

# BIFROST@ ESS & GAPS (CRG) @ ILL

Ph . Bourges (LLB)



- 1) ESS Symposium on spin dynamics in correlated electron systems, feb 2012 Abingdon, UK (A.T. Boothroyd)
- 2) Science and Scientists @ **ESS** - conference: Berlin in April **2012**.

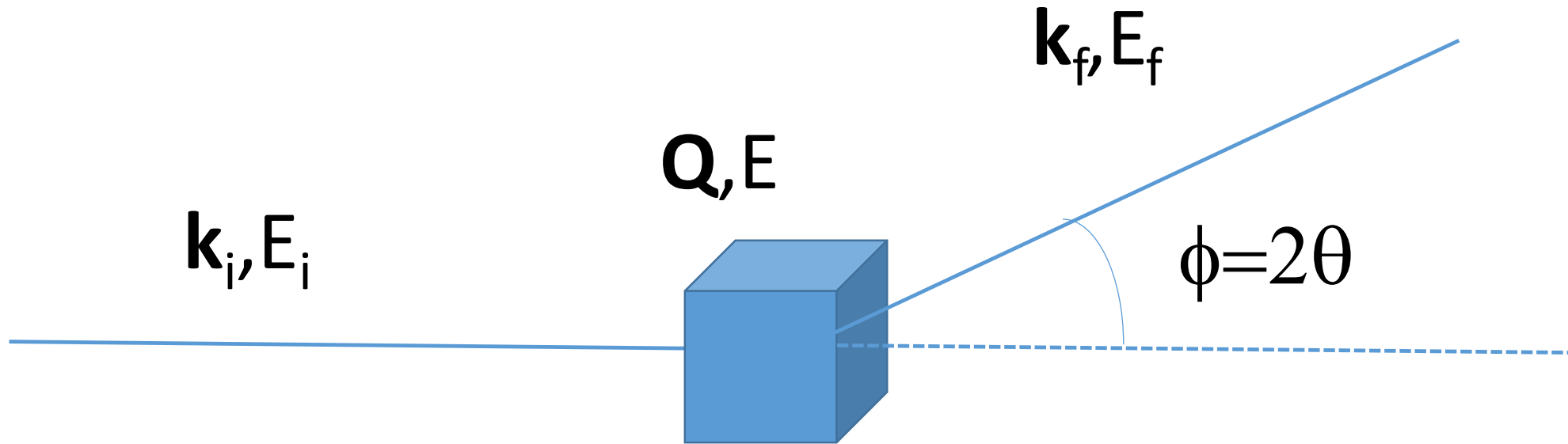
In addition to TOF instruments (Q,E-mapping), one needs:

- Parametric studies on external parameters (Temperature, Field, Pressure,...)
- Full Polarization Analysis (LPA, Polarimetry,...) → time-consuming

→ (Advanced) Triple-Axis

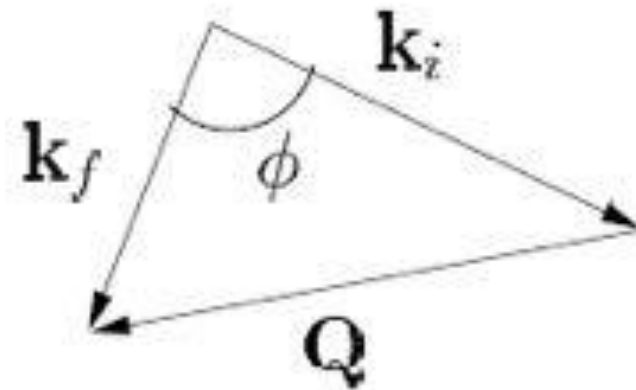
Diffusion inélastique de neutrons:

$$E = \frac{h^2}{2 M n \lambda^2} = \frac{\hbar^2 k^2}{2 M n}$$



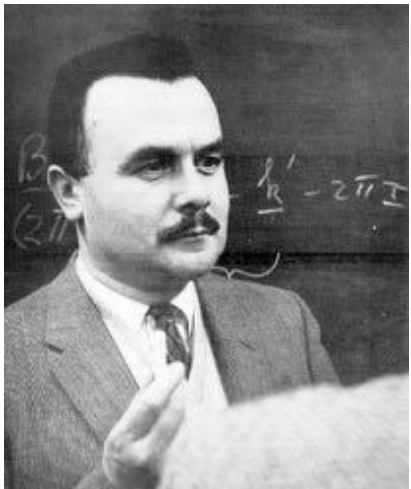
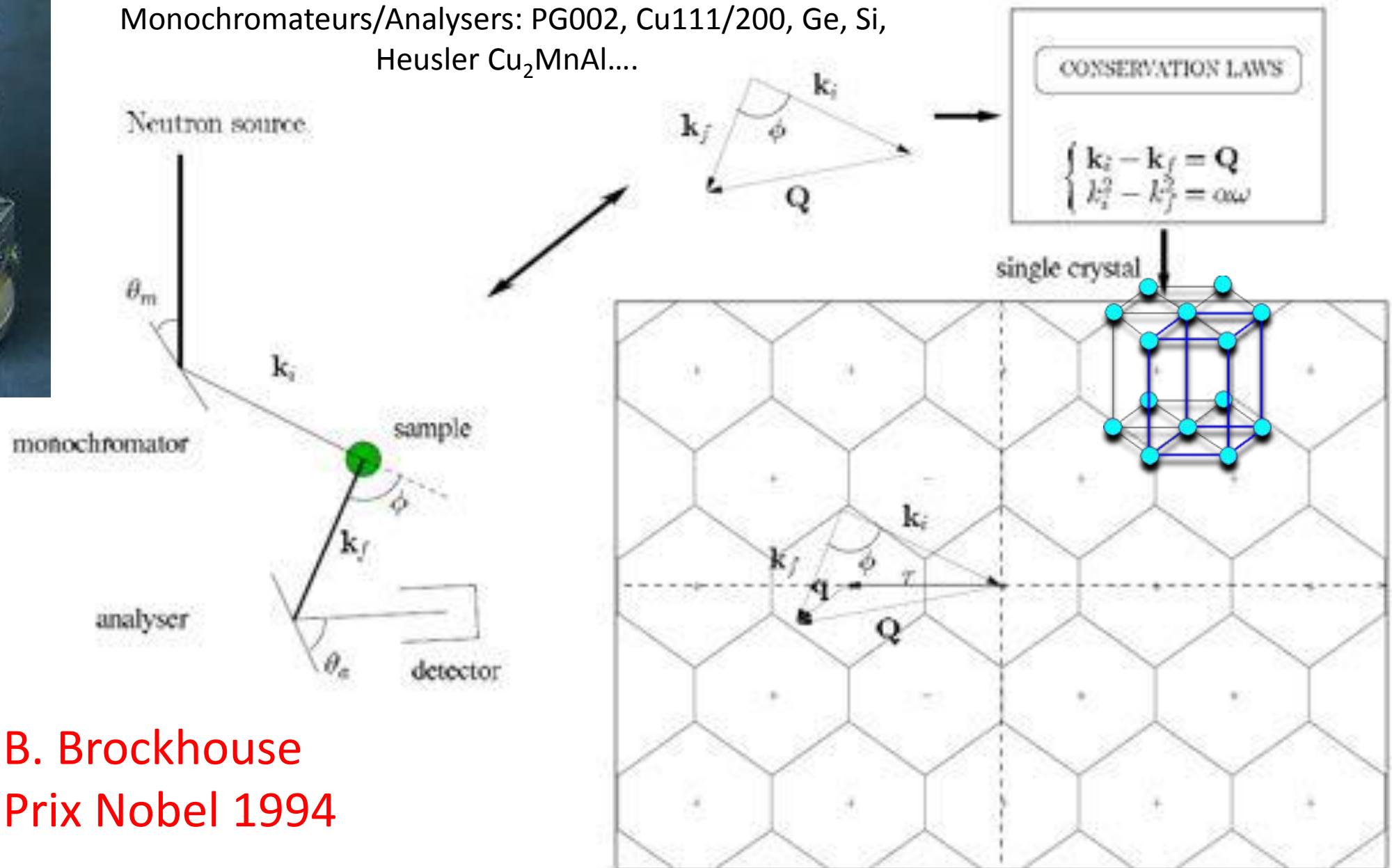
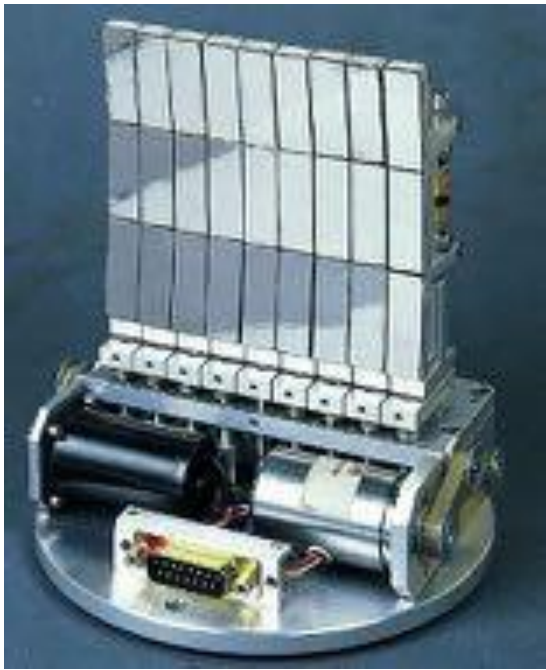
Lois de conservation:

