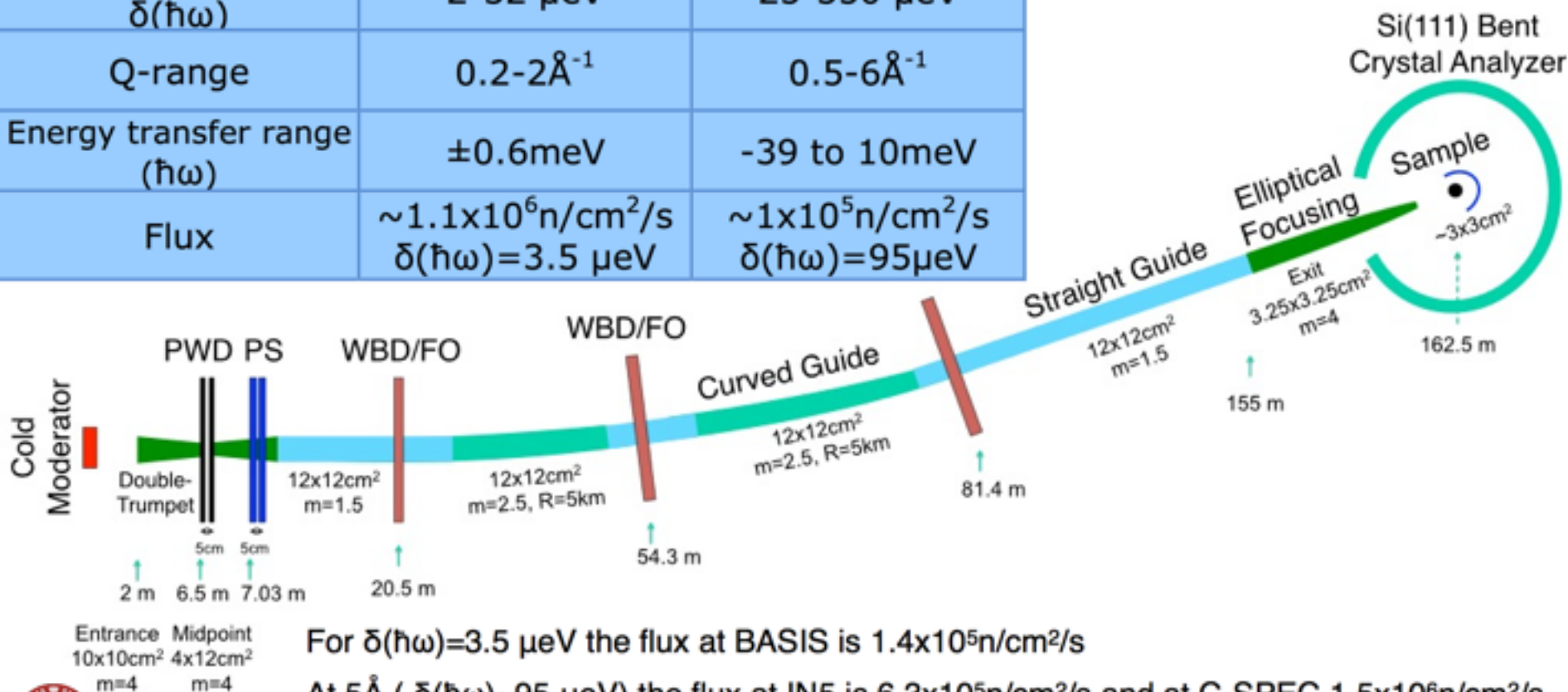
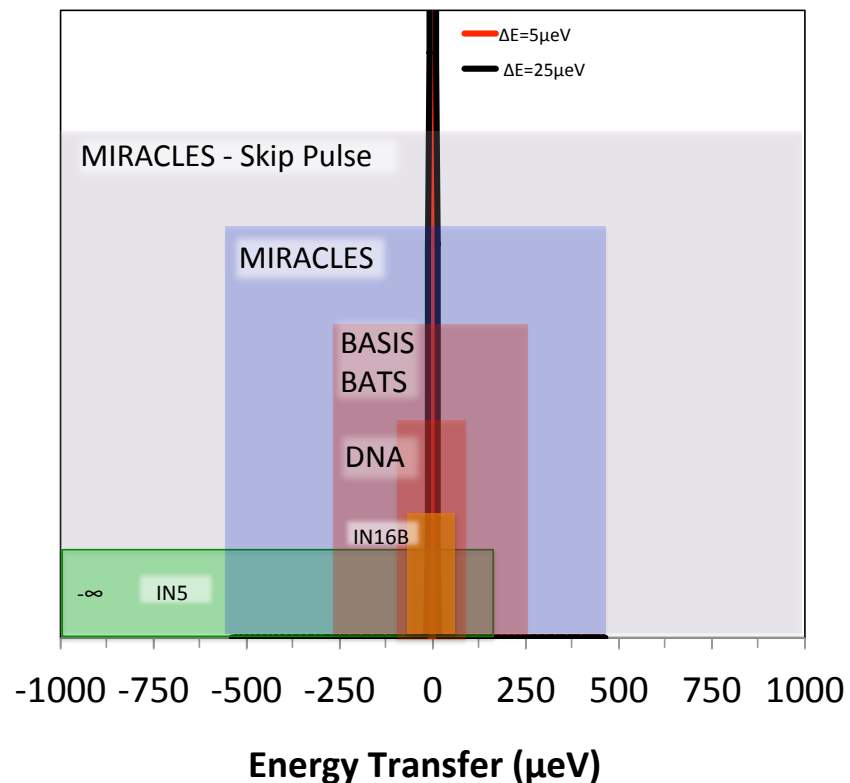
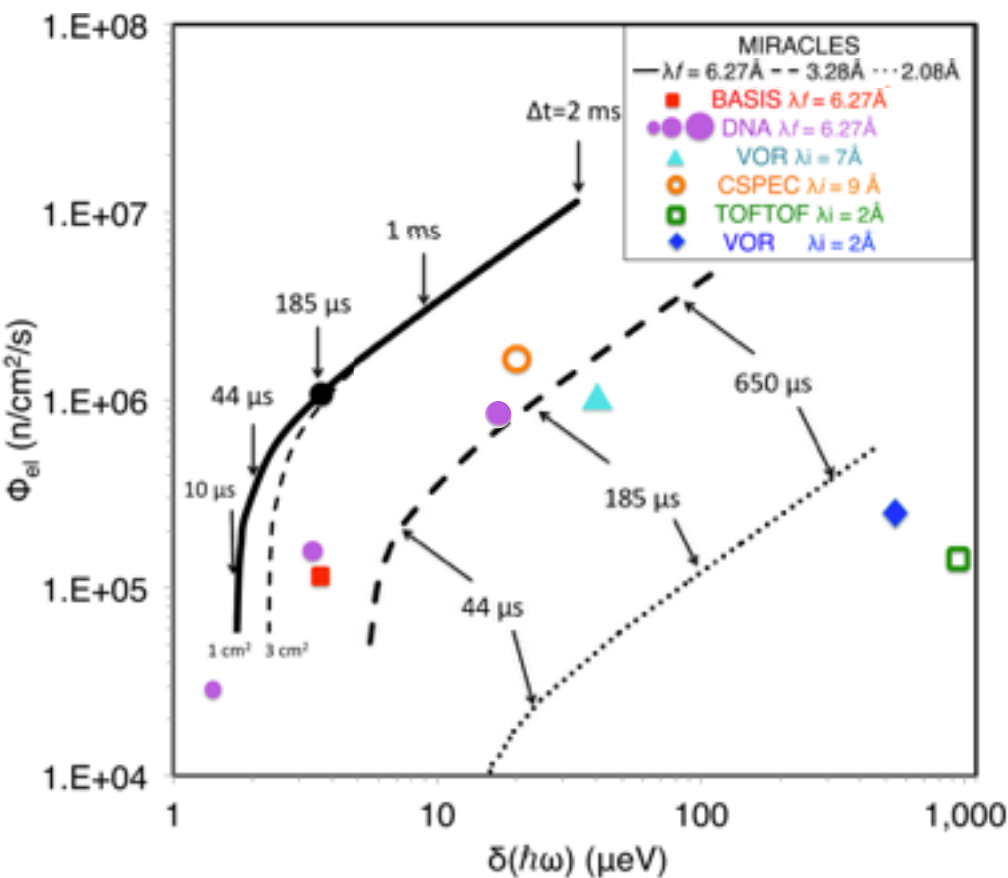


