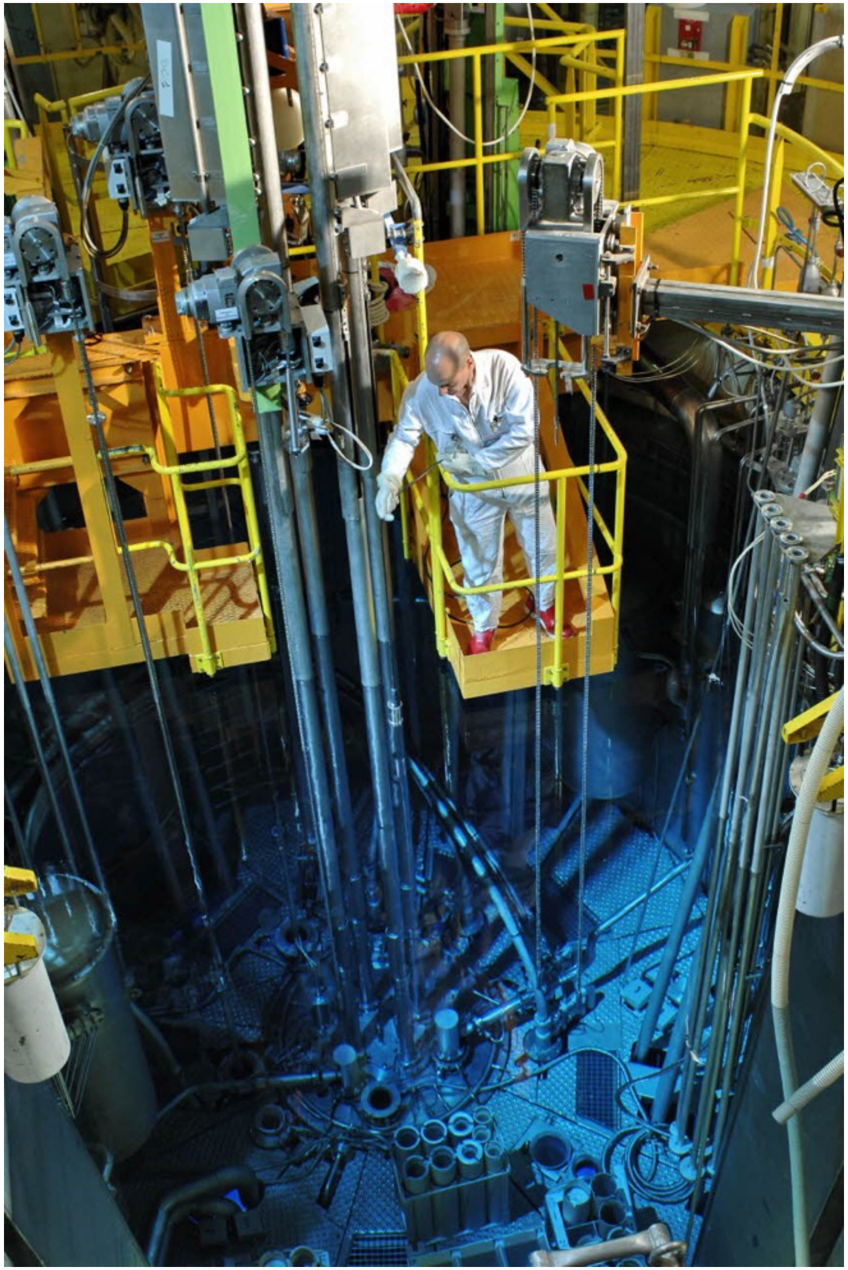
Neutron Resonance Spin Echo at the LLB.
Utility of transverse NRSE for quasi elastic scattering?

S. Longeville,
Laboratoire Léon Brillouin (LLB)
CEA-Saclay
France

Orphée reactor : 14 MW D_20 moderated reactor



Neutron Spin-Echo Spectroscopy at Saclay

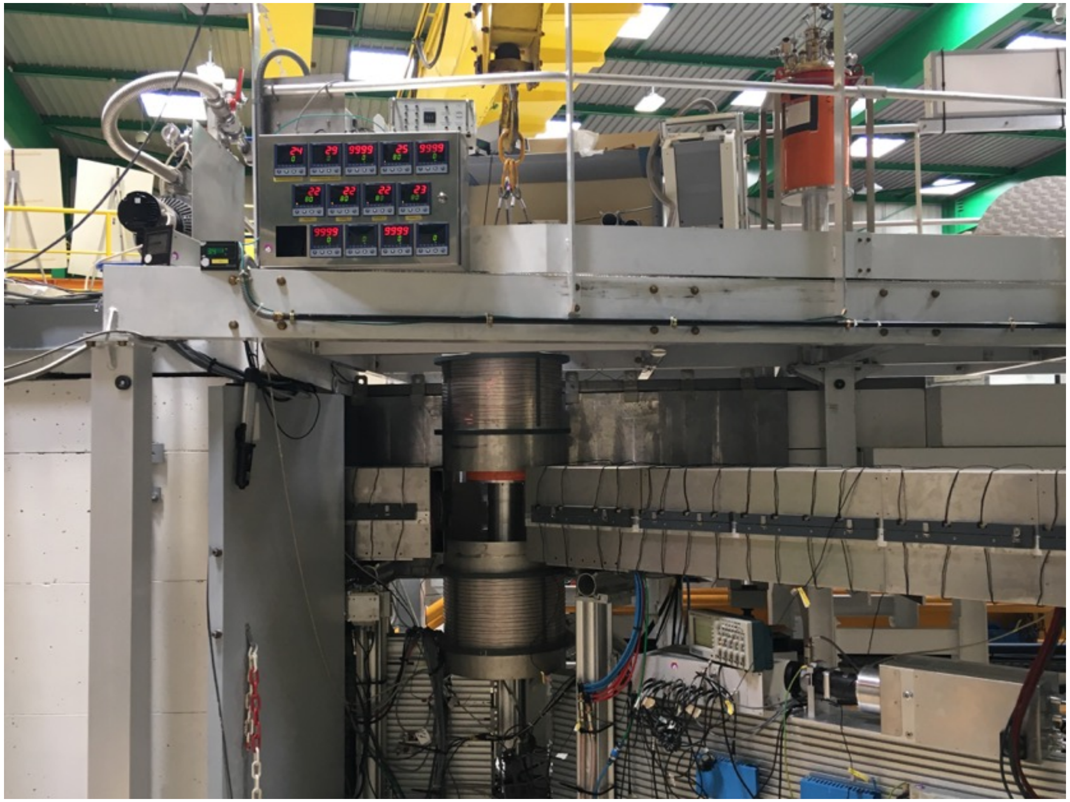
Mess : « Mezei » type

† 2005

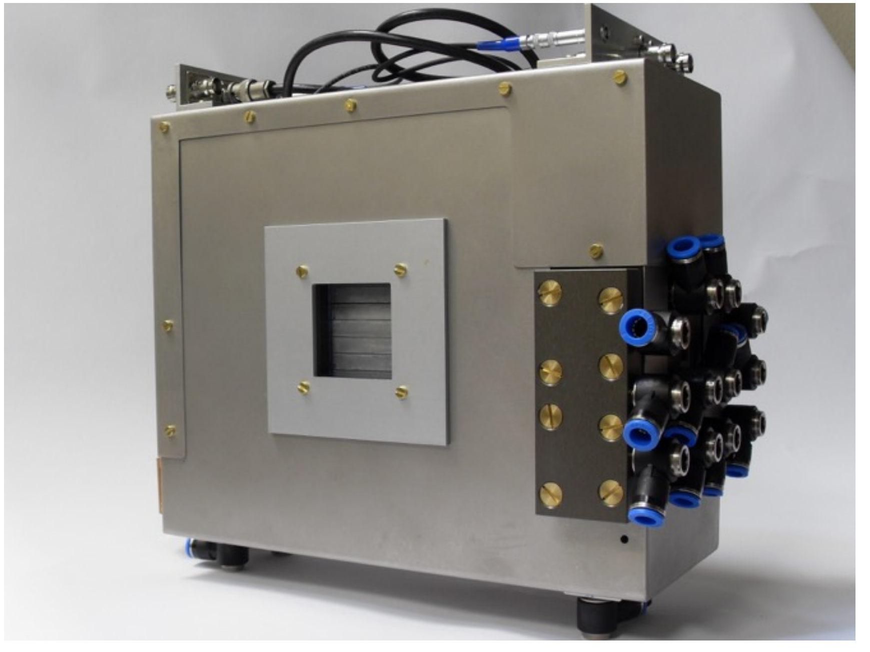
Neutron Spin-Echo Spectroscopy at Saclay

Mess : « Mezei » type

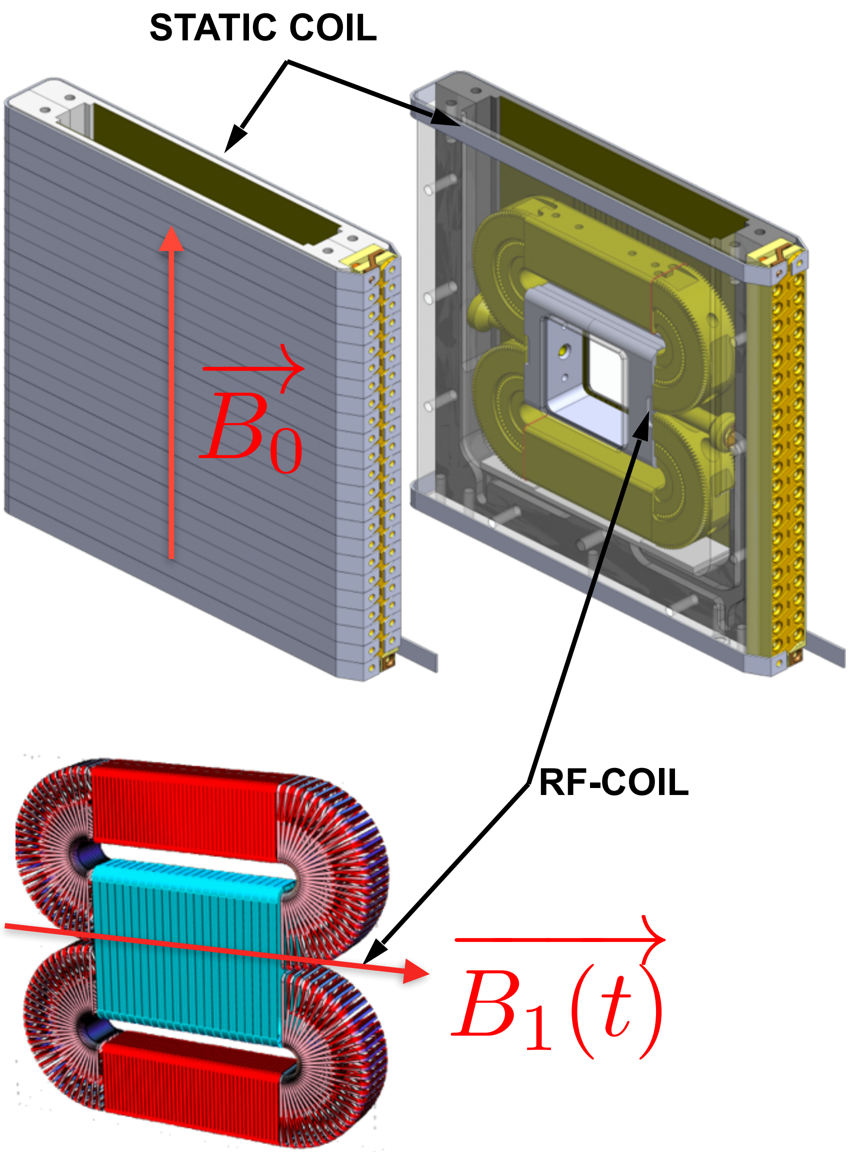
G1bis (Muses) Neutron Resonance Spin Echo