$$\mathbf{k}_i = \mathbf{Q} + \mathbf{k}_f$$
$$E_i = E + E_f$$



# Spectromètre à 3 axes → Excitations (phonons & magnons)

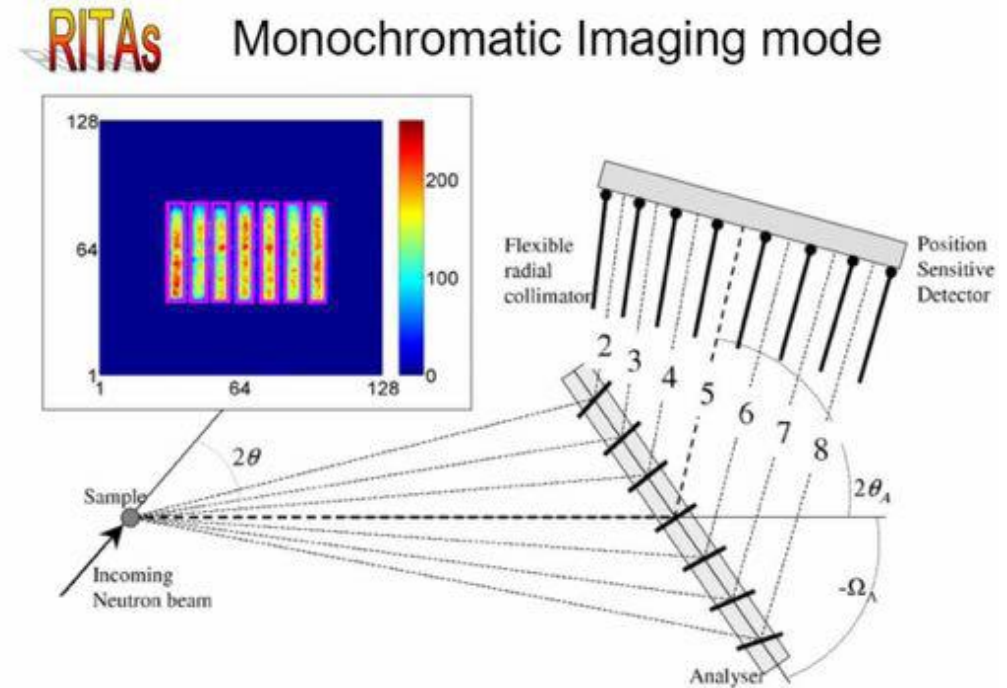
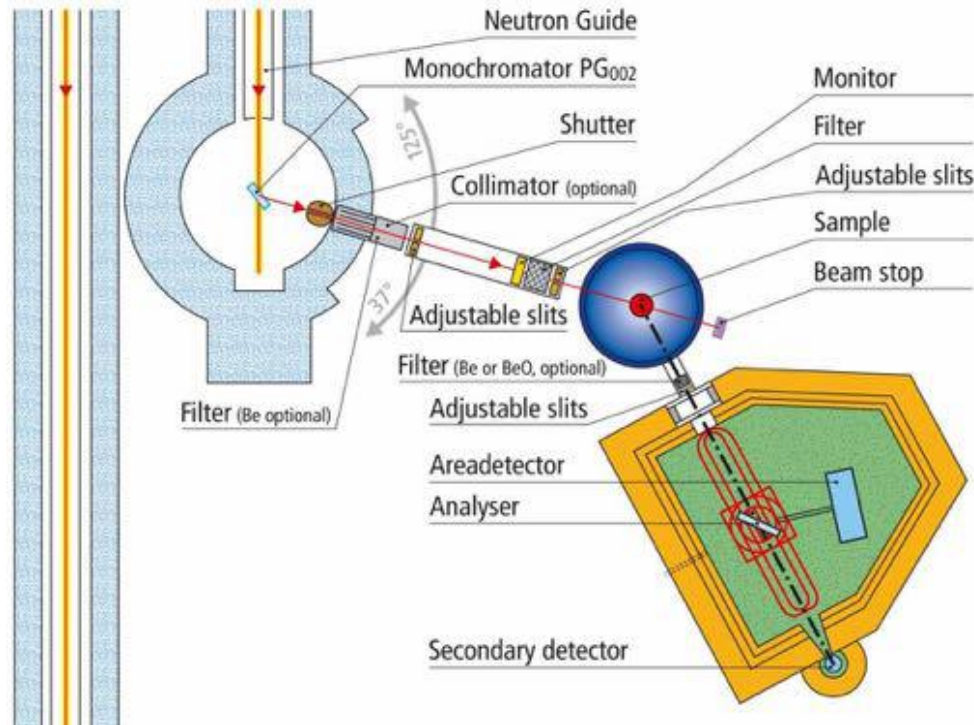
Monochromateurs/Analysers: PG002, Cu111/200, Ge, Si, Heusler  $\text{Cu}_2\text{MnAl}$ ....