# Disentangling time distribution

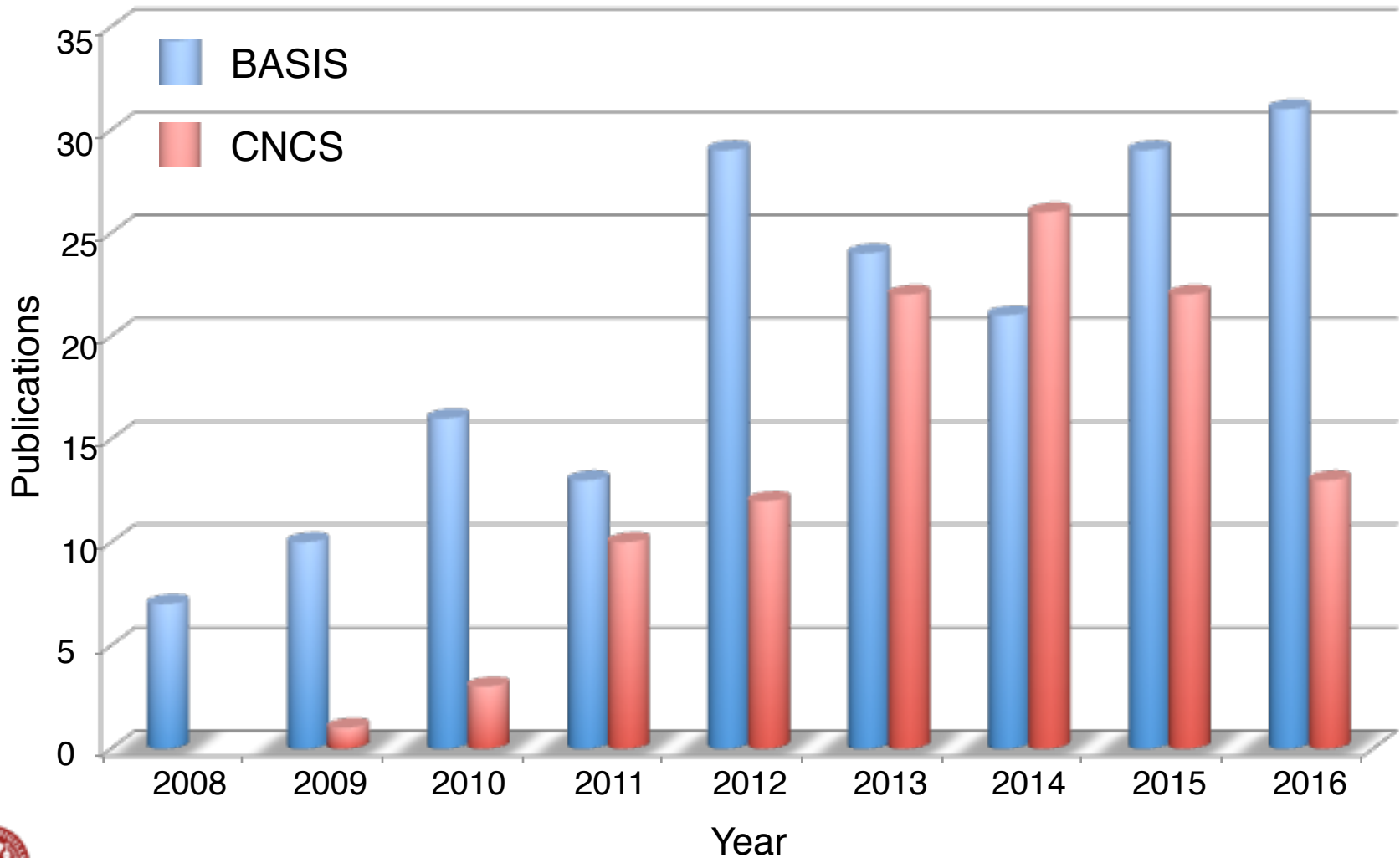
Analyzer crystals	Si(111)	Si(333)
	(6.267Å)	(2.08Å)
energy resolution - $\delta(\hbar\omega)$	2-32 $\mu\text{eV}$	25-350 $\mu\text{eV}$
Q-range	0.2-2Å <sup>-1</sup>	0.5-6Å <sup>-1</sup>
Energy transfer range ( $\hbar\omega$ )	$\pm 0.6\text{meV}$	-39 to 10meV
Flux	$\sim 1.1 \times 10^6 \text{n/cm}^2/\text{s}$ $\delta(\hbar\omega) = 3.5 \mu\text{eV}$	$\sim 1 \times 10^5 \text{n/cm}^2/\text{s}$ $\delta(\hbar\omega) = 95 \mu\text{eV}$



