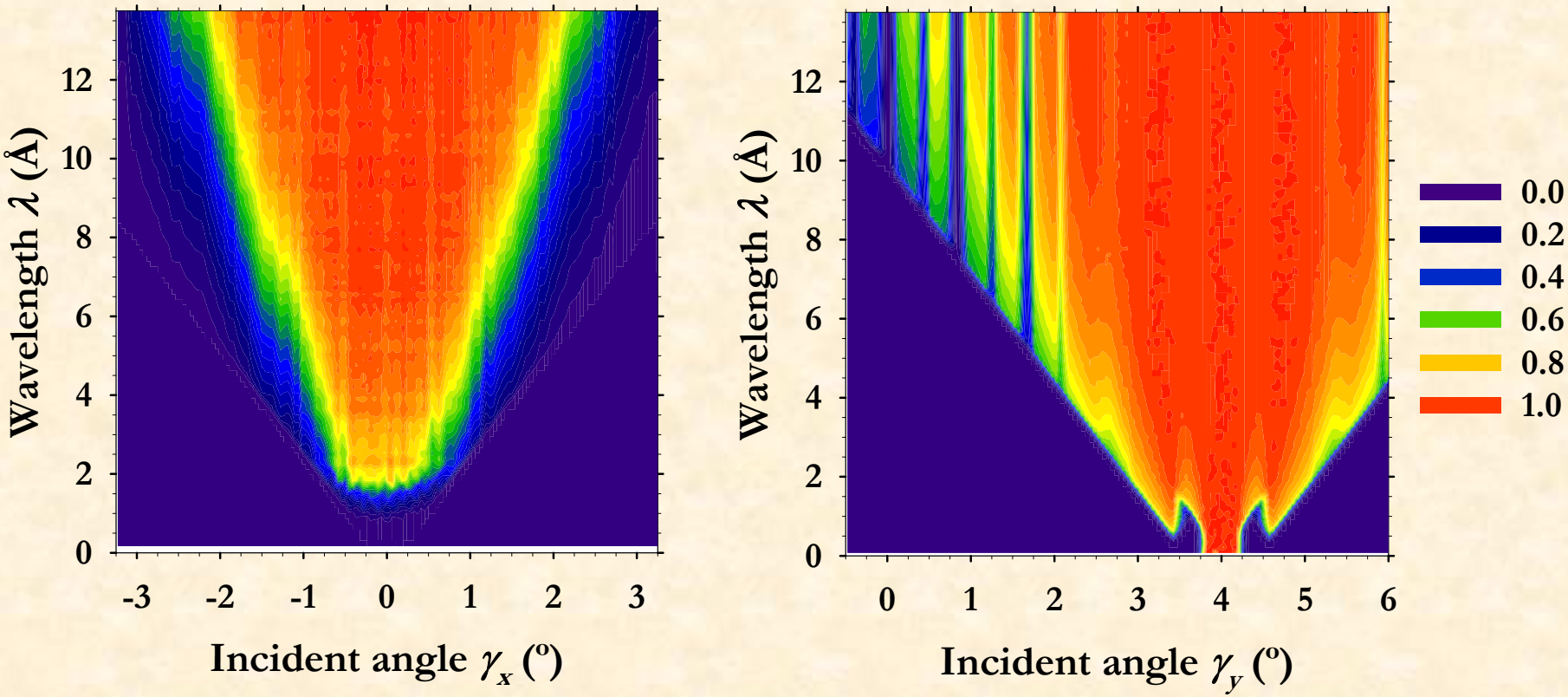


Installed

Four-channel bender



Simulated performance



[Calculations by J.F. Ankner and Ch. Rehm]