B. Brockhouse  
Prix Nobel 1994

# Multiplexing 3-axes (more than point by point)

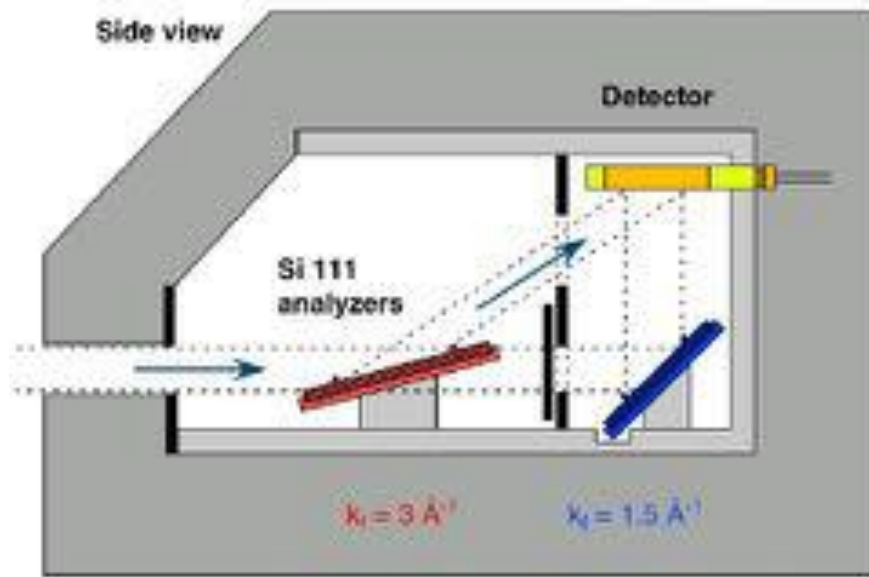
Multi-analyzer: RITA (Riso-1995), RITA-II (PSI-Riso, 2005), IMPS (IN8-ILL 2005), UFO (IN12-ILL, 2015)....



Problems: background, low ratio signal/noise...

M. Kempa et al, Physica B, 385-386, 1080 (2006)

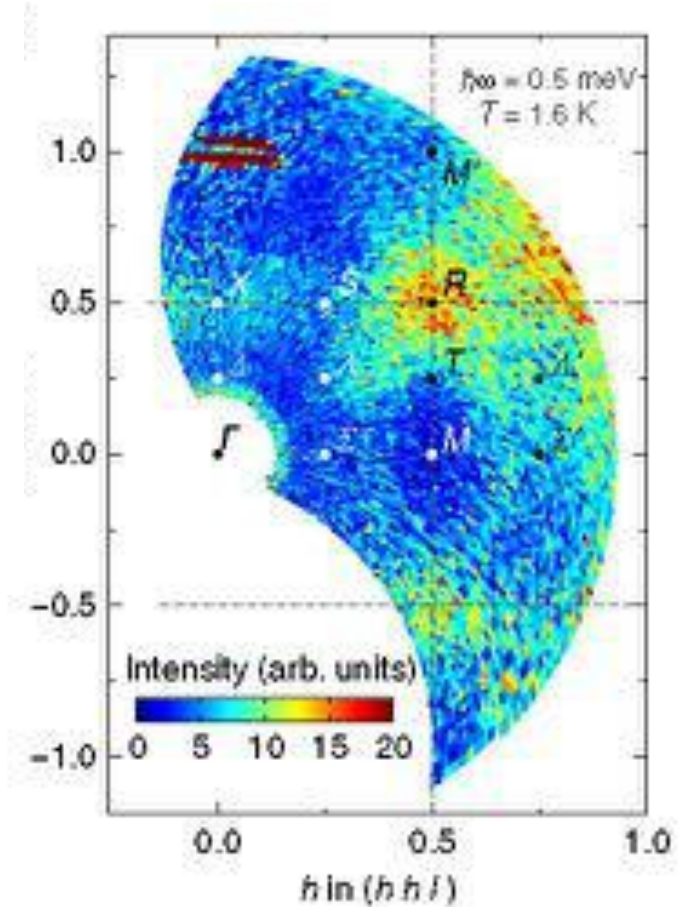
IN14 (ILL)



Covering scattering angle  $75^\circ$

Antiferro-Quadrupolar  
Phase in  $\text{CeB}_6$

« resonant magnetic  
exciton mode »



G. Friemel et al, Nat. Phys. 3, 830 (2012)

# The BIFROST (Indirect geometry)\* Spectrometer

\*3 Indirect-geometry instruments  
at ESS :  
BIFROST, VESPA and MIRACLES



BIFROST : 4 countries  
DTU/KU (Danemark) 22%  
PSI (Switzerland) 30%  
LLB (France) 24%  
IFE (Norway) 24%

## Géométrie indirecte:

« Quand l'énergie finale des neutrons est déterminée par une diffraction d'un cristal. »

(pas de vision directe de l'échantillon par le(s) détecteur(s).)



Philippe Bourges

Sylvain Rodrigues

Pascal Lavie

+ Bureau d'Etudes LLB

Yvan Sidis

**(France: 24%)**



H. Ronnov

K. Leffman

N. B. Christensen

....