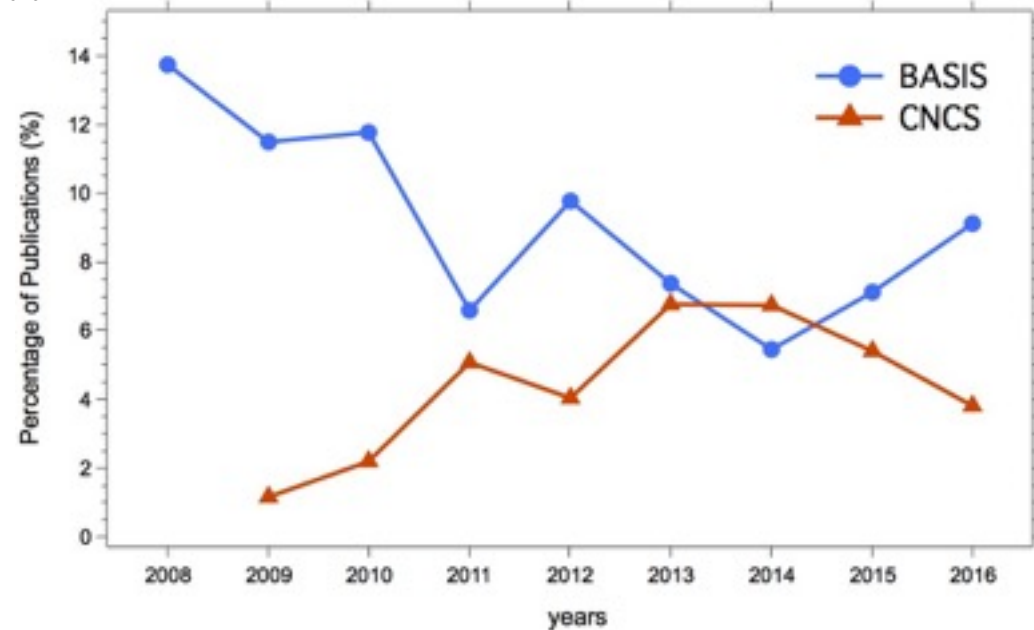
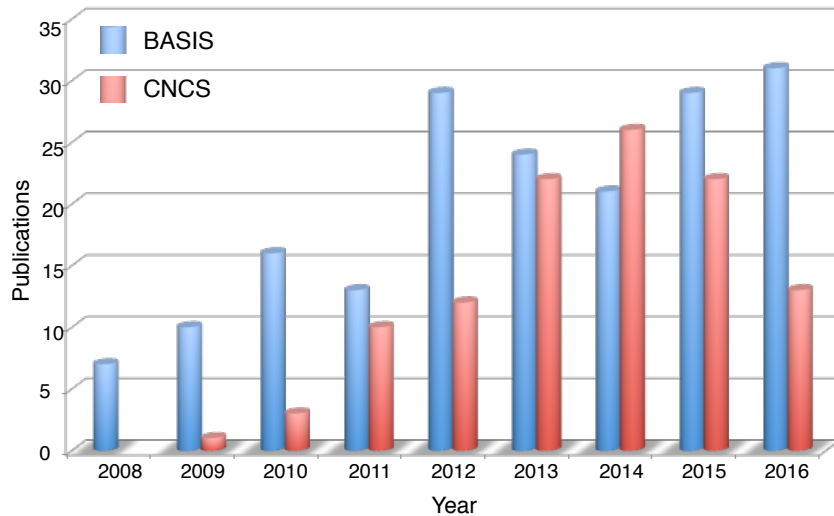
# MIRACLES outstanding performance



# Setting the world scenario: performance of two world leading spectrometers at SNS\*\*

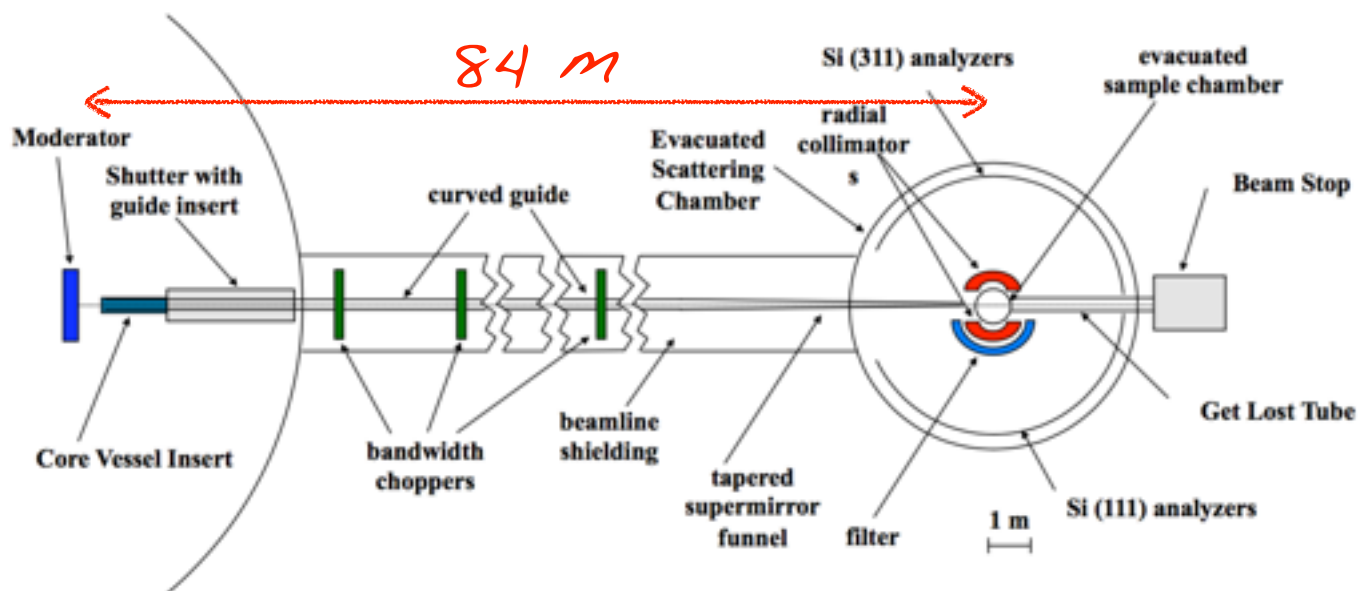


# Setting the world scenario: performance of two world leading spectrometers at SNS\*\*



# Success comes at a cost

1.07.04.01 - System Integration H R B S	1,159,245
1.07.04.02 - Data Acquisiton H R B S	318,651
1.07.04.03 - Detectors H R B S	273,198
1.07.04.04 - Choppers H R B S	671,624
1.07.04.05 - Sample Environment H R B S	37,643
1.07.04.06 - Optical Elements H R B S	1,940,026
1.07.04.07 - Shielding H R B S	1,941,570
1.07.04.08 - Instrument Specific H R B S	2,353,122
1.07.04.HIST - HIST - High Resolution Backscattering Sp	32,147
1.07.20.04 - Backscattering Spectrometer Installation	609,985
Total in 2004 *	9,337,211