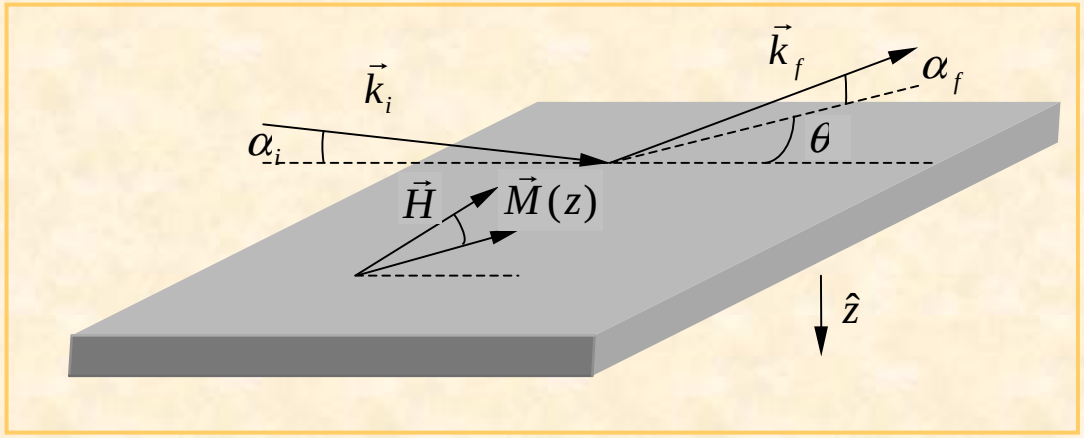
Neutron guide

Design Criteria

- Bender eliminates fast neutrons (λ < 2 Å)
- Beam centerline points down 4° below horizontal
- Vertical guide taper produces a "fire hose" effect to provide 0 < γ_v < 5.5° of angular divergence for liquid-surface measurements
- Horizontal angular divergence of ±0.75° available over 2 Å < λ < 15 Å
- Steel shielding intimately in contact with thin glass over entire guide length to reduce streaming

[Purchased from Swiss Neutronics]