**Lead scientist (DK):**

**Rasmus Toft-Petersen**

**Lead engineer (DK):**

**Liam Whitelegg**

# ESS Neutron instruments layout

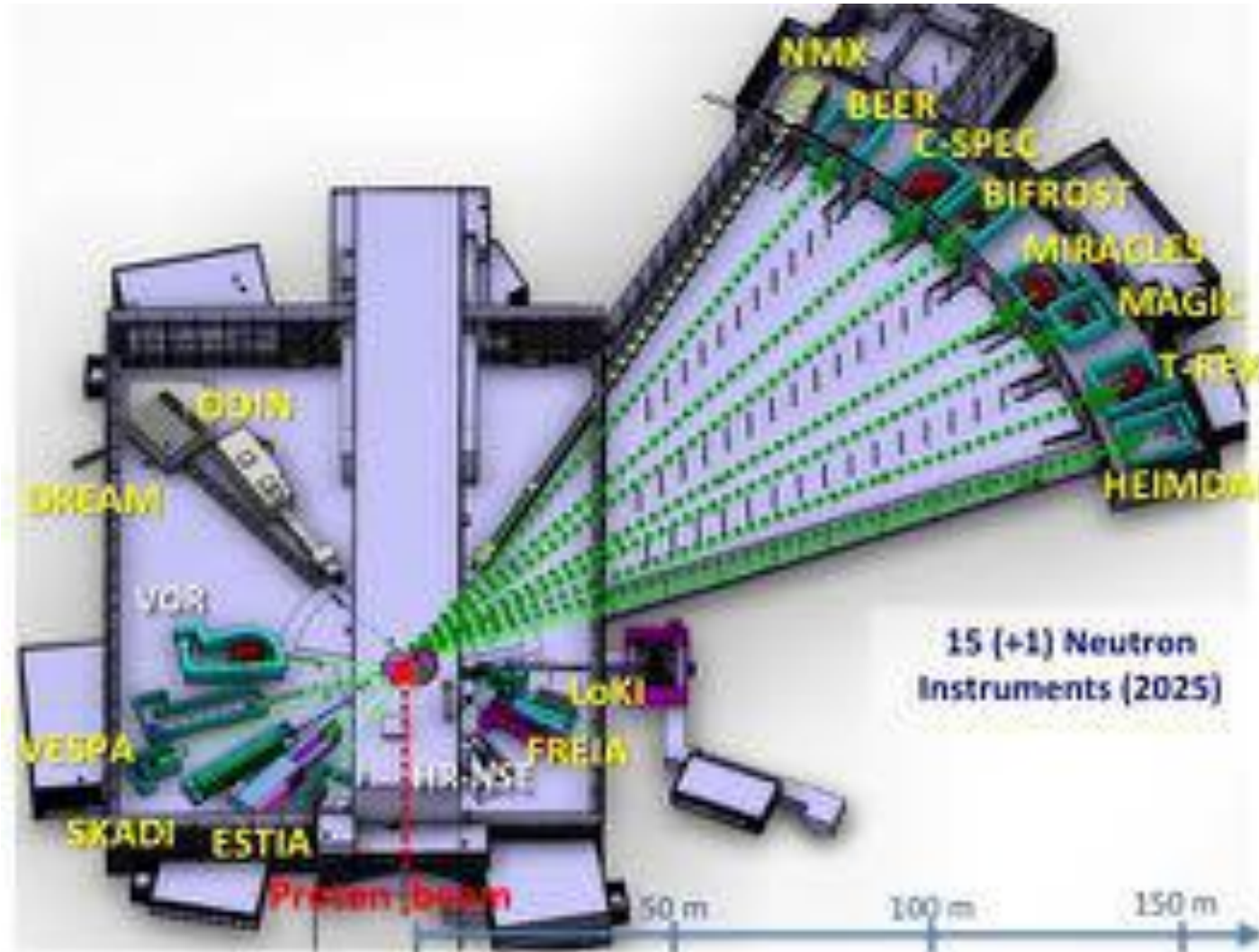
Magnetic excitations  
& Phonons

Primary Spectrometer

Time of flight  
 $E_f = 2$  to 40 meV

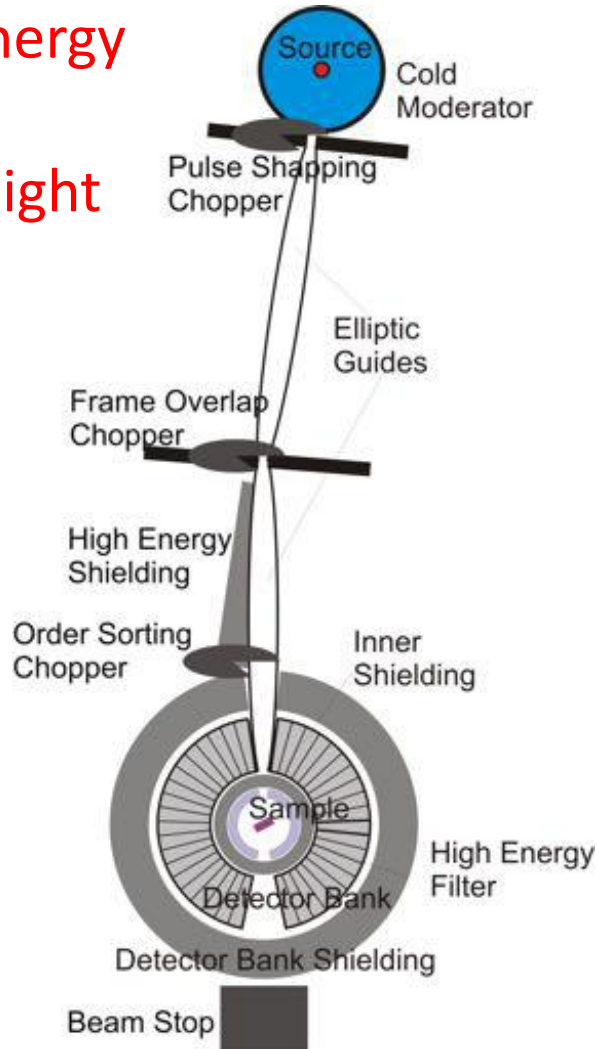
Secondary  
Spectrometer

45 HOPG analysers  
+ 45x3 PSD detectors  
(45 TAS at once)



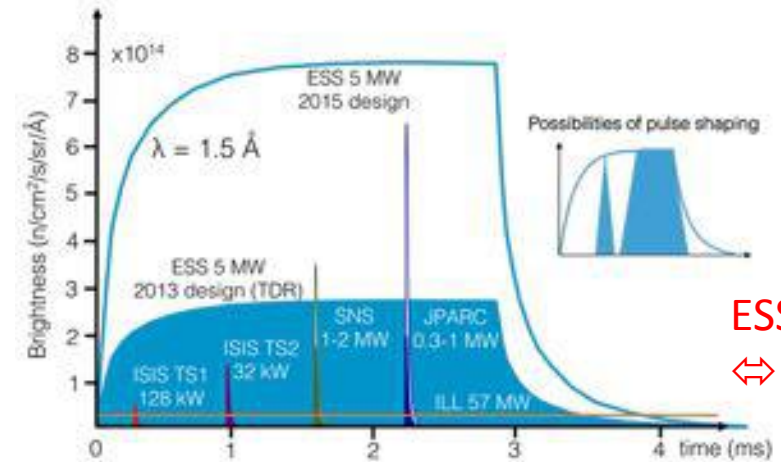
# Operating principle: primary spectrometer