EUROPEAN  
SPALLATION  
SOURCE



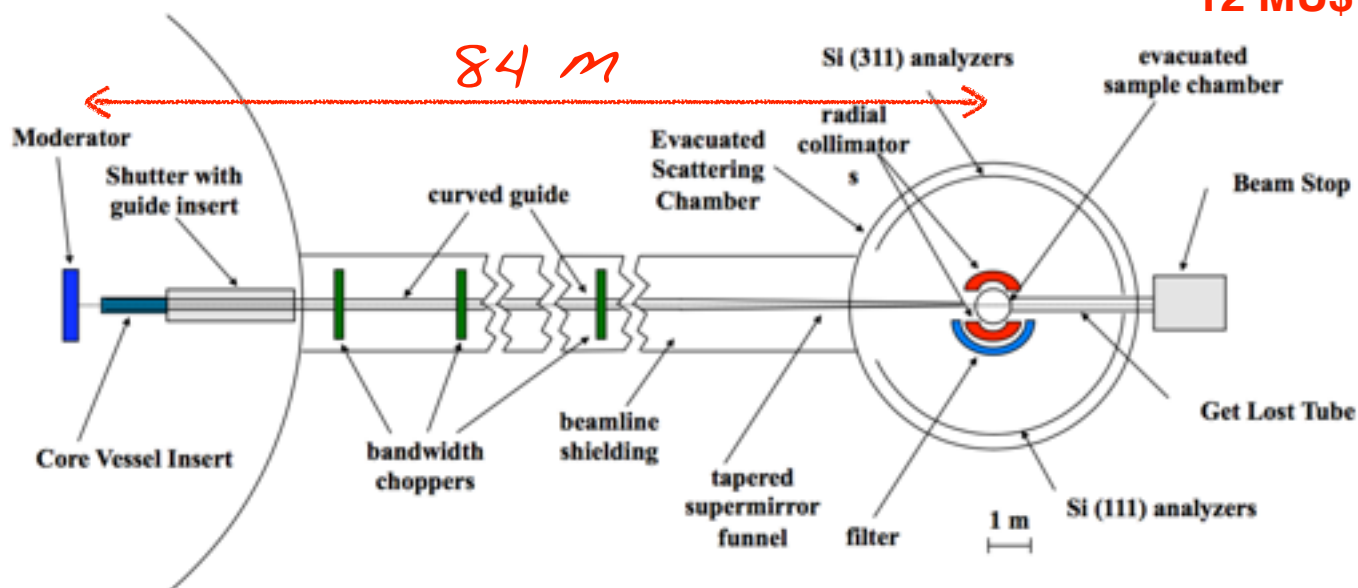
ESS  
bilbao

\*Kenneth W. Herwig, private communication by e-mail also to the ESS

# Success comes at a cost

1.07.04.01 - System Integration H R B S	1,159,245
1.07.04.02 - Data Acquisition H R B S	318,651
1.07.04.03 - Detectors H R B S	273,198
1.07.04.04 - Choppers H R B S	671,624
1.07.04.05 - Sample Environment H R B S	37,643
1.07.04.06 - Optical Elements H R B S	1,940,026
1.07.04.07 - Shielding H R B S	1,941,570
1.07.04.08 - Instrument Specific H R B S	2,353,122
1.07.04.HIST - HIST - High Resolution Backscattering Sp	32,147
1.07.20.04 - Backscattering Spectrometer Installation	609,985
Total in 2004 *	9,332,211

\*\*12 MUSD = 11M€ in 2016



EUROPEAN  
SPALLATION  
SOURCE



ESS  
bilbao

\*Kenneth W. Herwig, private communication by e-mail also to the ESS

\*\*<http://fxtop.com/en/currency-converter-past.php?C1=USD&A=12259637.60966&DD=18&MM=10&YYYY=2016>



### Anton Heidemann

**BACKSCATTERING SPECTROSCOPY: HOW IT ALL BEGAN EXACTLY 50 YEARS AGO**  
 AUGUST IS THE BIRTHDAY OF BACKSCATTERING SPECTROSCOPY.

PARFUMED AND HYGIENIC... CASUALTY OFFICERS WALKY GUYS LEAD PARTICIPATED IN OPENING A NEW FIELD. THIS DOES NOT APPROVE VERY FREQUENTLY TO THESE STUDENTS.

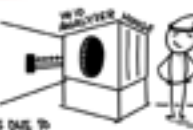
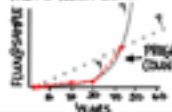


### Andreas Hagerl

**THE HISTORY OF NEUTRON BACKSCATTERING: FROM GARCHING TO GEMMING**

JOINED ILL. BSS GROUP

LEARNED ROTATIONAL TUNNELING FROM NOT'S NORDY BEEK



WHATEVER, HAD TO GO INTO THE HALLWAY HAD TO BE "SPICY"

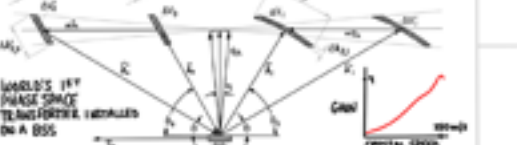
### Colin Carile

**BACKSCATTERING ON PULSED SOURCES: A PERSONAL ACCOUNT**

"IF A MAN CAN WRITE A BETTER BOOK, PUNCH A BETTER GOLF BALL, OR MAKE A BETTER HOLE-IN-ONE, THEN HE SHOULD BE BUILT HIS HOUSE IN THE WOODS, THE WORLD WILL MAKE A BEATFUL PATH TO HIS DOOR."  
 -RALPH WALDO EMERSON

WROTE 15% "AND ON END OF A LONG GOLF"

**Backscatterer Kroner**



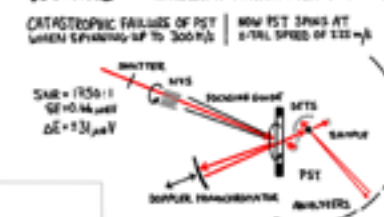
### Ken Herwig

**THE DESIGN AND CONSTRUCTION OF THE SWI-MARZ-BACKSCATTERING SPECTROMETER "BASSUS"**

TOO CLOSE! OUT-OF-FOCUS!  
 LIGHT... NEUTRON SOURCE EMITS SPHERICAL WAVES - SHOTS BY AND PARALLEL TO DIFFERENT FOCAL POINTS.