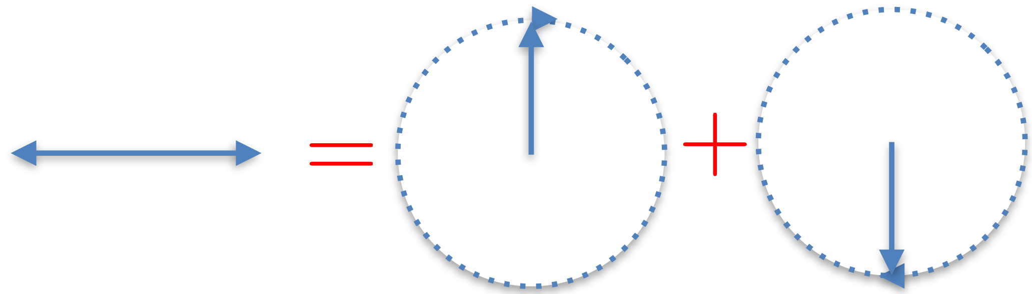


Resonance method for quasi-elastic scattering ?



courtesy : S. Klimko





$$\overrightarrow{B_1(t)} = \overrightarrow{B_1^{\alpha}(t)} + \overrightarrow{B_1^{\beta}(t)}$$

$\overrightarrow{B_0}$ spin precession counter clockwise

$\gamma_n < 0$

if $\overrightarrow{B_1^{\alpha}(t)}$ is in the direction of rotation then

$\overrightarrow{B_1^{\beta}(t)}$ is in the opposite direction

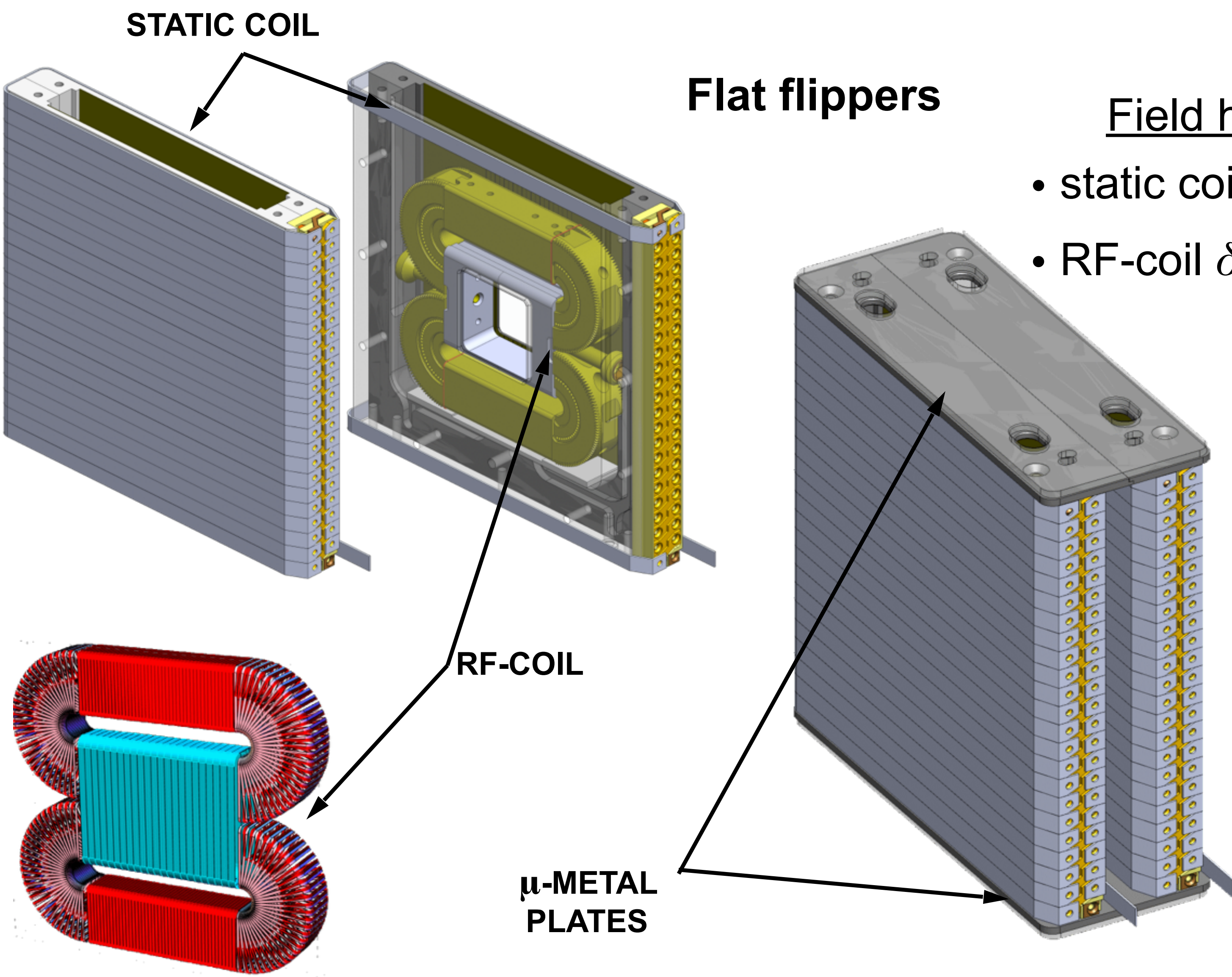
$$\|\overrightarrow{B_0}\| >> \|\overrightarrow{B_1(t)}\|$$

~~$\overrightarrow{B_1^{\beta}(t)}$~~ Not short times

Bloch-Siegert shift

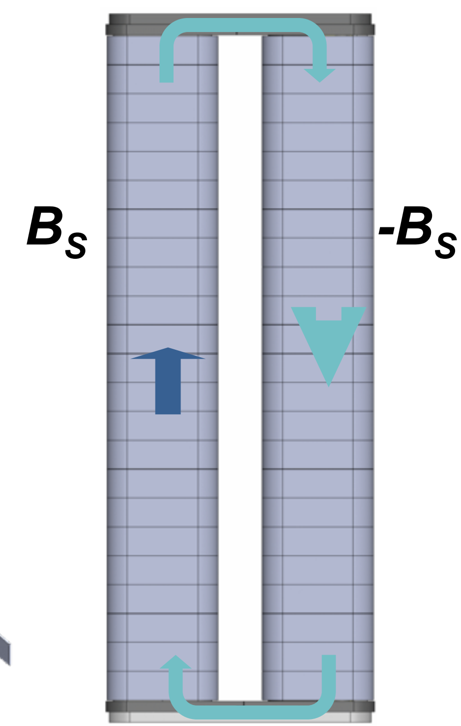
New Flat Resonance Flippers (1rst Arm)

Flat flippers

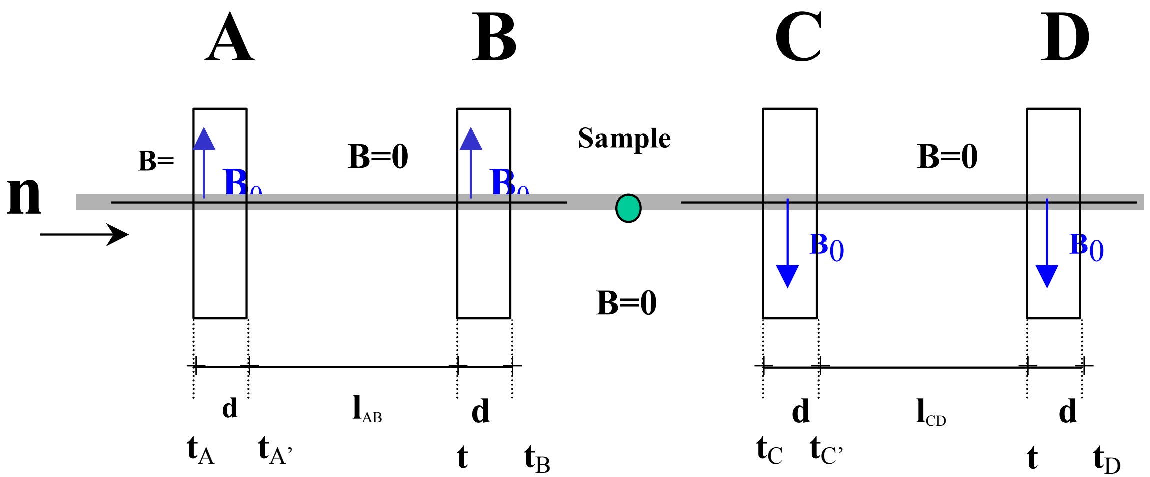


<u>Field homogeneity:</u>

- static coil $\delta B_S/B_S \sim 10^{-3}$
- RF-coil $\delta B_{RF}/B_{RF} \sim 10^{-2}$



NRSE spectrometer



1

Table 1. Spin orientation

	Time t	Phase field B_r	neutron Spin phase S
A	t_A	ωt_A	0
A'	$t_{A'} = t_A + \frac{d}{v}$	$\omega t_{A'}$	$2\omega t_A + \omega \frac{d}{v}$
B	$t_B = t_A + \frac{l_{AB}+d}{v}$	ωt_B	$2\omega t_A + \omega \frac{d}{v}$
B'	$t_{B'} = t_A + \frac{l_{AB}+2d}{v}$	$\omega t_{B'}$	$2\omega \frac{l_{AB}+d}{v}$
C	t_C	$-\omega t_C$	$2\omega \frac{l_{AB}+d}{v}$
C'	$t_{C'} = t_C + \frac{d}{v}$	$-\omega t_{C'}$	$-\omega \frac{d}{v'} - 2\omega t_C - 2\omega \frac{l_{AB}+d}{v}$
D	$t_D = t_C + \frac{l_{CD}+d}{v'}$	$-\omega t_D$	$-\omega \frac{d}{v'} - 2\omega t_C - 2\omega \frac{l_{AB}+d}{v}$
D'	$t_{D'} = t_C + \frac{l_{CD}+2d}{v'}$	$-\omega t_{D'}$	$2\omega(\frac{l_{AB}+d}{v} - \frac{l_{CD}+d}{v'})$