Incident energy  
↔  
Time of Flight

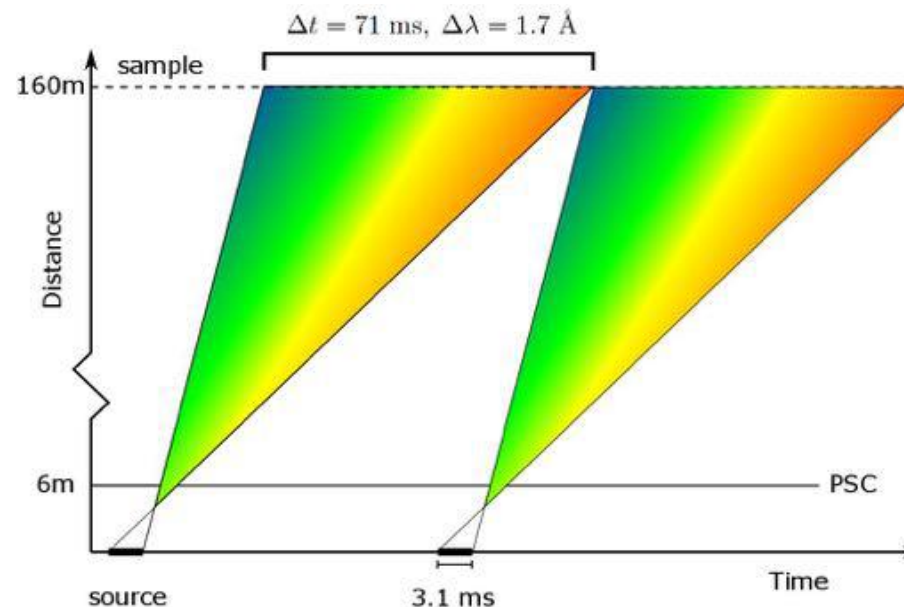


Combine a long instrument with long-pulsed source.