### Joachim Wutke

**SPINELS: THE SPECTROMETER FOR HIGH ENERGY NEUTRONS AT ILL**  
 IN HONOR OF MICHAEL FRANK (1910-2000)



### Bernhard Frick

**A PERFORMANCE BOOST FOR BRAGG BACKSCATTERING - IN ILL AT ILL**

OLD ILL - 334 PAGES / 18 YEARS  
 1991 - BEGAN LABORTING FOR PST  
 2001 - GREEN LIGHT FOR PST

**IN ILL & ILL**

**PST - THE HEART OF ILL**

GAIN - 2.1-2.5  
 RANGE -  $3.8 \cdot 10^{-4}$  nm<sup>-1</sup>  
 SIZE - 100000  
 ANALYZER - 2-TAL (SIL)  
 CENTERED BACKSCAT.  $4\theta_{1/2} = 2.0^\circ$

Qmax ( $0.210 - 3.94^\circ$ )  
 SE ( $0.210 - 1.9^\circ$ )  
 SE ( $0.11 - 0.9^\circ$ )

# 50 YEARS OF NEUTRON BACKSCATTERING

FOR ADDITIONAL INFORMATION VISIT: [www.ill.eu](http://www.ill.eu)

ANTON HEIDEMANN

### Valeria Arrighi

**USING BACKSCATTERING TO STUDY DYNAMICS OF SOFT MATTER AND COLLOID SYSTEMS**

POLYMER NETWORKS → MANY DECADES IN TIME

MS  
 BRAD LENGTH (Å) → CHAIN LENGTH (100 nm)

### DiDier Blanchard

**GENS STUDIES OF THE THERMAL STABILITY**

DEVELOP MATERIALS TO HARVEST, STORE, AND CONVERT BIOETHANOL

COMPUTATIONAL (QMC) AND EXPERIMENTAL RESEARCH

ML STORAGE IN METAL HALIDE SALTS

IN  $NaCl_2$ , WITH FULL  $H_2$  PROTONS AND EQUIVALENT

T-DEPENDENT MOBILITY

### Andreas Meyer

**NEUTRON PROBE DYNAMICS ON HYBRID SILICATE MEMBRANES AS DESIGN BY GEANTS AT ELEVATED TEMPERATURES AND PRESSURES**

BACKSCATTERING GOOD FOR PROBING NETWORK RELAXATION

ALUMINUM SILICATE MEMBRANE - NO TUNNEL RELAXATION

REPRODUCTION: BUILD BSS INSTRUMENTS WITH SMALLER BEAMS → EXTREME ENVIRONMENTS

### Early OENS

EXTRACTED LANGUAGES DEPEND ON RESOLUTION AND DYNAMIC RANGE OF QENS TO APPROPRIATE MATERIALS

USE DISTRIBUTION OF ISOTOPIAL FREE QUANTITIES - NOT JUST ONE

QENS

SYNTHESIZING

CHARACTERIZING

PROBE PROPERTIES

OPTIMIZING QENS AND INTERPRETATION

LIBRARY

HO STORAGE IN BORONTRIDES

### Christiane Agre-Simonescu

**SUPERCOOLED LIQUIDS, POLYMERS, PLASTICS, METALS, SPIN GLASSES**

CHARACTERIZED BY DEMERSED STRUCTURE WITH SLOW RELAXATION CAPTURES BRIDGING NEARBY EFFECTS

POLYMERS & PLASTICS

FROM STRETCHES AT T<T<sub>g</sub>

ON MEMBRANE SCALE, PLASTIC DEFORMATION REMAINS

BSS VALIDATES MODELS & THEORIES

BSS: WIDER PART OF WHY MAT'L'S AT NANOSCALE

### Denise Morneau

**ON THE CHARACTERIZATION OF LIQUIDS IN PRESSURIZED HOSTS: RECENT AND LESS RECENT ACHIEVEMENTS FROM NEUTRON STUDIES**

CONFINEMENT CAN DYNAMICALLY CHANGE DYNAMICS W/ I.E. BULK BEHAVIOR

WHY?

PORE SIZE (HETEROGENEITY) SURFACE EFFECTS (CHARACTERISTIC)

SURFACE HETEROGENEITIES & HYPHENOC/HYDROPHILIC

WHOLE CHANNEL CONFINEMENT & EFFECTS ON BUNNET LINKAGES

### Wolfgang Doster

**THE PROTON DYNAMICAL TRANSITION FROM BACKSCATTERING-DISPLACEMENTS**

APPLICATION OF BSS TO MOLECULAR BIOLOGY

PROTON DYNAMICAL TRANSITION

PST

INTERNAL ROT TRANSITIONS OF SUGARS, CH<sub>3</sub> GROUP OF PEPTIDE BLM & VIBRITY

SOLVENT VISCOSITY DEPENDENT DISPLACEMENTS CHANGED TO TRANS DIFFUSION OF HYDRATING WATER

### Werner Press

**HISTORY & 50 Y. ROTATIONAL TUNNELING WITH HIGH RESOLUTION NEUTRON SCATTERING**

PEOPLE ARE AS DIFFICULT AS SPECTRA!

ALFRED, FRANK, HEDDICH, HEIDEMANN, COOPER, BRÄUER, SCHWETS...

HITACHI CH<sub>4</sub> IN H<sub>2</sub>O (LARGE)