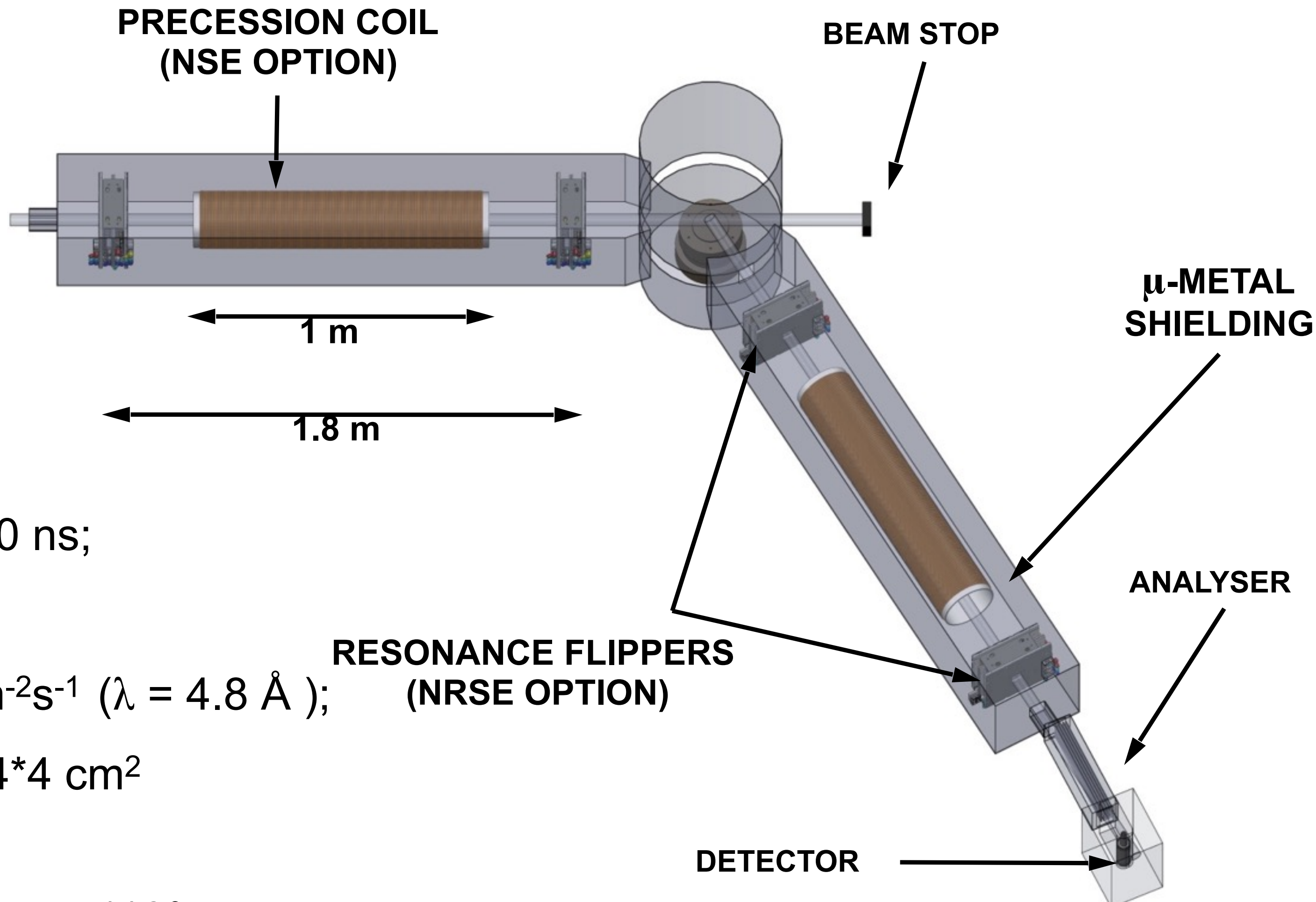
Echo condition NRSE $\frac{L_{AB}}{v} = \frac{L_{CD}}{v'}$

NSE $\frac{\int B_0 dl}{v} = \frac{\int B_1 dl}{v'}$

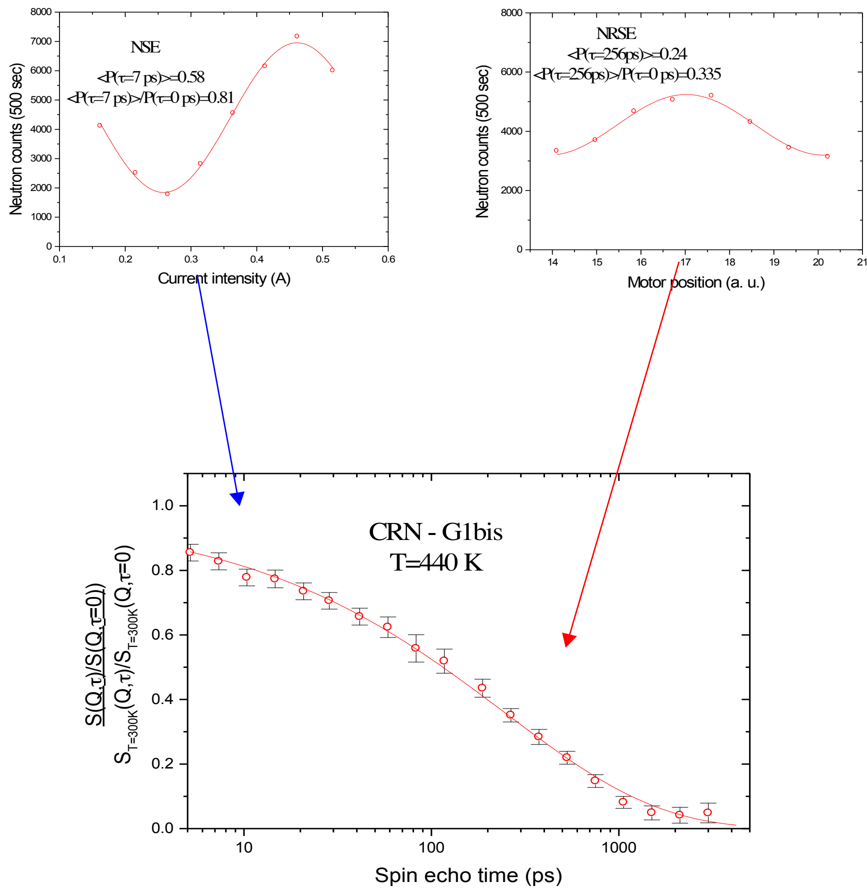
$$\langle P \rangle \cong \int_0^\infty I(\lambda) \int_{-\infty}^\infty S(Q,\omega) \cos(\omega \tau_{NRSE}) d\omega d\lambda$$

$$\tau_{NRSE} = 2\omega_f \frac{l+d}{2\pi} \frac{m^2}{h^2} \lambda^3$$

MUSES (G1bis) - mixed NSE / NRSE



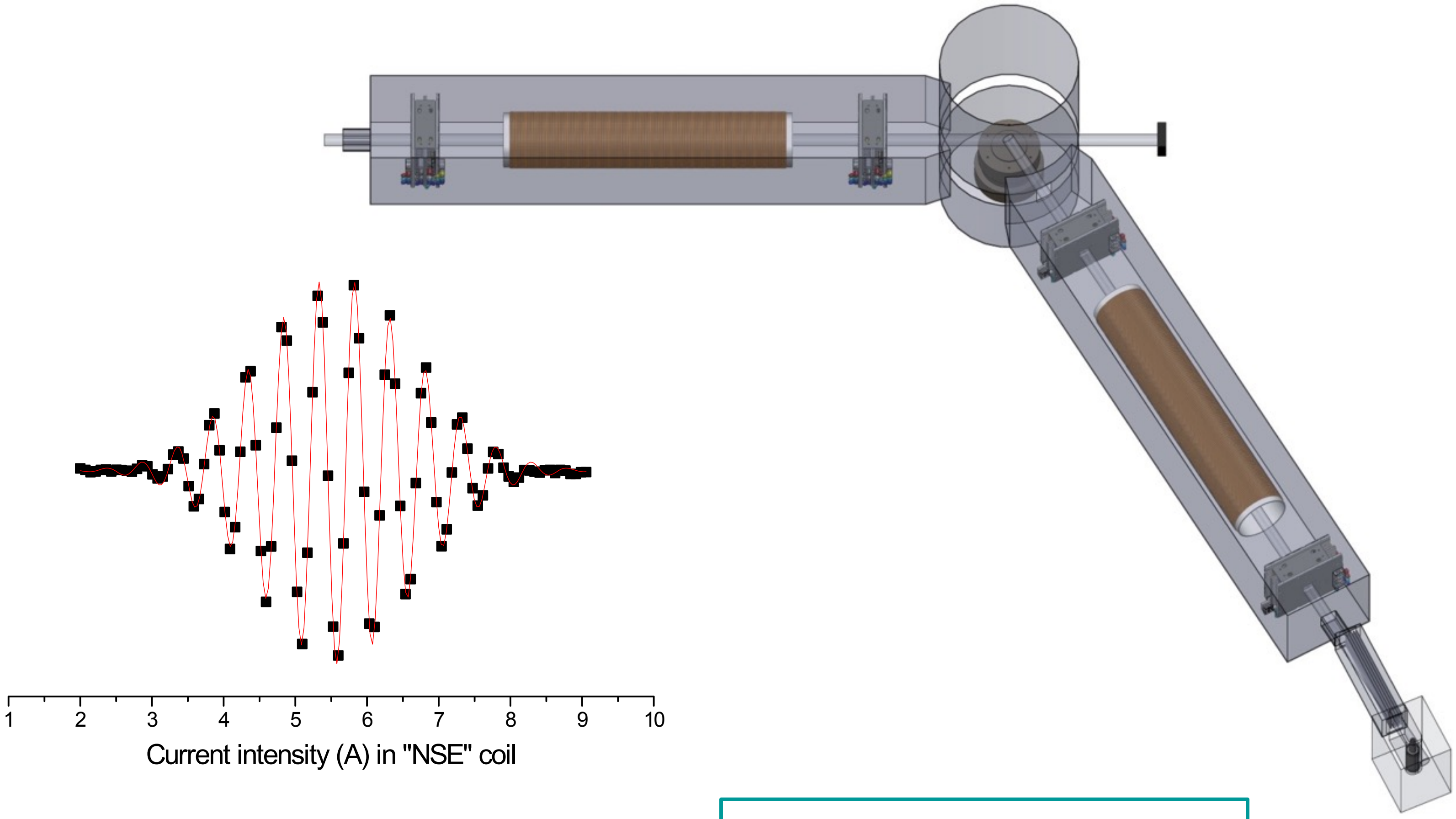
- τ_{NSE} : 0.2 ps - 20 ns;
- $\Delta\lambda/\lambda \approx 15\%$;
- $\Phi s = 2.10^{7}$ n $cm^{-2}s^{-1}$ (λ = 4.8 Å);
- beam section: 4*4 cm^2
- λ: 3.5 - 14 Å
- Scattering angle: 5 - 110°
- Q range: 0.05 - 4 $Å^{-1}$