Flight time: 100 ms



ESS 14Hz  
↔ 71 ms

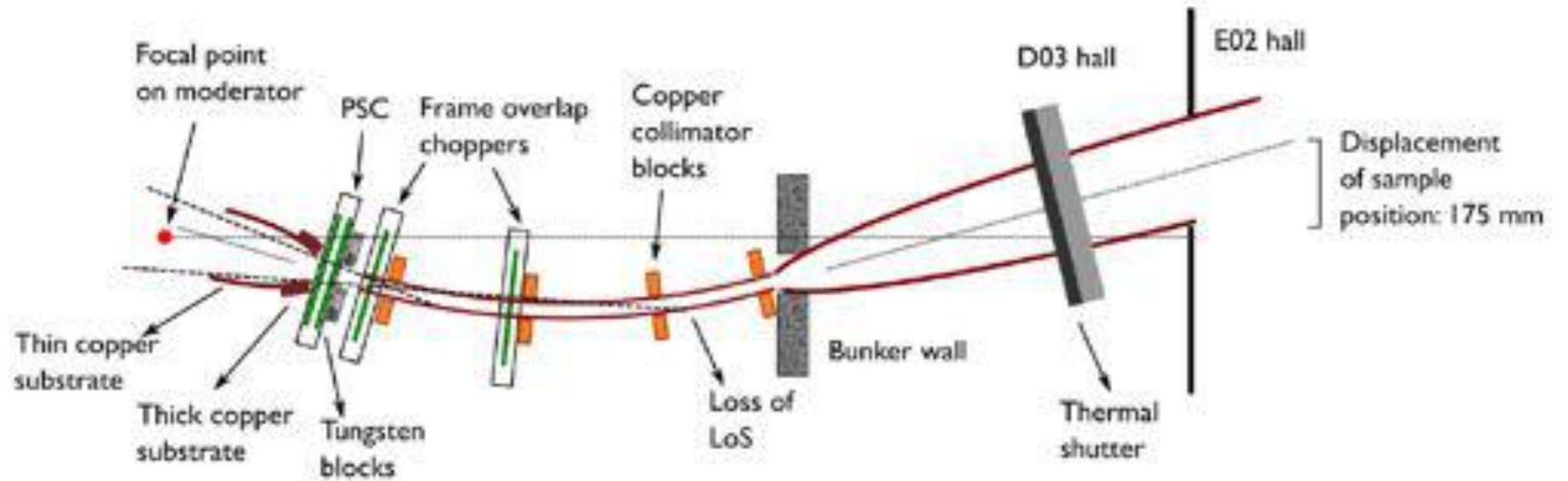


Non-stop  
Measurements  
Band 1.7 Å

Pulse shaping  
Chopper

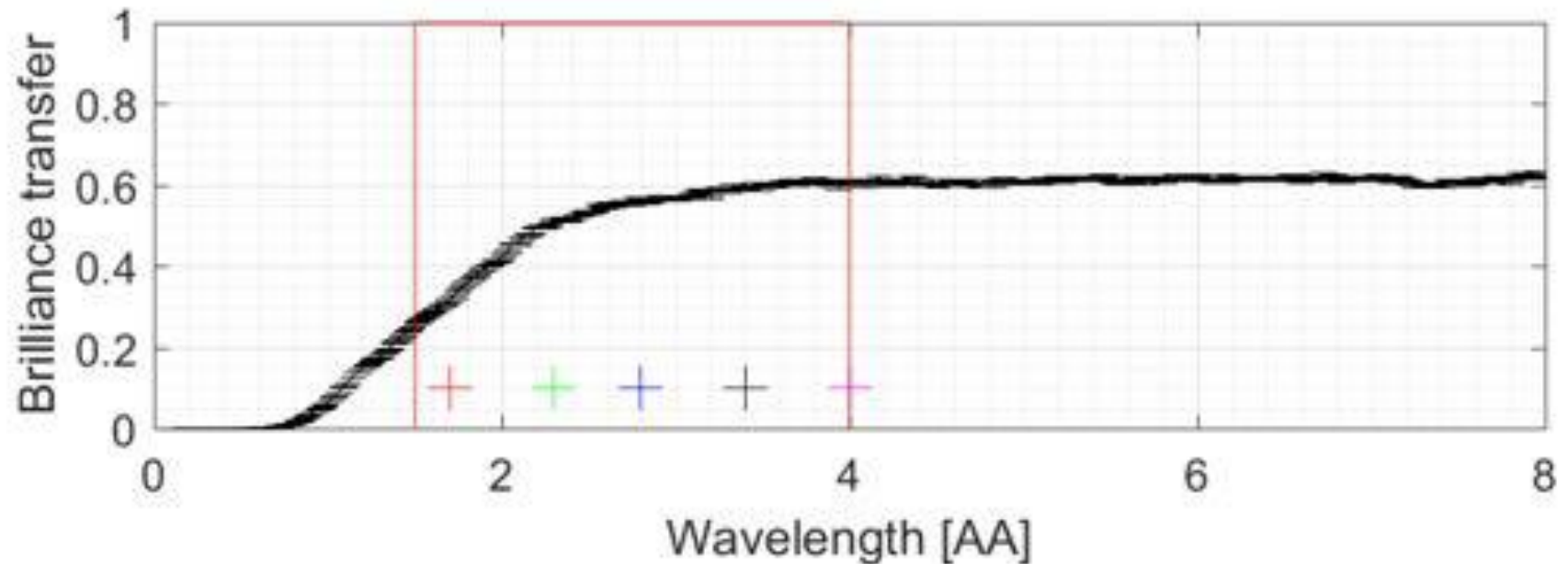
# Guide system: 150 m

Horizontal kink  
to remove  
Line of sight

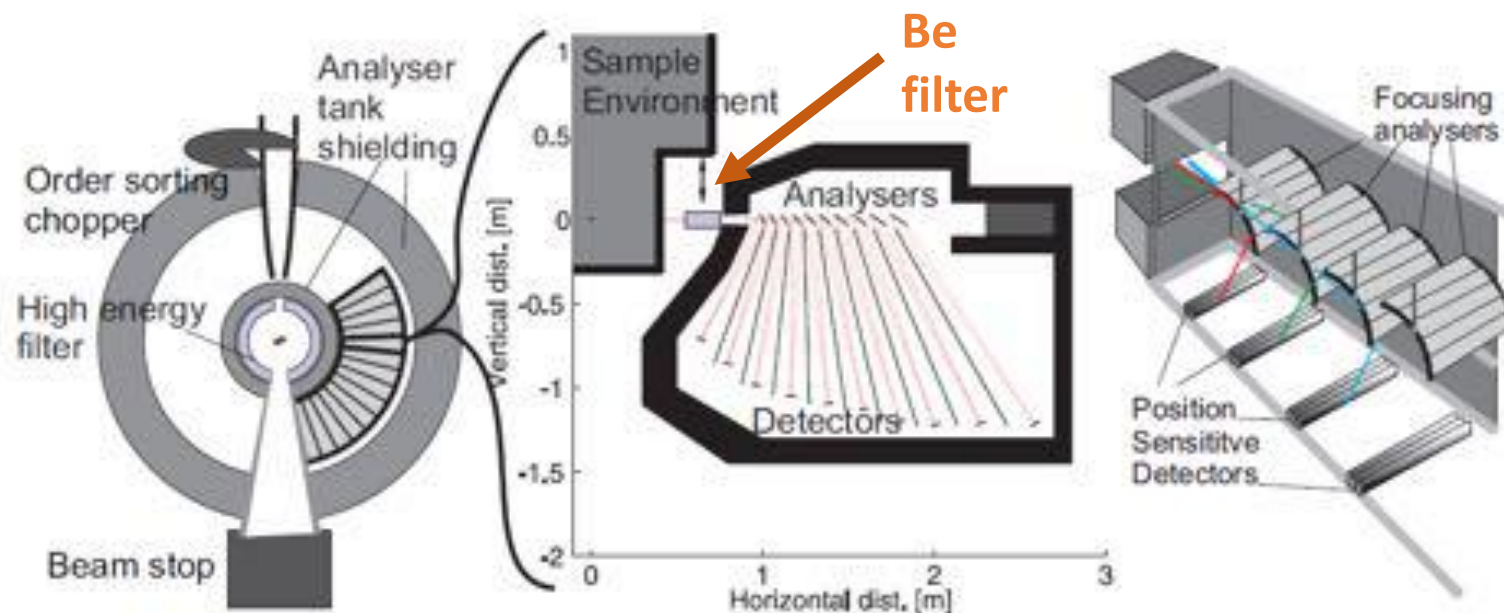


McStas simulations:

Jonas Birk,  
Kim Leffman  
KTU/DK

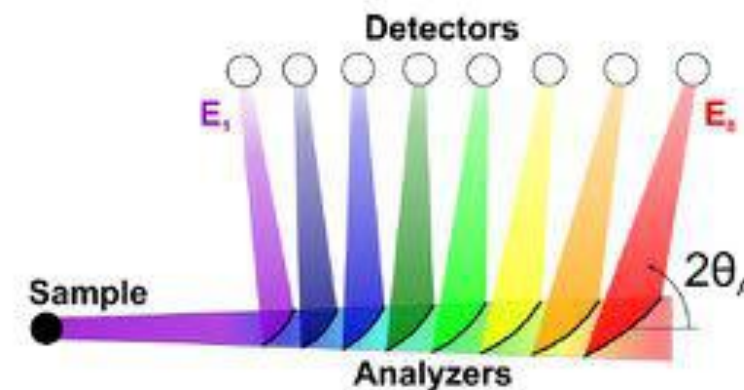


# Operating principle: secondary spectrometer



Final energy  
↔  
Diffraction PG 002

H. Ronnov: CAMEA- PSI  
(2018/2019)

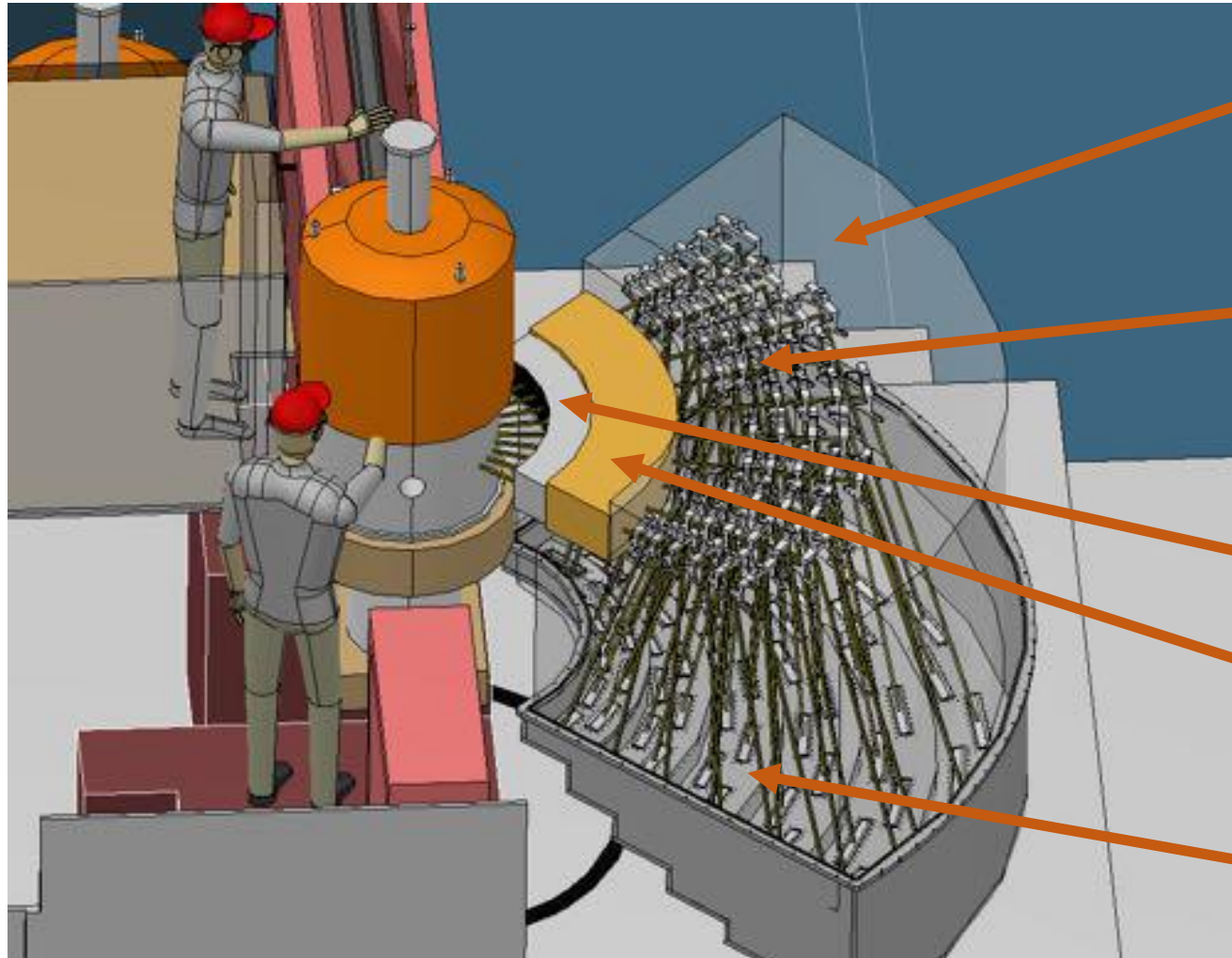


- Out-of-plane scattering (as flatcone): downward
- Pyrolythic graphite is transparent at  $E < 5$  meV  
(Be filter for low background)
- We can over 0.5 ster in the **horizontal scattering plane**:  
**A compression of the capabilities of a TOF spectrometer**

F. Groitl et al, Rev. Sci. Int. 87 035109 (2016)

Future Projects: MARMOT, BAMBUS,...