CH<sub>4</sub> SPIN - ROTATIONAL TUNNELING

ROTATIONAL TUNNELING IS LARGELY A QUANTUM-BIASED PHENOMENON - FELI GROUPS

### Arantxa Arbe

**POULTRY DYNAMICS HIGHLIGHTS FROM NEUTRON BACKSCATTERING**

RICH DYNAMICS OBSERVED ON THE LENGTH SCALE OF OBSERVATION

POULTRY DYNAMICS

SIDE GAP HATHING MEMBERS → 2<sup>nd</sup> ORDER RELAXATION

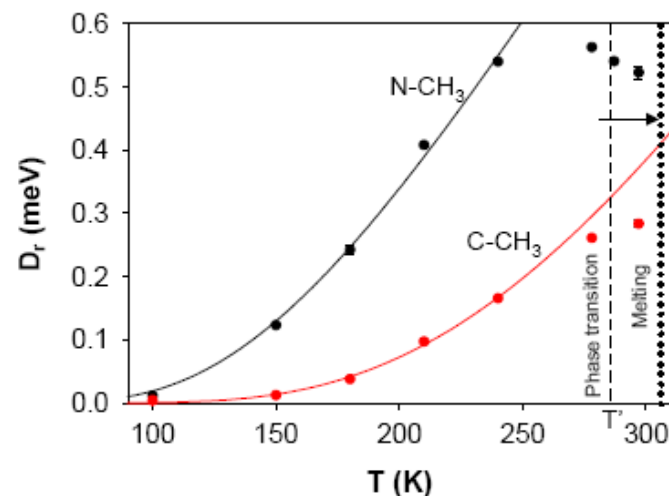
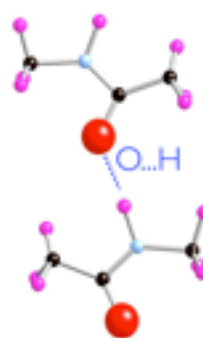
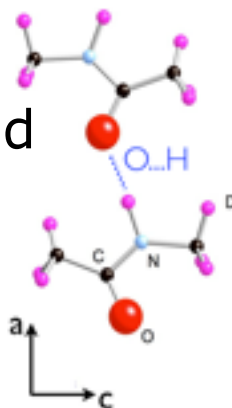
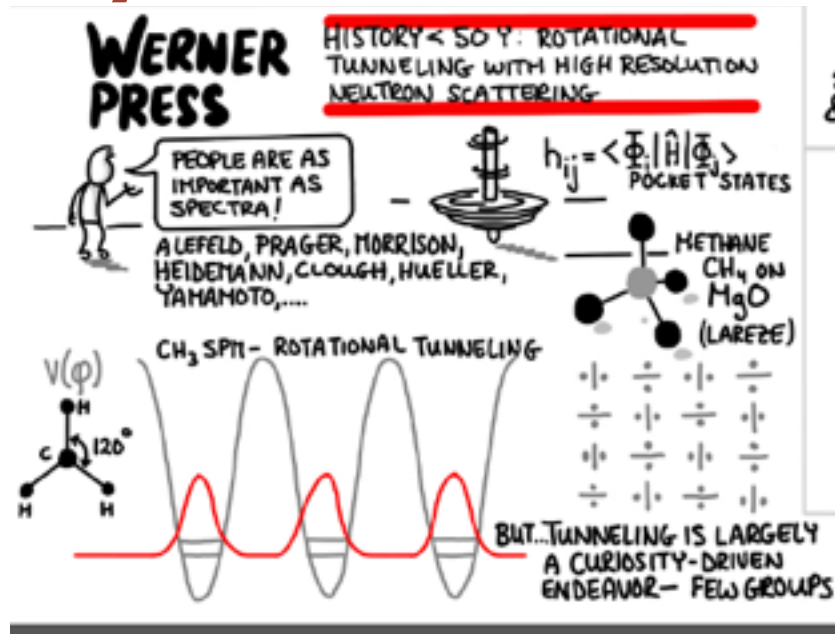
INTERNAL ORDER → RELAXATION CHAIN → CURE DYNAMICS

CLASSICAL TO QUANTUM

TUNNELING IN GLASSES TO

# MIRACLES allows for curiosity driven science with 12M€

- ✓ Considerable reduction of analyser angle, as well as detector area.
- ✓ Critical loss of detection flux, with a subsequent significant increase of the measurement time.
- ✓ Lack of the collimator and Be-filter will result in low signal/noise ratio.

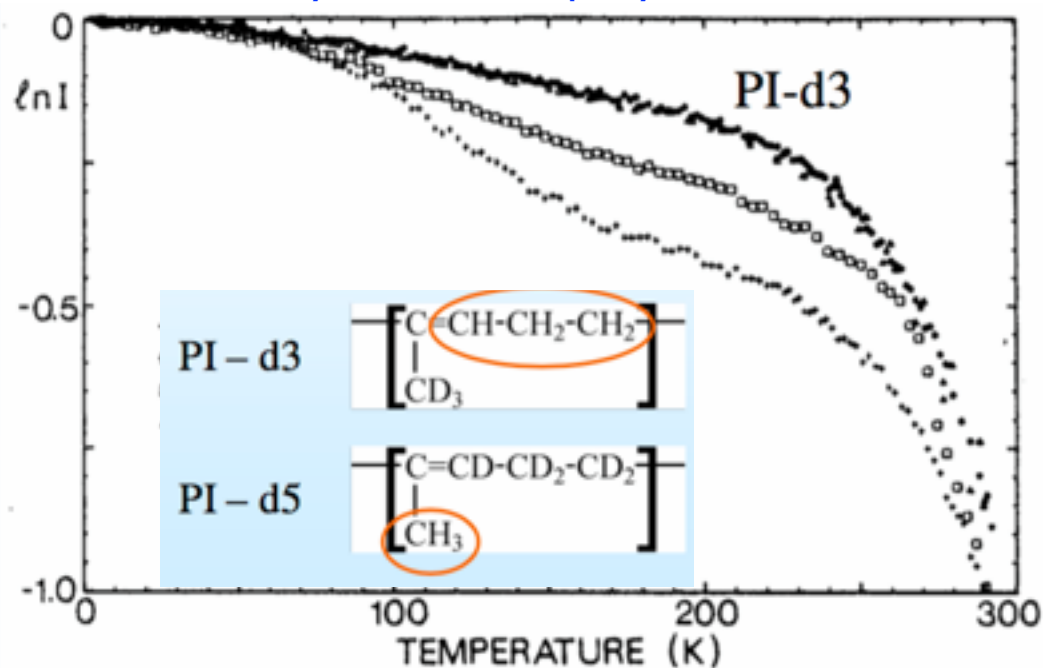




# MIRACLES allows for **curiosity driven science** with 12M€

- ✓ Considerable reduction of analyser angle, as well as detector area.
- ✓ Critical loss of detection flux, with a subsequent significant increase of the measurement time.
- ✓ Lack of the collimator and Be-filter will result in low signal/noise ratio.

separating methyl group & main chain dynamics in polymers



Frick, B. and Fetters, L.J. ; *Macromolecules* **1994**, 27, 974.

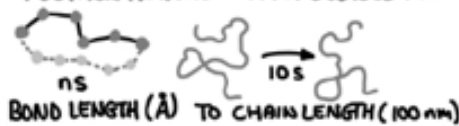
# MIRACLES provides outstanding science with 15.9M€

- Almost full coverage of the analyser angle, as well as detector area.
- Increased flux and reduction of the measurement time.
- Lack of Be-filter might result in low signal/noise ratio.