NSE
<P(τ=7 ps)>=0.58
<P(τ=7 ps)>/P(τ=0 ps)=0.81
Neutron counts (500 sec)
Current intensity (A)
NRSE
<P(τ=256ps)>=0.24
<P(τ=256ps)>/P(τ=0 ps)=0.335
Neutron counts (500 sec)
Motor position (a. u.)
CRN - G1bis
T=440 K
S(Q,τ)/S(Q,τ=0))
S_T=300K(Q,τ)/S_T=300K(Q,τ=0)
Spin echo time (ps)

Neutron spin echo for quasi-elastic scattering

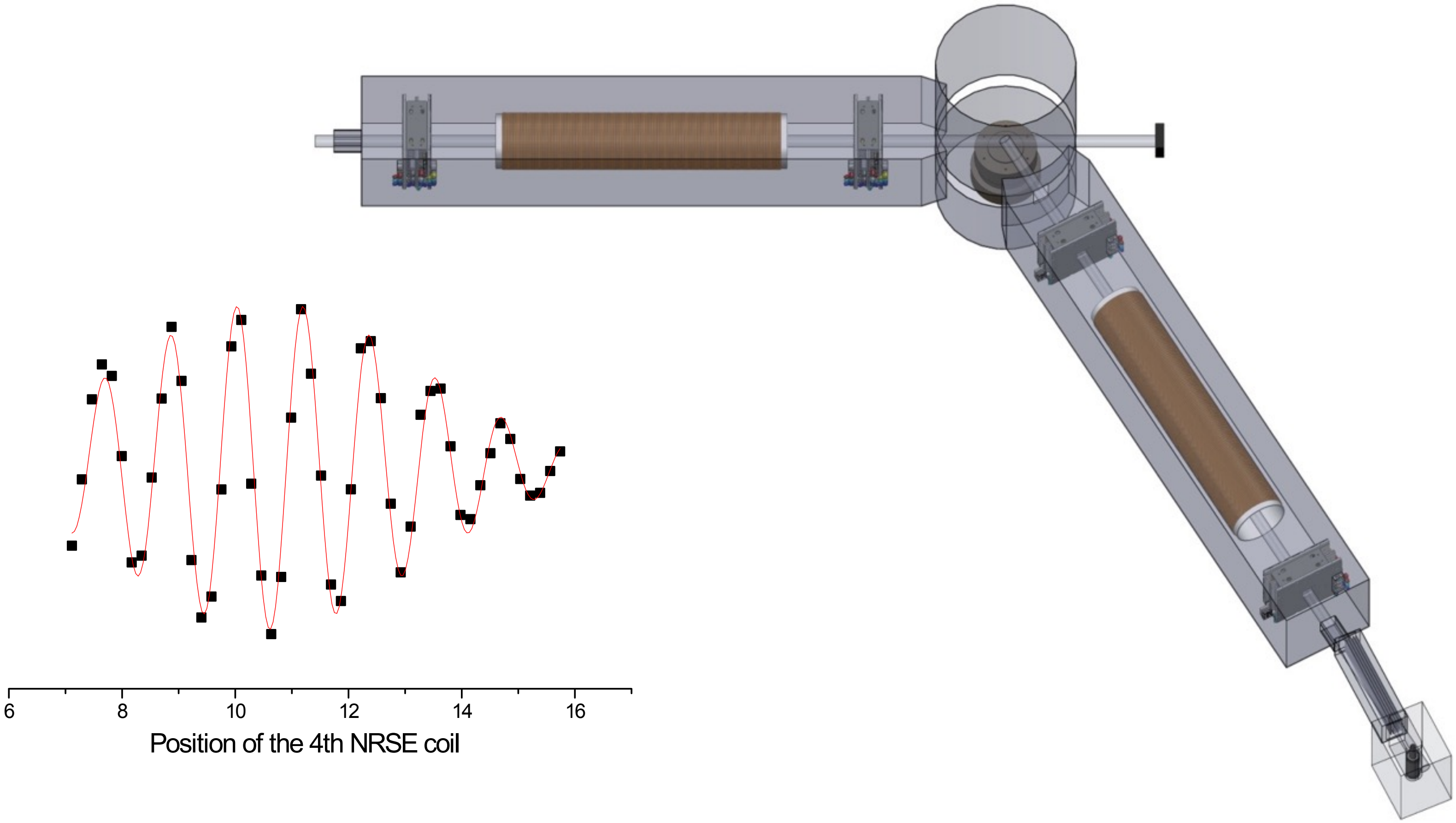
Small times –> NSE option !



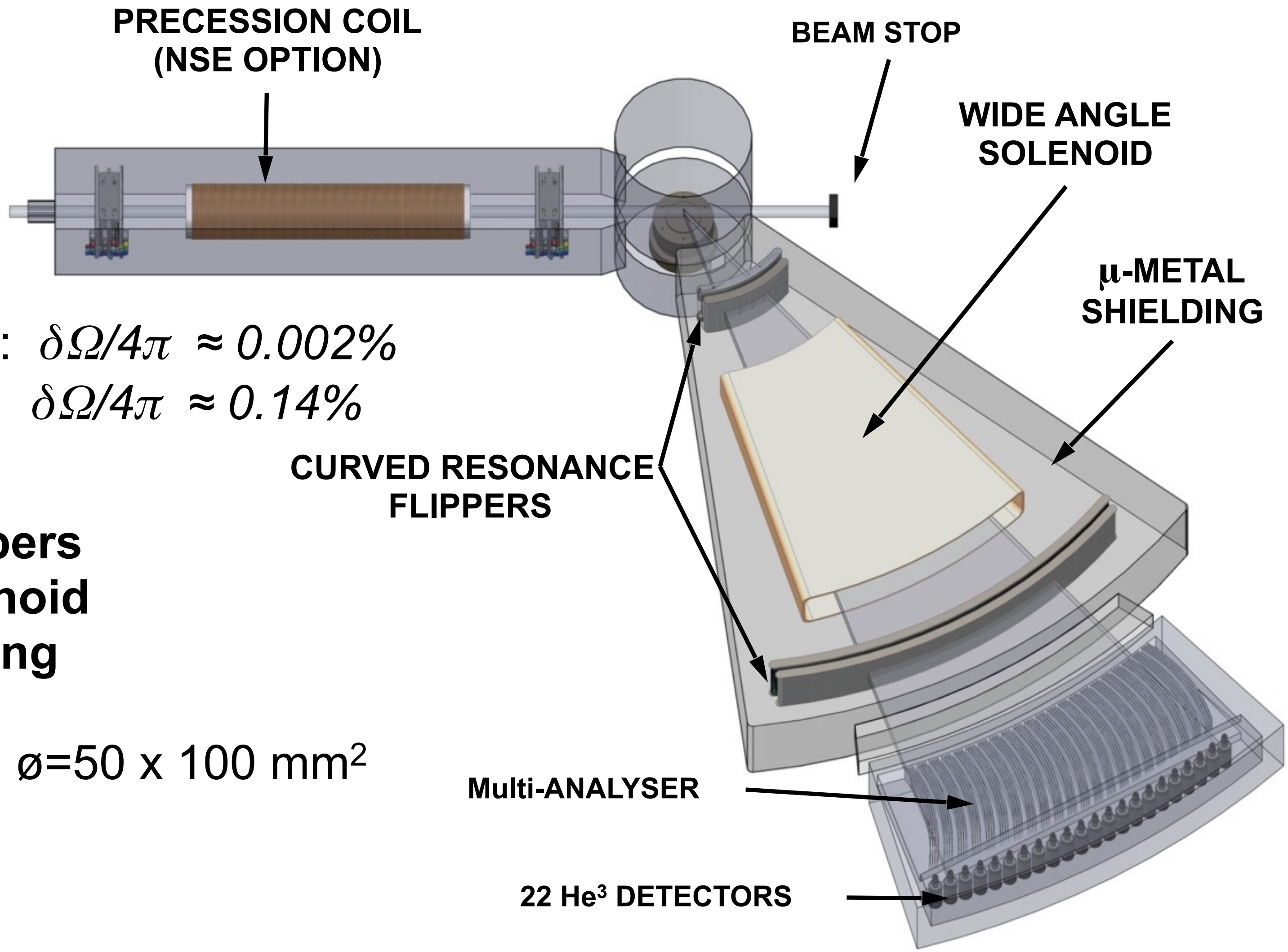
$$\int |B_1| dl = \int |B_2| dl$$

Neutron spin echo for quasi-elastic scattering

long times –> NRSE option !



Multi - MUSES



Single detector : $\delta\Omega/4\pi \approx 0.002\%$

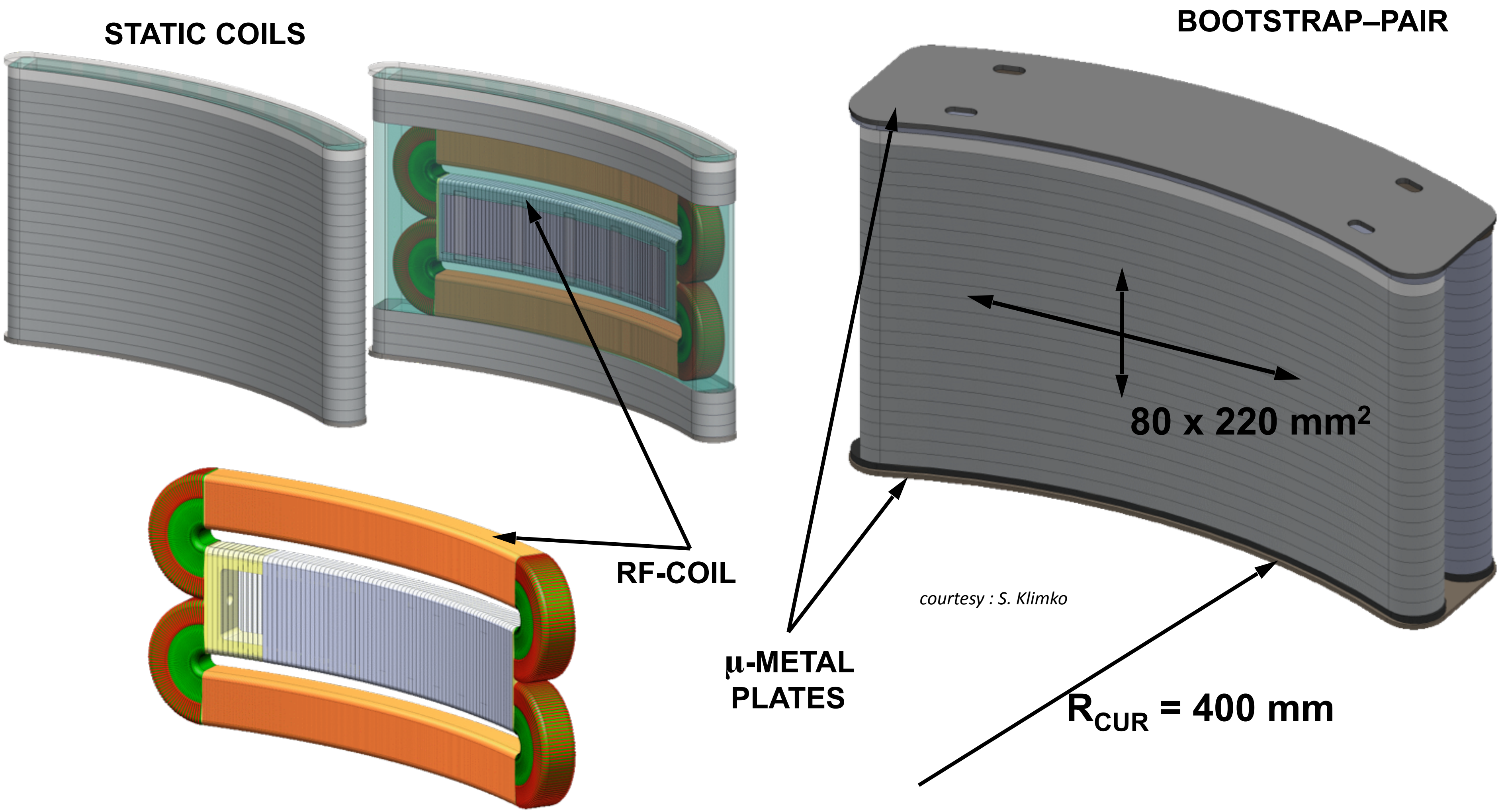
'Multi'- detector : $\delta\Omega/4\pi \approx 0.14\%$