Access all reflection geometries



Specular: $Q = 4\pi \sin\alpha / \lambda$

Specular

$\alpha_i = \alpha_f$

$\theta = 0$

Off-Specular

$\alpha_i \neq \alpha_f$

$\theta = 0$

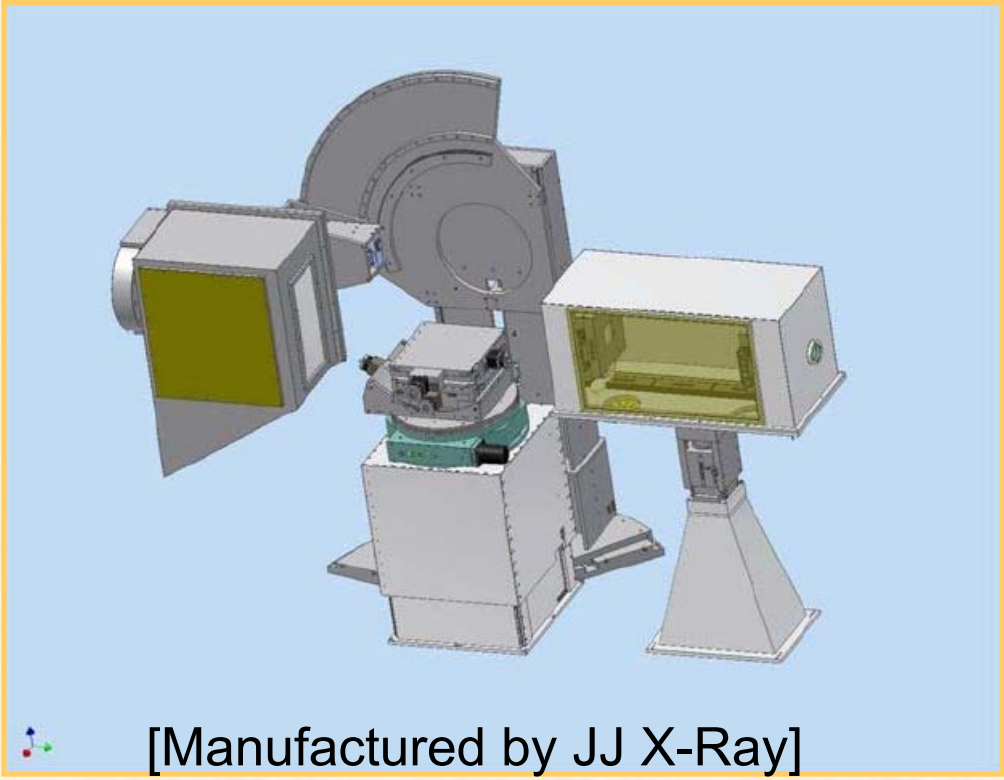
GISANS

$\alpha_i \neq \alpha_f$

$\alpha_i , \alpha_f < \alpha_c$

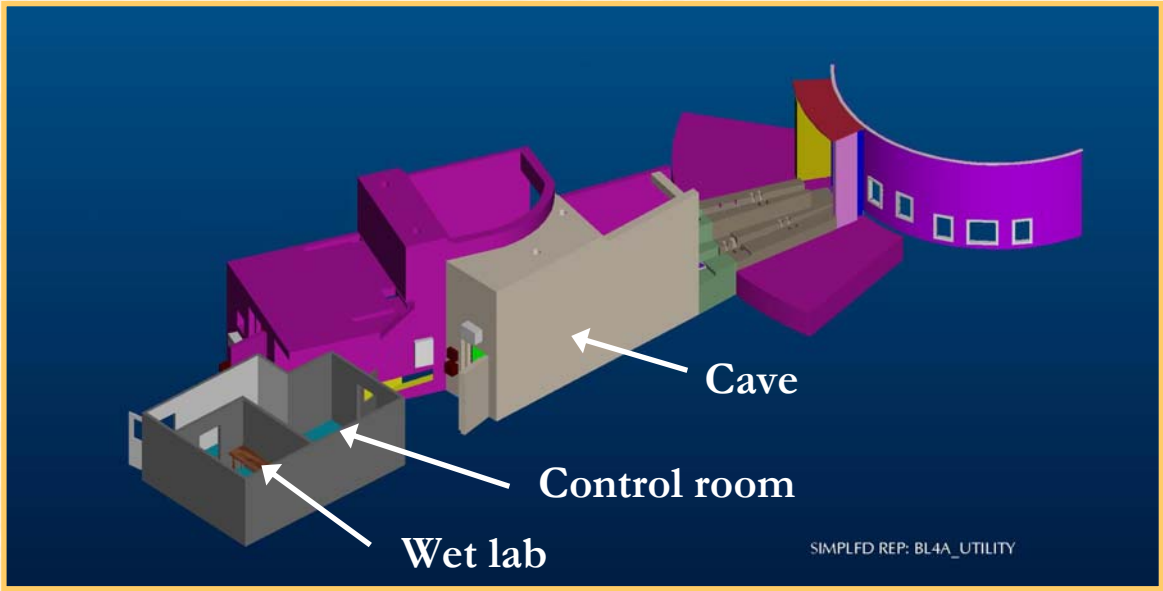
$\theta \neq 0$

Goniostat



$$0 \le \alpha_{liquid} \le 5.5°$$
$$0 \le 2\alpha \le 90°$$
$$0 \le 2\theta \le 30°$$