**Valeria Arrighi**

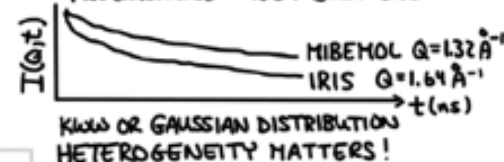
USING BACKSCATTERING TO STUDY DYNAMICS OF SOFT MATTER AND COMPLEX SYSTEMS

POLYMER MOTIONS → MANY DECADES IN TIME



EARLY QENS | EXTRACTED LINEWIDTHS DEPEND ON RESOLUTION AND DYNAMIC RANGE LEADS TO INAPPROPRIATE MODELING

→ USE DISTRIBUTION OF ROTATIONAL FREQUENCIES — NOT JUST ONE



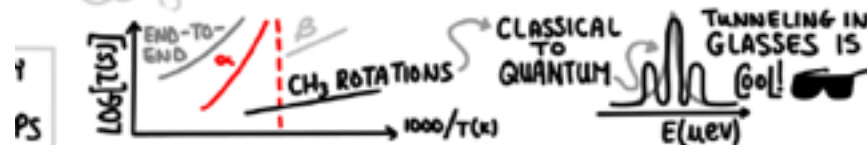
**ARANTXA ARBE**

POLYMER DYNAMICS: HIGHLIGHTS FROM NEUTRON BACKSCATTERING



RICH DYNAMICS DEPEND ON THE LENGTH SCALE OF OBSERVATION

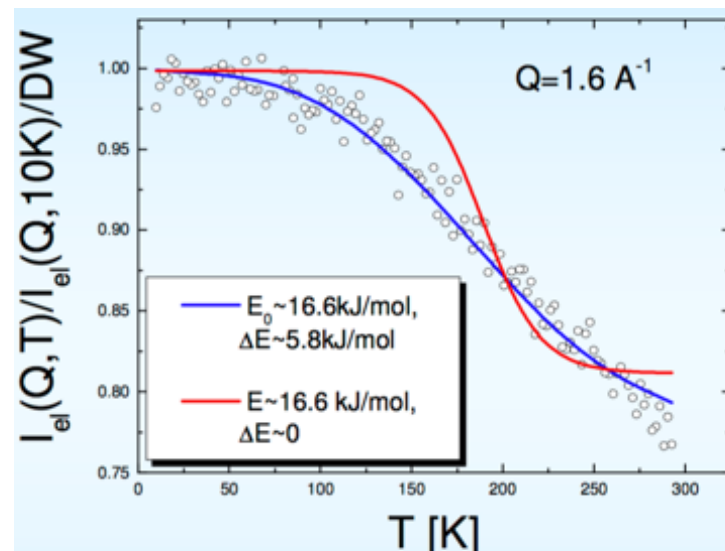
MONOMERS → SIDE GRP MOTIONS  
INTERMOLECULAR → 2<sup>ND</sup>-ARY RELAXATIONS  
CHAIN → CHAIN DYNAMICS



# MIRACLES provides **outstanding science** with 15.9M€

describing methyl group & main chain dynamics in proteins

- ☑ Almost full coverage of the analyser angle, as well as detector area.
- ☑ Increased flux and reduction of the measurement time.
- ☐ Lack of Be-filter might result in low signal/noise ratio.



$$I_{el}(Q, T, \omega \sim 0) = DW(Q, T) \left[ 1 - p_m + p_m \int_{-\infty}^{\infty} S_{met}(Q, \omega') R(\omega - \omega') d\omega' \Big|_{\omega=0} \right] \propto DW(Q, T) \left[ const(Q) + \int_{-\infty}^{\infty} R(\omega - \omega') \int_0^{\infty} g(E_i) \frac{\tau_i}{1 + \omega^2 \tau_i^2} dE_i d\omega' \Big|_{\omega=0} \right]$$

Zaccai G, Bagyan I, Combet J, et al. *Scientific Reports*. **2016**, 6, 31434.

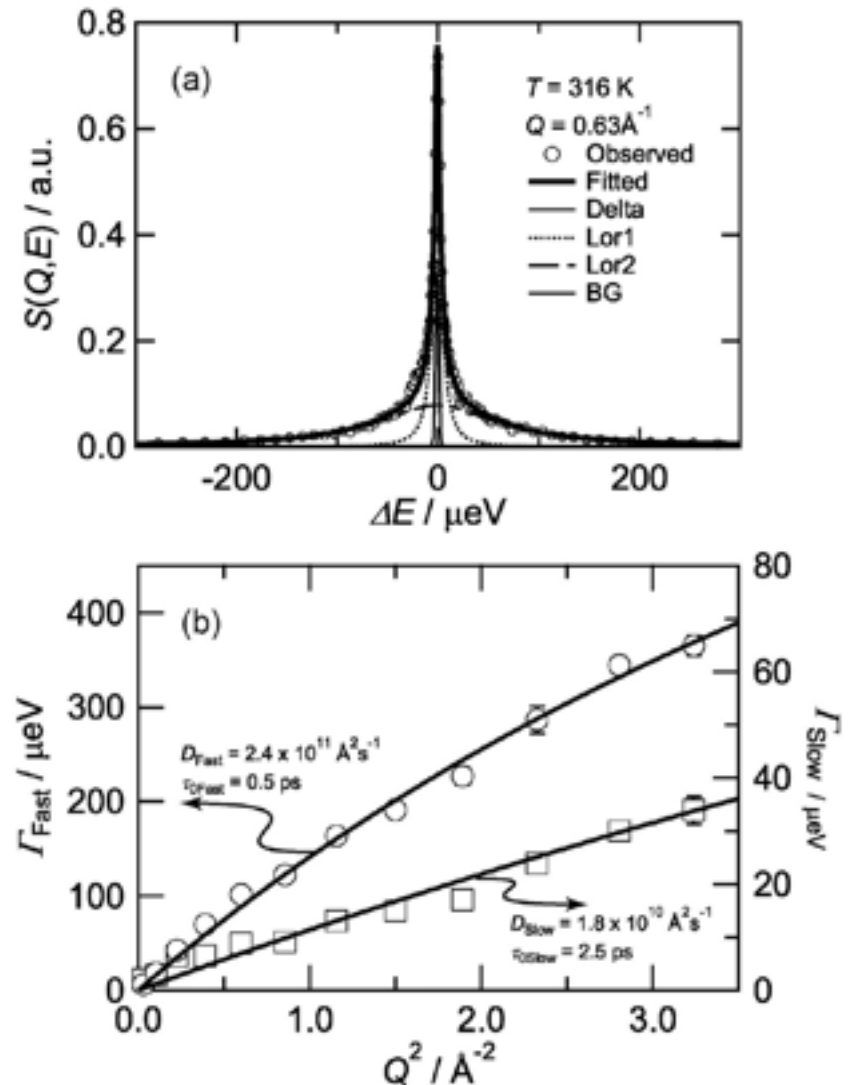


Example inspired by A. Sokolov in <http://cns.che.udel.edu/files/2014/03/Sokolov-reloyj.pdf>

# MIRACLES provides outstanding science with 15.9M€

- ☑ Almost full coverage of the analyser angle, as well as detector area.
- ☑ Increased flux and reduction of the measurement time.
- ☐ Lack of Be-filter might result in low signal/noise ratio.

broad range water dynamics in biological systems: DNA first results



# MIRACLES brings a paradigm shift to neutron backscattering with 17.7M€

- ✓ Full coverage of the analyser angle, as well as detector area.
- ✓ Matchless flux and excellent sample environment.
- ✓ Outstanding signal/noise ratio.
- ✓ Very large Q-range and even broader elastic energy resolution coverage.