- **Resonance flippers**
- **Wide angle solenoid**
- **Magnetic shielding**
- **Multi – Analyser**
- **22 He^3 detectors** ø=50 x 100 mm^2

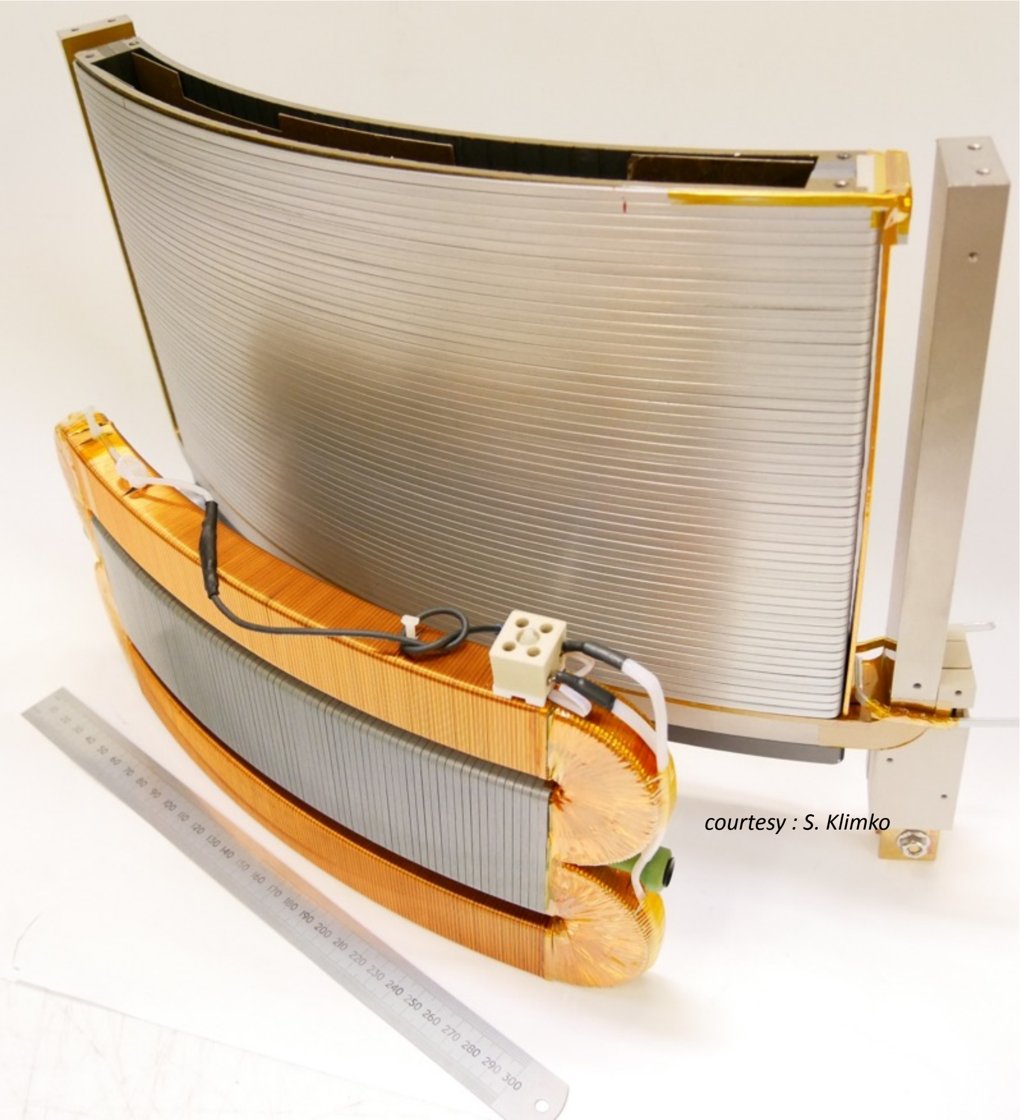
Orphée Laboratoire Léon Brillouin

Curved Resonance Flippers

Curved flippers

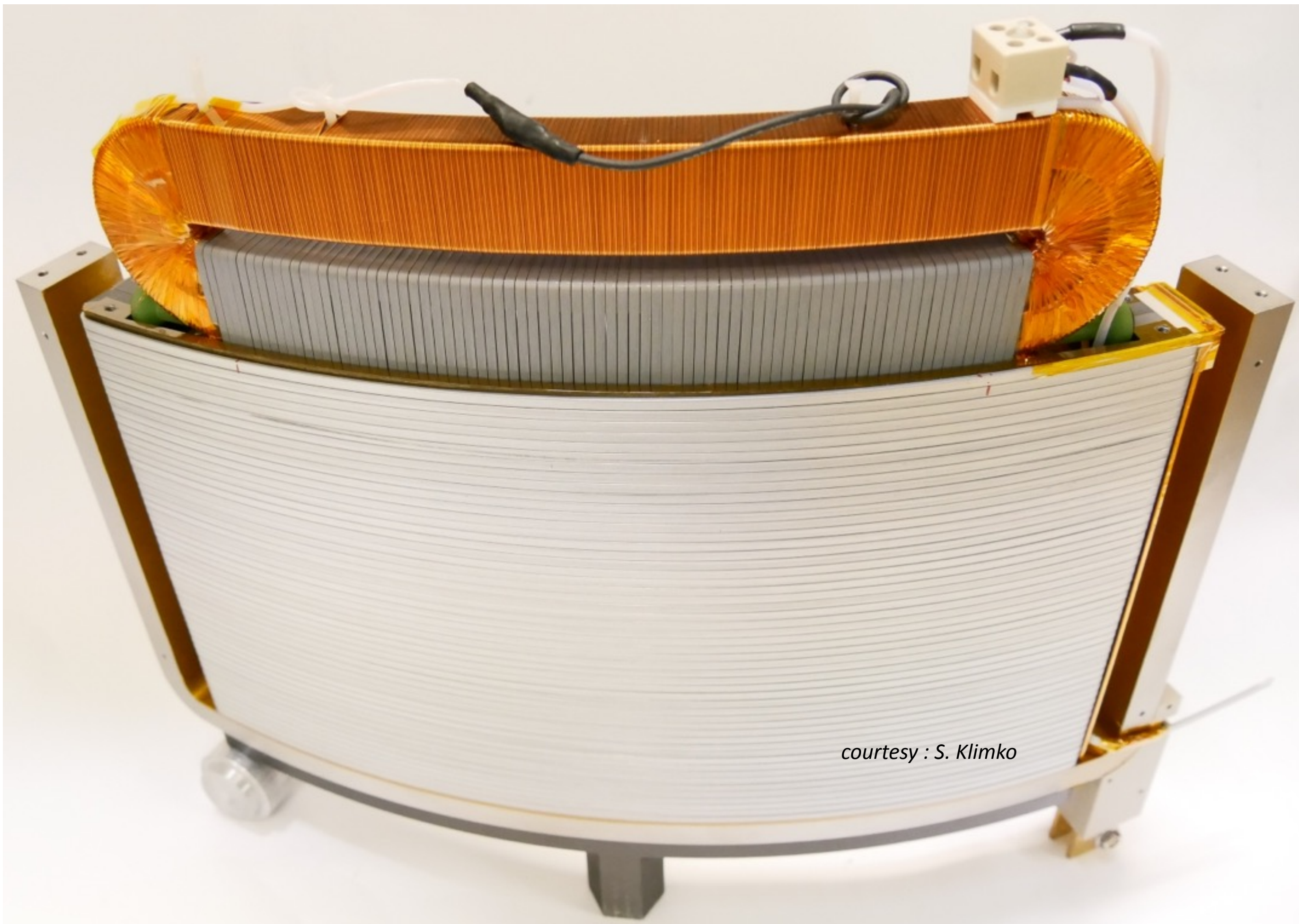


Curved Resonance Flippers

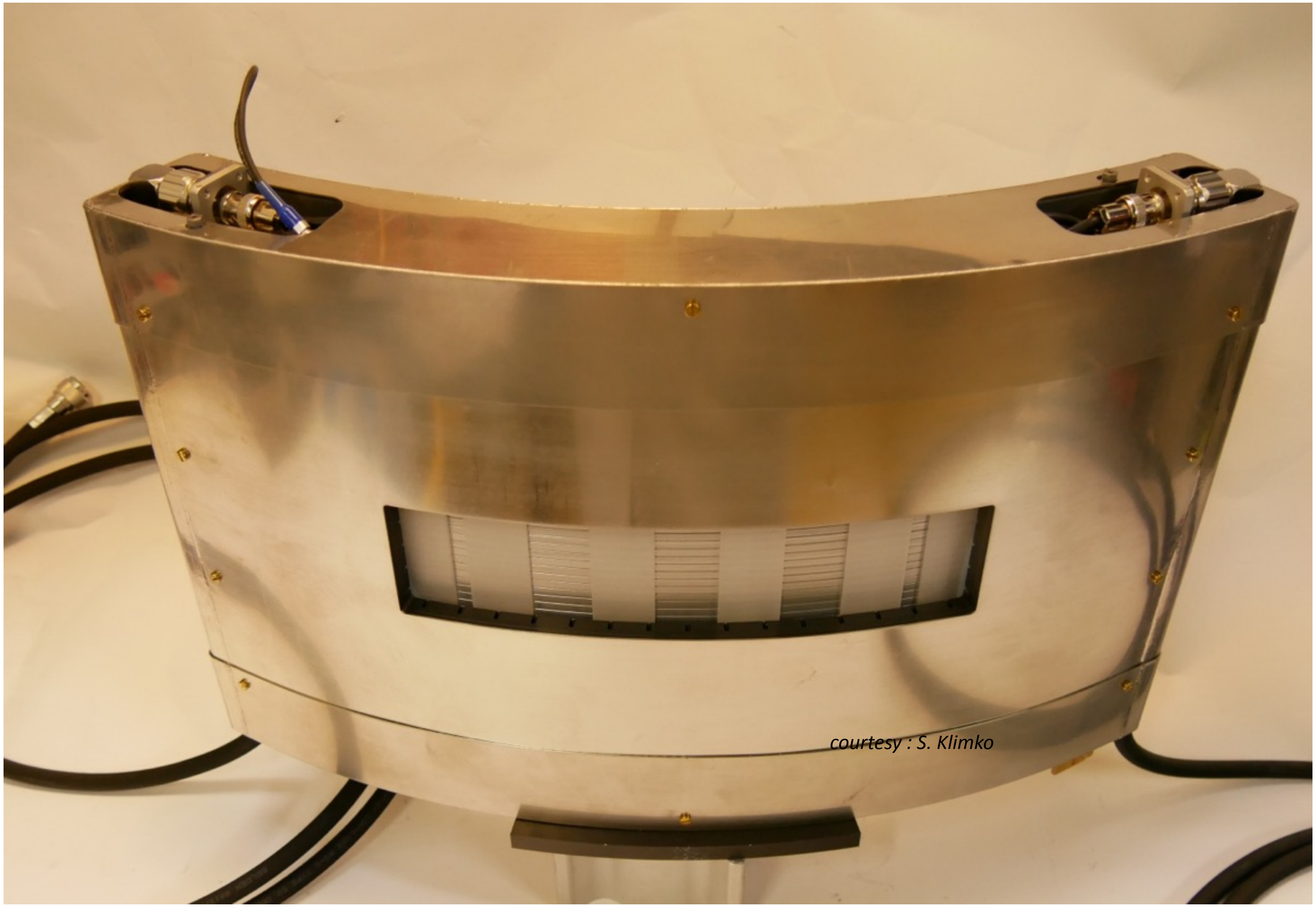


courtesy : S. Klimko

Curved Resonance Flippers

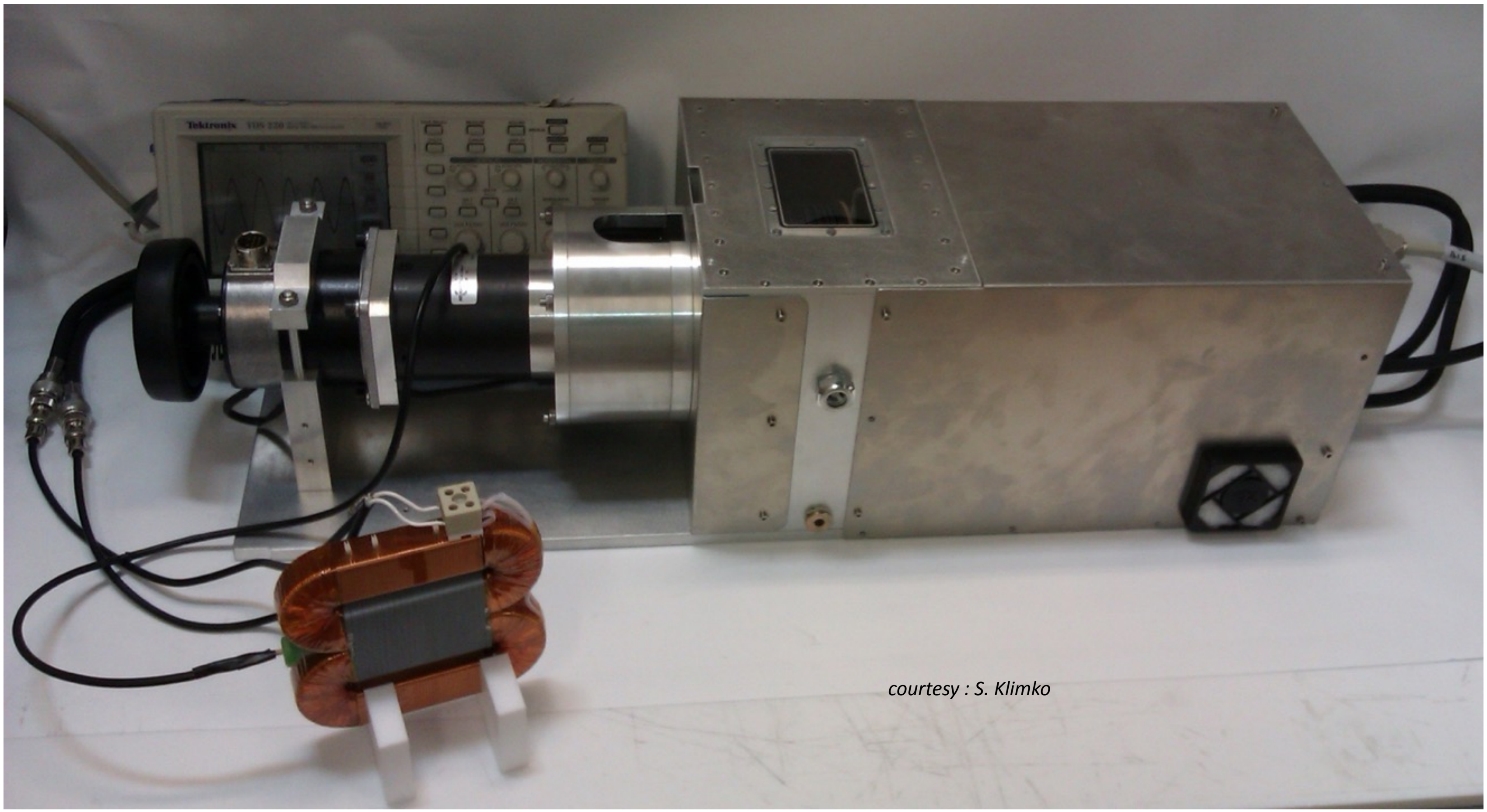


Curved Resonance Flippers

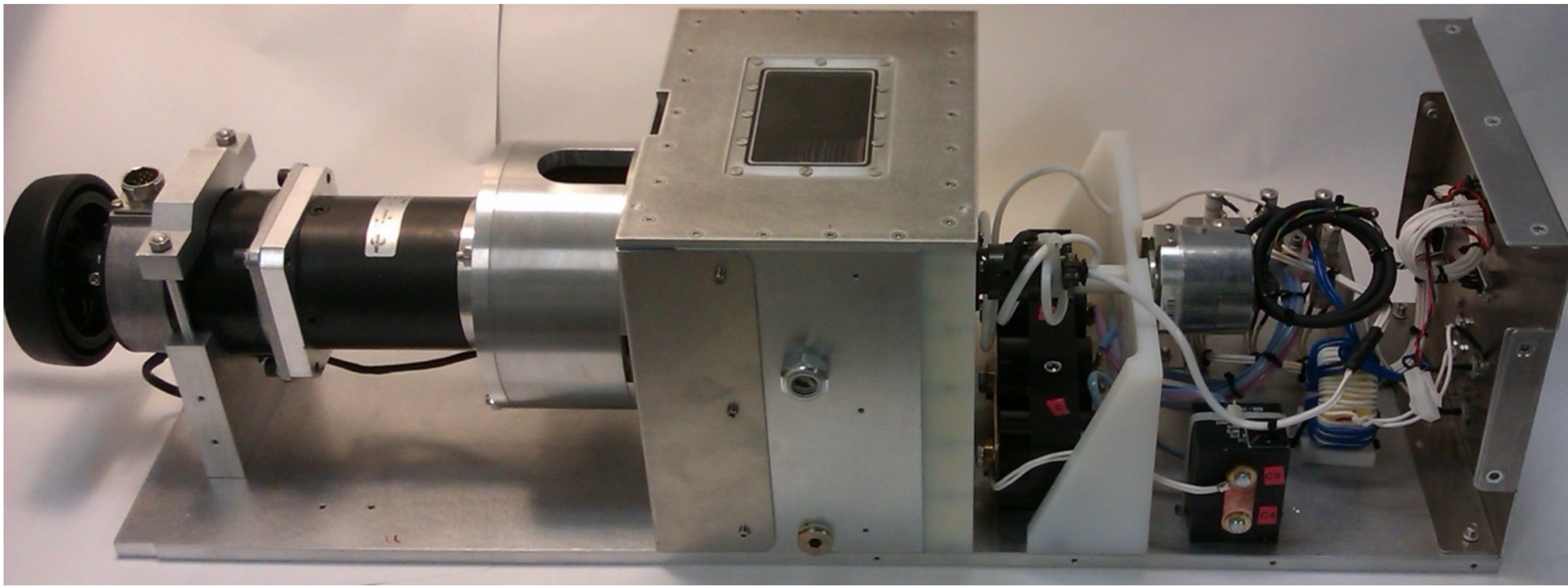


Curved Resonance Flippers

HF circuit : impedance adaptation

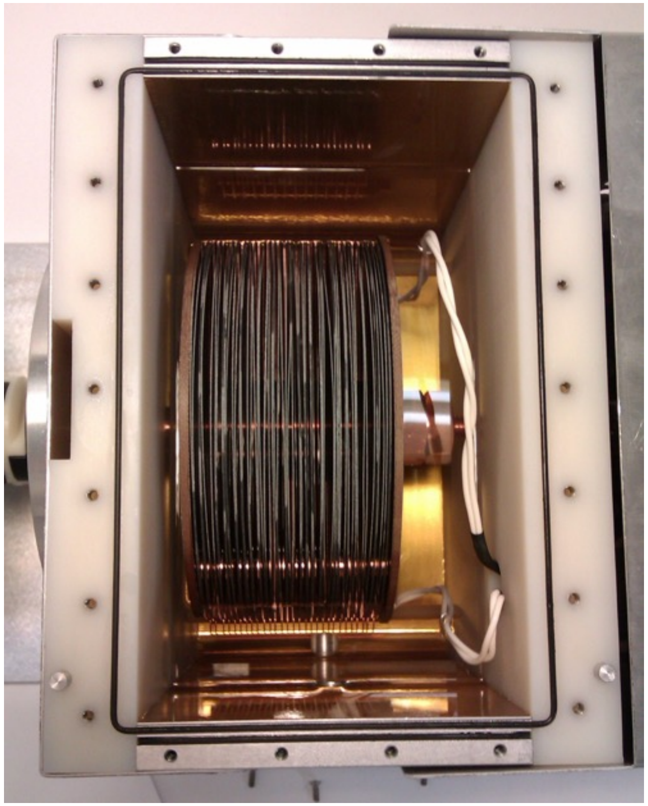


HF circuit : impedance adaptation



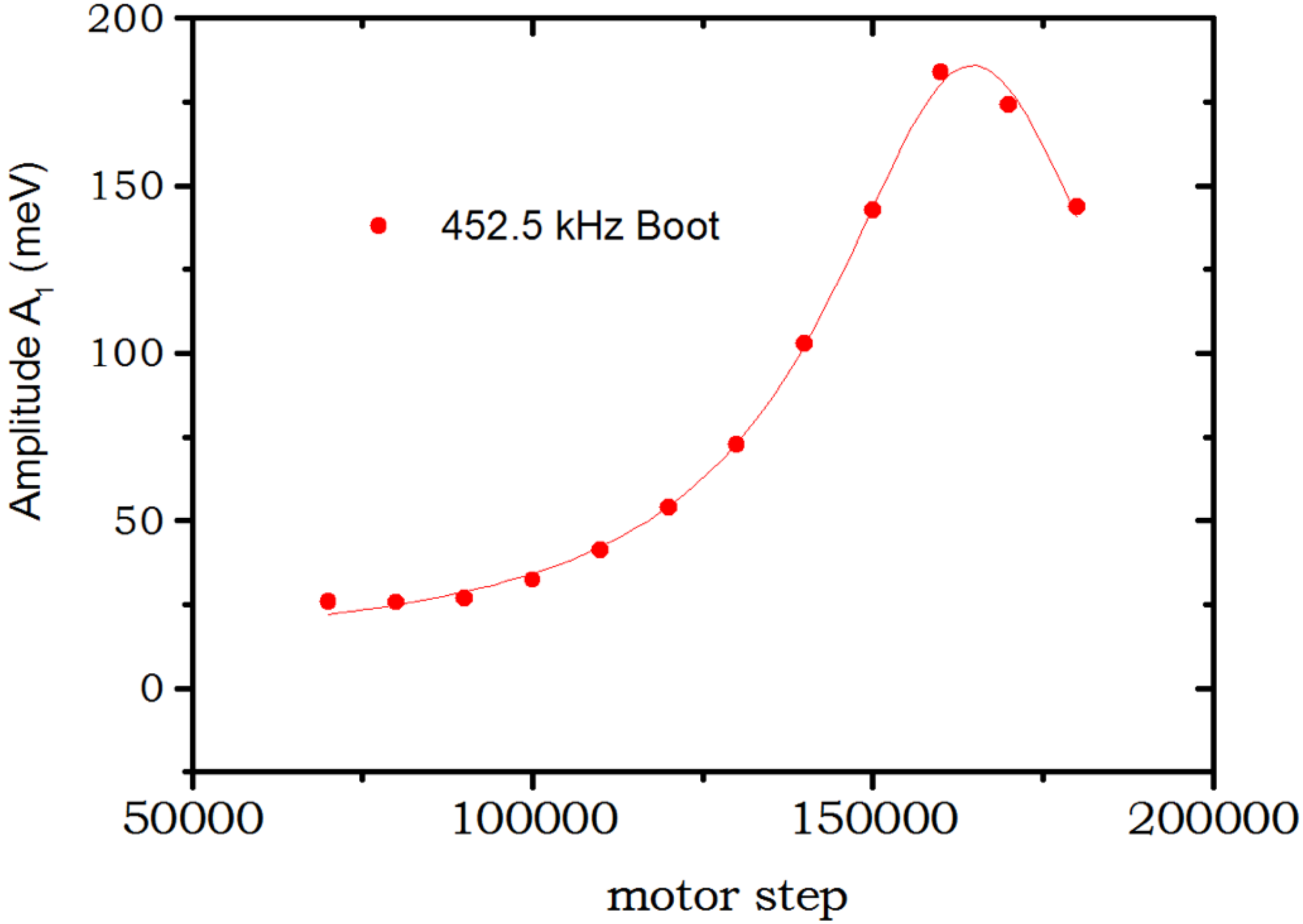
courtesy : S. Klimko

HF circuit : impedance adaptation



courtesy : S. Klimko

HF circuit : impedance adaptation



NRSE versus NSE@ Saclay

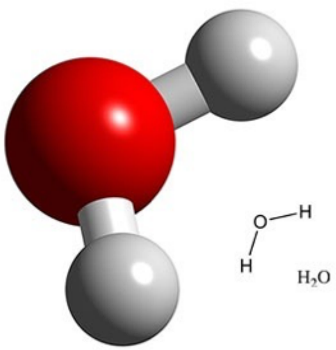
- Mixed spectrometer
  - Not the short times (Bloch-Siegert shift)