Instrument infrastructure

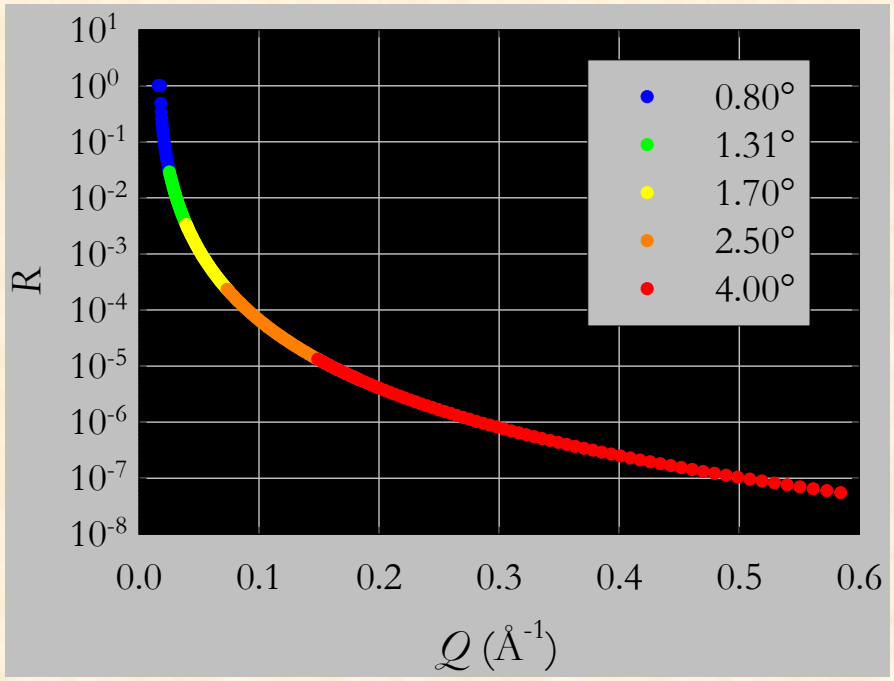


Inside wet lab

Inside control room

III. Performance and Challenges

Performance for liquid surface

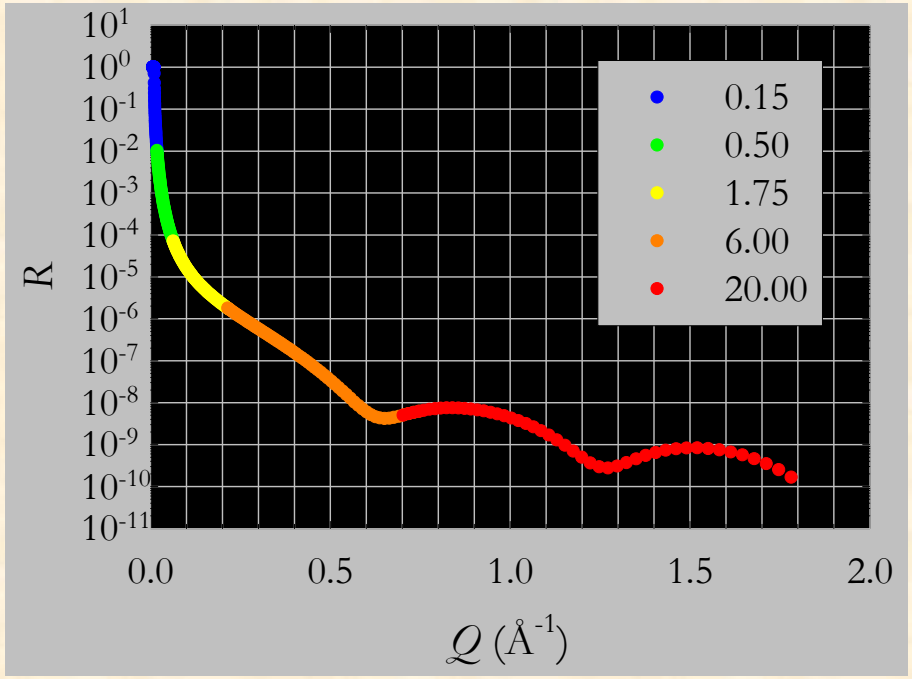


D_2O surface

θ (°)	t_{100} (sec)	Σt_{100} (sec)
0.80	0.4	0.4
1.31	0.4	0.8
1.70	0.9	1.7
2.50	4.8	6.5
4.00	282.9	290.4

$Q = 4\pi \sin\alpha / \lambda$

Performance for solid surface



10 Å SiO_2/Si

θ (°)	t_{100} (sec)	Σt_{100} (sec)
0.15	2	2
0.50	22	24
1.75	76	100
6.00	1960	2060
20.00	4062	6022

$$Q = 4\pi \sin\alpha / \lambda$$

Software challenges

1. Develop/adapt direct methods
2. Process piece-wise data
3. Efficiently model parametric data
4. Improve ties to molecular dynamics, micro-magnetic modeling, etc.
5. Simulate the instrument to fit the data
6. Model off-specular data

Milestones

- Construction complete: June 2006
- First neutrons: July 2006
- First users: November 2006
- Start of general user program: Spring 2007

Credit

This instrument is a product of the labor of many people, primary contributors being

- **Tim Chae, Lead Engineer**
- **Roger Kellogg, Lead Engineer**
- **Tammy McHargue, Scientific Associate**
- **Rick Goyette, Scientific Associate**
- **Rob Connatser, Installation Coordinator**
- **Frank Klose, Instrument Scientist**
- **Andre Parizzi, Engineer**
- **Steve Proffitt, Engineer**
- **Peter Rosenblad, Engineer**
- **George Rennich, Engineer**
- **Several Dozen Other Dedicated Folks**

Tim Chae