**ANDREAS MEYER**

INTRINSIC PROTON DYNAMICS IN HYDRATED SILICATE MELTS AS SEEN BY QENS AT ELEVATED TEMPERATURE AND PRESSURE

WANT TO UNDERSTAND LAVA FLOWS & MELTS ON A MOLECULAR LEVEL USING NEUTRON SCATTERING → QENS

BACKSCATTERING GOOD FOR PROBING NETWORK RELAXATION  $\tau \sim ns$

ALKALI SILICATE MELT - NETWORK RELAXATION

300K, 1300K

$E(\mu eV)$

$Na_2O \cdot 2SiO_2$

$S(q,t)$

Na RELAXATION

NETWORK RELAXATION

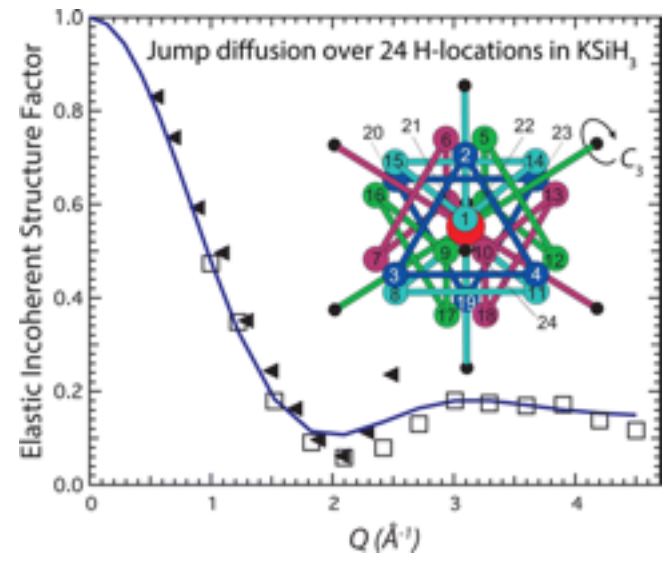
$t(ps)$

RECOMMENDATION: BUILD BSS INSTRUMENTS WITH SMALLER BEAMS → EXTREME ENVIRONMENTS

Lava FLOW vs. Explosive Volcanism

HOW IS WATER DISSOLVED IN SYSTEM? → IN MOLECULAR H<sub>2</sub>O & OH GROUPS

## Hydrogen as an energy source



Österberg, C. et al. *J. Phys. Chem C* **2016**, 120, 6369.

Remember: Q-range determines the spatial properties that are observable. A typical range (IN16, IN5) is  $0.2 - 2 \text{ Å}^{-1}$   $3 - 30 \text{ Å}$ , a  $Q_{max} = 5 \text{ Å}^{-1}$  gives  $d_{min} = 1 \text{ Å}$ .



# MIRACLES brings a **paradigm shift to neutron backscattering** with 17.7M€

- ✓ Full coverage of the analyser angle, as well as detector area.
- ✓ Matchless flux and excellent sample environment.
- ✓ Outstanding signal/noise ratio.
- ✓ Very large Q-range and even broader elastic energy resolution coverage.

DSC data: M.L. Martins & H.N. Bordallo,  
private communication.

# MIRACLES brings a **paradigm shift to neutron backscattering** with 17.7M€

- ✓ Full coverage of the analyser angle, as well as detector area.
- ✓ Matchless flux and excellent sample environment.
- ✓ Outstanding signal/noise ratio.
- ✓ Very large Q-range and even broader elastic energy resolution coverage.

A relative large number of intracranial diseases can show restricted diffusion and may therefore appear bright on diffusion-weighted images. An incomplete listing by category of disease is shown below, with the most common examples highlighted in red:

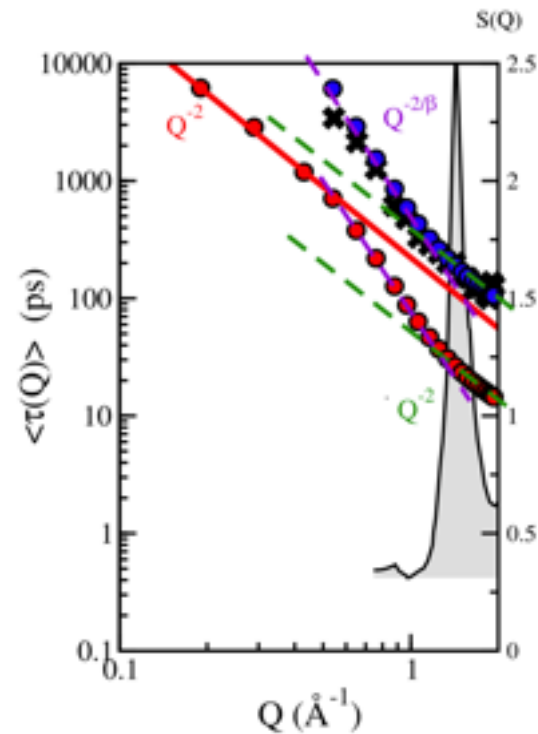
Category	Examples
Vascular	<b>Infarction (venous or arterial), diffuse hypoxic injury, posterior reversible encephalopathy (PRES)</b>
Neoplastic	<b>Lymphoma, epidermoid, xanthogranuloma</b> of choroid plexus, medulloblastoma, malignant glioma, malignant meningioma, primitive neuroectodermal tumor (PNET), atypical teratoid-rhabdoid tumor, metastases
Infectious	<b>Abscess, empyema,</b> meningoencephalitis (herpes), Creutzfeldt-Jakob disease
Traumatic	<b>Hematoma, diffuse axonal injury (DAI), Wallerian degeneration, status epilepticus,</b> contusion
Toxic/Metabolic	<b>Carbon monoxide (CO), drugs</b> (heroin, vigabatrin, carbamazepine, methotrexate), <b>hypoglycemia,</b> hyperglycemia, Wernicke's, congenital biochemical disorders (phenylketonuria, glutaric aciduria, urea cycle defects, maple syrup urine disease, Canavan's, many others)
Demyelinating	<b>Acute disseminated encephalomyelitis (ADEM),</b> osmotic demyelination, multiple sclerosis, delayed post-anoxic encephalopathy, Marchiava-Bignami

Intracranial diseases with restricted diffusion (bright on DW images)

DSC data: M.L. Martins & H.N. Bordallo, private communication.

The mechanisms responsible for restricted diffusion are incompletely understood and depend on the particular disease being considered. For many disorders several processes may act in concert to reduce the ADC.

# We have yet another benchmark: EMU



Busselez, R. et al. *J. Phys.: Condens. Matter*  
**2011**, 23, 505102.

Correct spectra of glycerol at 310K in blue and at 10K in red at  $Q=0.5 \text{ \AA}^{-1}$  measured for only 2 hours after one week of QENS data collection on EMU. Private communication.



EUROPEAN  
SPALLATION  
SOURCE



ESS  
bilbao



Jose Luis Martinez  
Project Leader



Felix J. Villacorta  
Instrument Scientist



Paula Luna  
Mechanical Design and  
CAD

Iñigo Herranz  
Neutronic Design