  - Not the long times (no correction coils)
- NSE inside the mu-metal shielding : short times (no depolarization of the beam)
- Small to medium times (0.5 ps to 20 ns)
- Compact spectrometer : High flux (2.10^7 $n.cm^{-2}.s^{-1}$ polarized neutrons @ sample position 4*4 cm^2)
- Zero field in the sample position :
  - resolution is very little Q dependent
  - not sensible to flight path distribution in the sample
- Multi detector is limited
- Stability of the RF current requires appropriate design of the circuits
- high Q measurements
- Beam is passing through 3*2 mm aluminium per coil *8 = 48 mm without sample environment

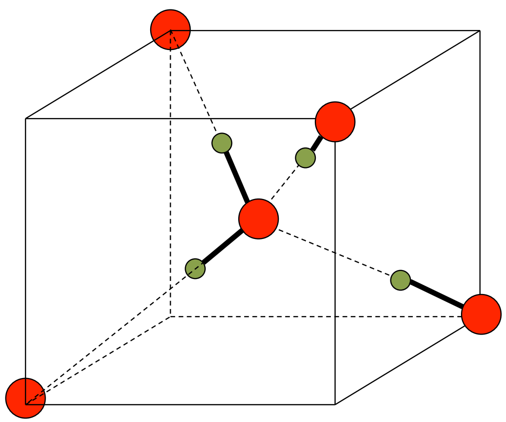
1- The dynamics of supercooled water - hydrogen bond lifetime

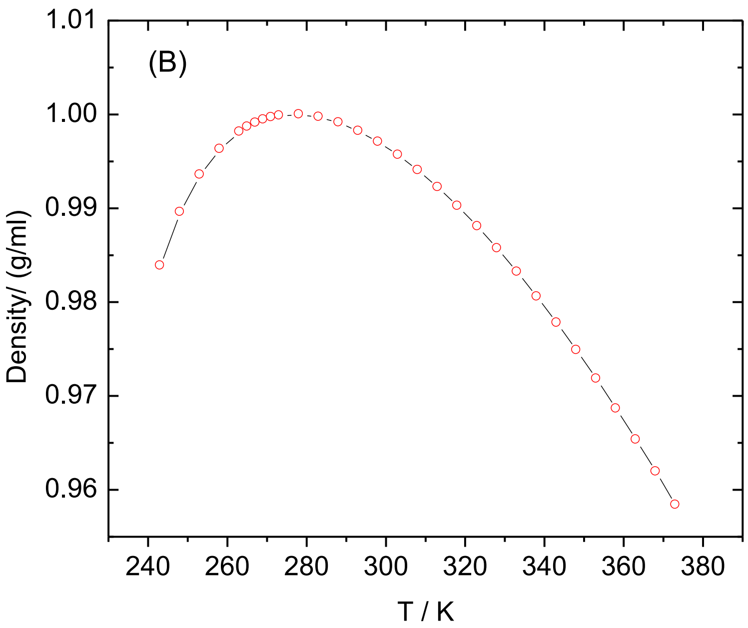
J. Teixeira, A. Luzar and S. Longeville, J. Phys.: Condens. Matter ***18*** *(2006) S2353–S2362*

Water: a common liquid with « anomalous properties »

Why is water so complex ?







G. Johari and J. Teixeira,
J. Phys. Chem. B ***119****, 14210 (2015)*

- Large number of hydrogen bonds
- Local tetrahedral order
- Short life time of H bonds

Density, compressibility, heat capacity viscosity, isotopic effects …

1- The dynamics of supercooled water - hydrogen bond lifetime

J. Teixeira, A. Luzar and S. Longeville, J. Phys.: Condens. Matter ***18*** *(2006) S2353–S2362*

PHYSICAL REVIEW A VOLUME 31, NUMBER 3 MARCH 1985

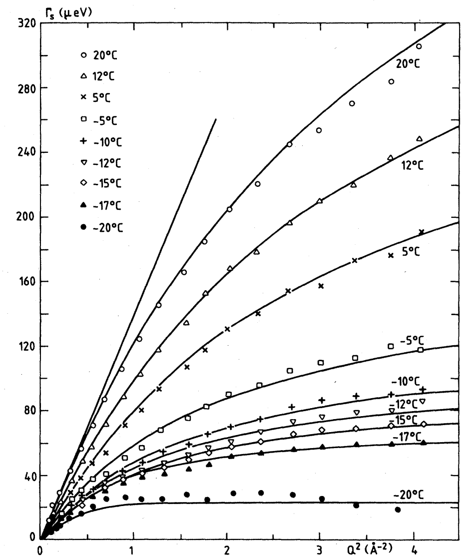
Experimental determination of the nature of diffusive motions of water molecules at low temperatures

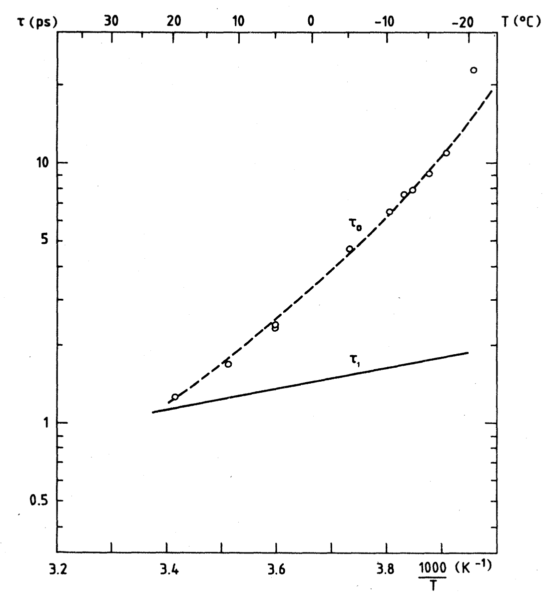
J. Teixeira and M.-C. Bellissent-Funel
Laboratoire Léon Brillouin, Centre d'Etudes Nucléaires Saclay, 91191 Gif-Sur-Yvette Cédex, France*

S. H. Chen
Department of Nuclear Engineering, 24-209 Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

A. J. Dianoux
Institut Laue Langevin, 156 X, 38042 Grenoble Cédex, France

(Received 27 April 1984)



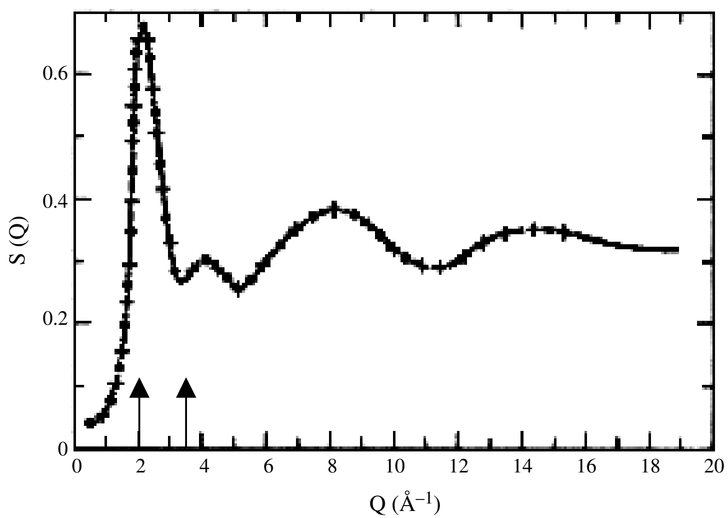


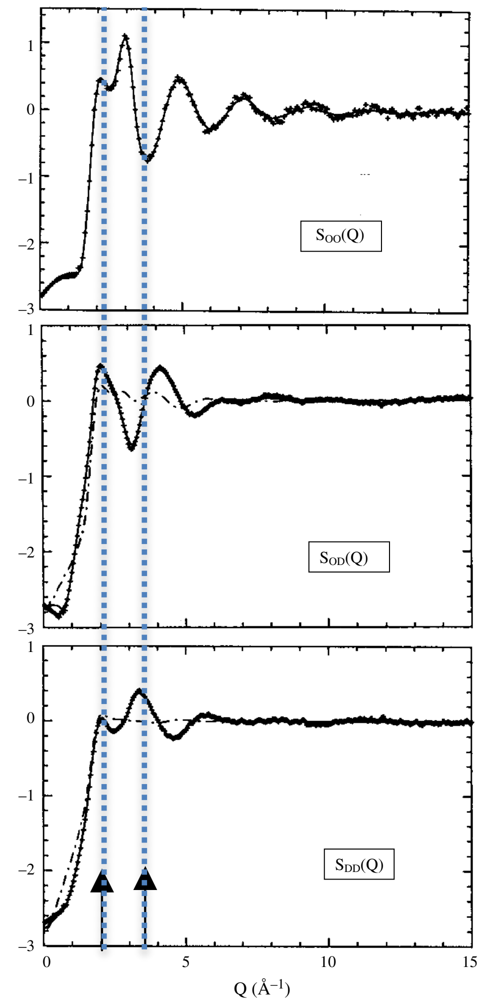
1- The dynamics of supercooled water - hydrogen bond lifetime

*J. Teixeira, A. Luzar and S. Longeville, J. Phys.: Condens. Matter **18** (2006) S2353–S2362*

D-D

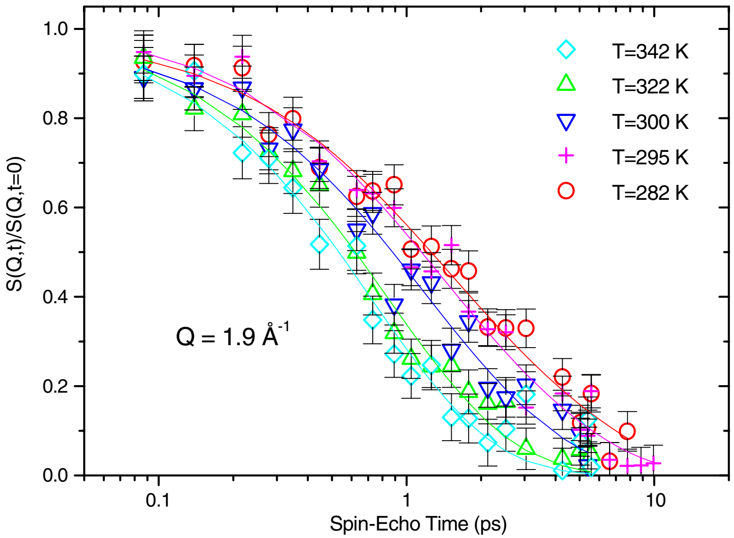
Can we have a more precise measurement of τ_{HB}

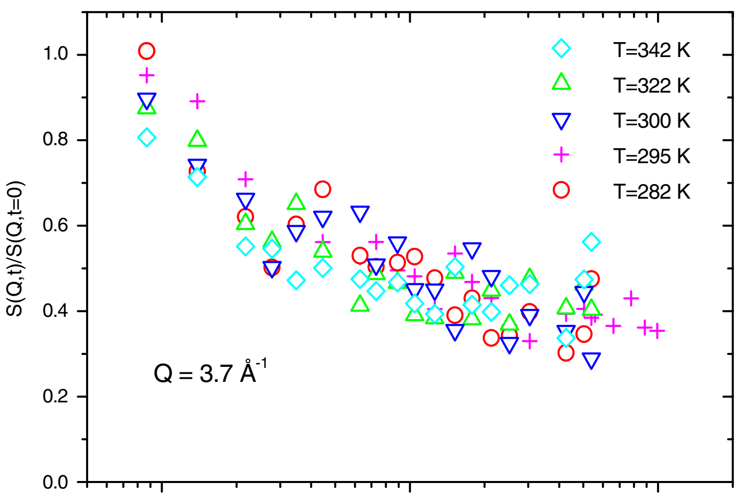




1- The dynamics of supercooled water - hydrogen bond lifetime

J. Teixeira, A. Luzar and S. Longeville, J. Phys.: Condens. Matter ***18*** *(2006) S2353–S2362*





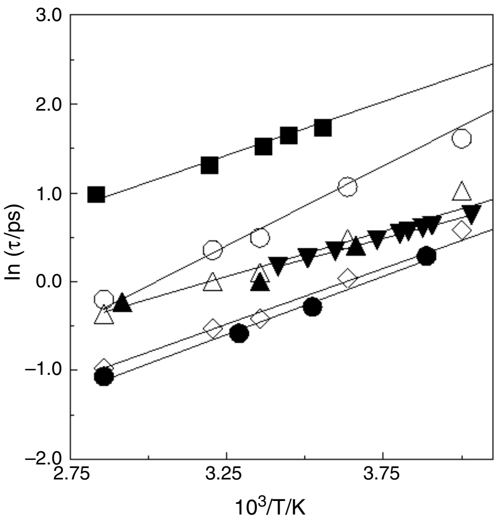


Figure 7. Arrhenius temperature dependence of the hydrogen bond dynamics determined by several different experimental techniques (filled symbols) and theoretical calculations (open symbols); experimental points: coherent QENS (this work, squares), incoherent QENS ([4], triangles down), IR transient hole burning ([11], triangles up), depolarized Rayleigh light scattering ([7], circles). Theoretical points obtained by means of molecular dynamics and the reactive flux correlation function approach [23], using the SPC model of water: hydrogen bond lifetime (circles), hydrogen bond reforming time (triangles up), time of switching hydrogen bond partners [32]. Slopes represent activation energies between 8 and 11 kJ mol^{-1}.

2- Structural relaxation in supercooled $(Na_2O–Li_2O)–2P_2O_5$: a neutron spin-echo study

B. Rufflé

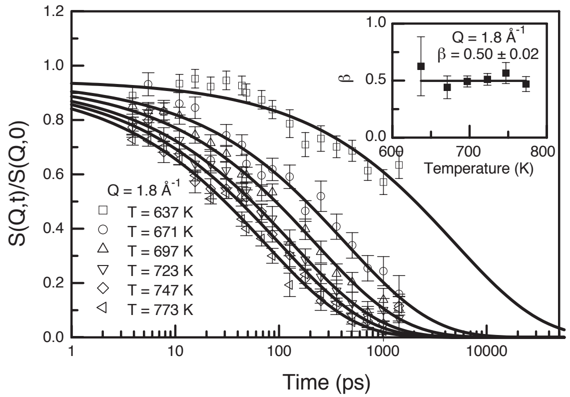


Fig. 1. Intermediate scattering function $\phi(Q,t) = S(Q,t)/S(Q,t=0)$ measured on $(Na_2O–Li_2O)–2P_2O_5$ at $Q = 1.8$ Å^{-1} for six temperatures ranging from 637 to 773 K. Lines are the resulting KWW fit curves (Eq. (1)) described in the text. The inset shows the temperature dependence of the Kohlrausch stretching exponent.

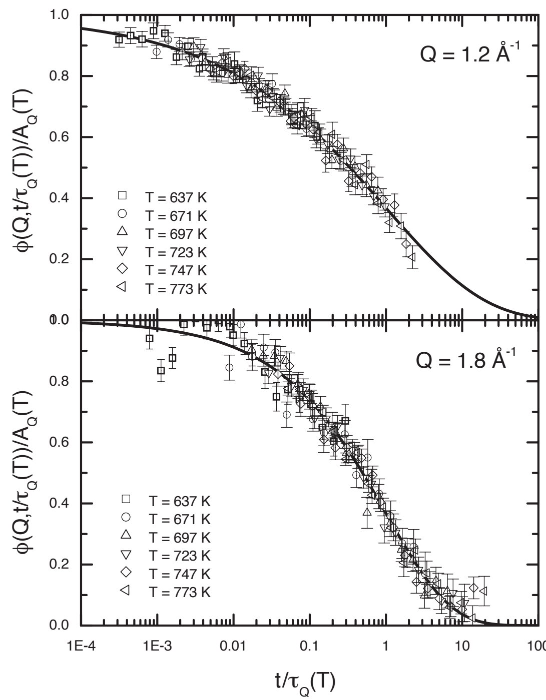


Fig. 2. Scaling analysis of the α relaxation in $(Na_2O–Li_2O)–2P_2O_5$: master curves $\phi(Q, t/\tau_Q(T))/A_Q(T)$, where $A_Q(T)$ and $\tau_Q(T)$ are obtained from iterative fits with Eq. (1).

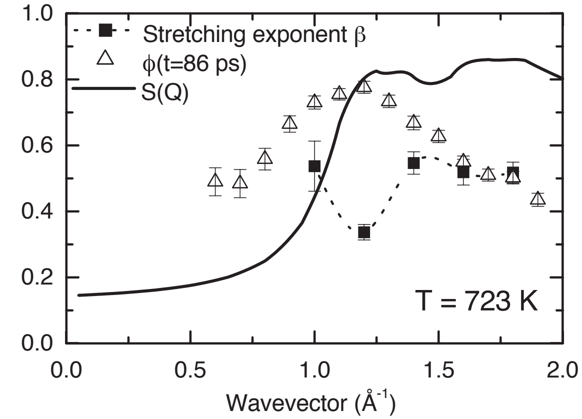


Fig. 3. Dependence on scattering vector Q: (■) stretching exponent β_Q obtained by the three-step procedure described in the text; (△) intermediate scattering function at a fixed time $\phi(t = 86$ ps) revealing a maximum of the structural relaxation time around $Q = 1.2$ Å^{-1}, the position of the pre-peak; (solid line) static structure factor $S(Q)$ of $(Na_2O–Li_2O)–2P_2O_5$ at $T = 723$ K.

$$\Phi(\tau = 86ps) = \frac{S(Q, \tau = 86ps)}{S(Q, \tau = 0)}$$