# Compact secondary spectrometer



Spectrometer  
vacuum tank

9 tranches x 5 analysers  
→ 45 independent  
PG analysers

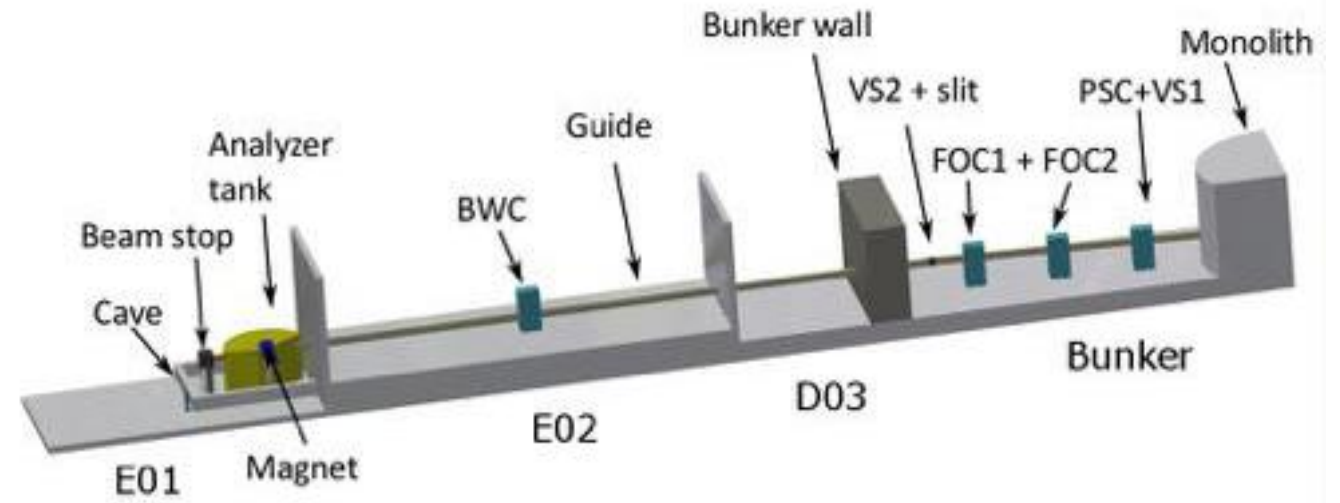
**$E_f = 2.7, 3.2, 3.8, 4.4, 5$  meV**

Be filter

Radial  
collimator

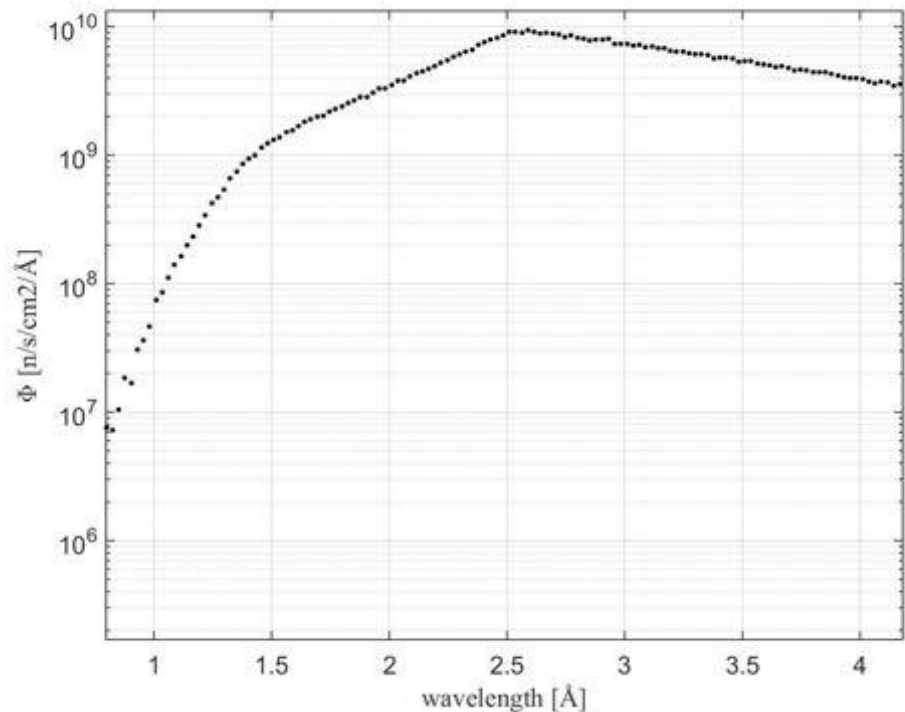
45x3=135 He<sup>3</sup> PSD  
detectors

# Accepted project: 13.44 M€



- Couverture angulaire réduite ( $2\theta_s$ ): 90 deg (9 tranches de 10 deg)
- 5 analyseurs par tranche → 45 detecteurs
- Polarization en option possible.... Idem champ magnétique intense (>15T) → 2030 ?
- Sample Environment: will need cryostat (SAS cryogenerator), 10T magnet and dilution fridge  
→ many sample sticks (due to activation)
- France:
  - 4 Choppers: 1 Pulse Shaping Chopper (PSC) 14Hz-210Hz + 3 choppers lents 14Hz
  - Detecteurs:  $^3\text{He}$  tube PSD à 5 bars ( $\Phi = 12$  mm): 9 tranches x 5  $E_f$  x 3 = 135 dectecteurs de 230 mm)(Suisse: Guides, Pg Analysers, Be filter, Norvège: Shielding, Cave., Danemark: Enceinte, Collimator...)

# High Performance : 45 TAS + 1.7 Å incident neutron band



Energy resolution: from TOF to TAS  
 $\Delta E/E \sim 1-5\%$

- Very high incident flux  
(up to  $10^{10}$  n/s/cm<sup>2</sup>)
- Versatile sample environment:
  - High magnetic field (0-15T)
  - High pressure cell ....
- Small samples
- Parametric studies
- High Energy-resolution achievable

Day 1 Performance (2MW)  
world-leading

\*Upgrade path : Polarization analysis with either He<sup>3</sup> filter or wide-angle bender (>2030)

# science topics today

Courtesy  
A. Hiess (ESS)



data: ILL

# Science case

from Quantum Matter & Magnetism .....  
to Geoscience, Bioscience (with small samples)

## Resonance modes in **unconventional superconductors**

Stock et al, Raymond et al PRL 2008, 2012, 2015, 2017

## Quantum Magnetism, **Quantum phase transitions, Frustration**

Coldea et al, Science 2010, Petit et al, Nature Phys (2016), Faure et al, Nature Phys (2018)

## **Strongly correlated electrons. Mapping Q- $\hbar\omega$ space, multiferroics**

Jang et al, Nat. Comm (2014); Portnichenko PRL 2016

## **Cuprate high-temperature superconductors: Resonance mode dispersion & Field**

Bourges et al, Science (2000) Dai et al, Nature (2000); Tranquada, PRB (2004)

## **High-field: The resonance mode as a spin triplet?**

(Today we have insufficient resolution at high energies)

Lorenzo et al, PRB (2007).

## **Discrete spin waves in multilayers / magnonics**

Grünwald et al, PRB (2010)

## **High-pressure: Phonons in 200K superconductor**

Drozdov et al, Nature 2015

## **Dynamics in organic superconductors**

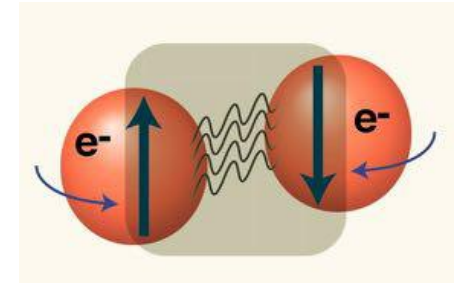
Dressel, Crystals 2012

## **Water diffusion in the GPa range**

Bove et al PRL 2013

## **Collective dynamics in membranes**

Rheinstädter et al PRL 2004



## Example: superconducting pairing ?

Some ideas requiring high energies/polarization/field

- The normal state spin fluctuations as **pairing glue**?
- **Loop current** fluctuations ?
- Tuning competing orders and their excitations with a field

- Complex continuous spin excitation spectra in quantum magnet and strongly correlated electrons:  $Q_{2D}-\hbar\omega$  maps with polarized neutrons to disentangle spin and lattice
- Spin-waves in more & more complex **helimagnets**
- **Pressure studies:** Magnetic phase diagram (spectrum) ?
- High energy resolution & pressure for Phonons  
(**Thermoelectrics & Photovoltaics**)

• ...

When: among the first 8 instruments → 2024/25



# GAPS

## ***Get Access to a Polarized Spectrometer !***

**3-axes LLB group :**

Ph. Bourges, J.P. Castellan,  
J.M. Mignot, S. Petit, Y. Sidis

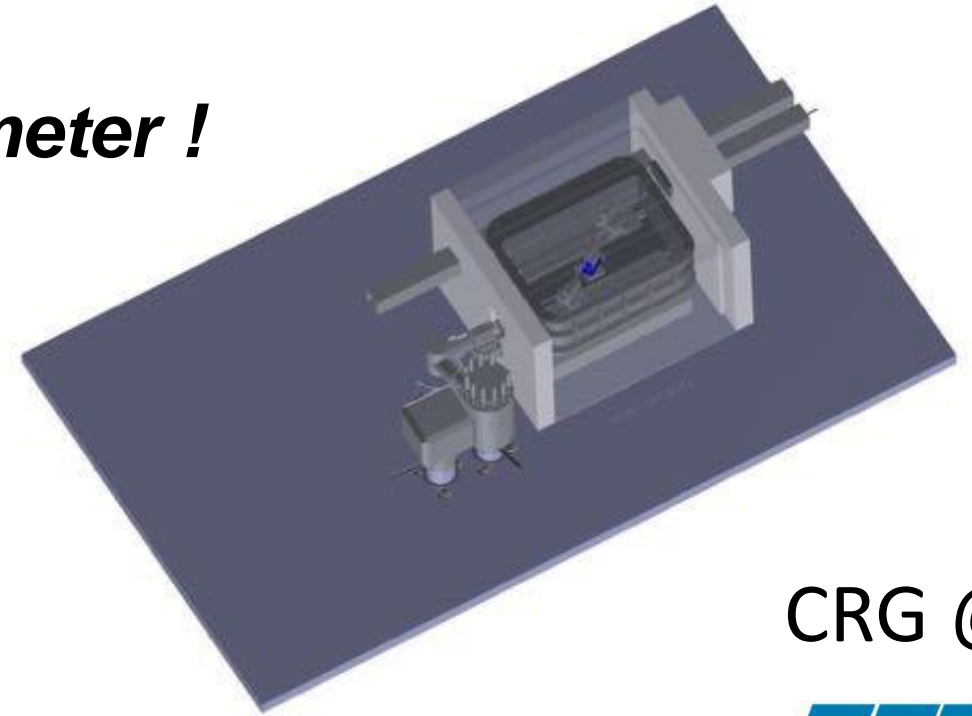
Ph. Boutrouille, F. Maignen, C. Meunier

*TAS fully equipped with polarization analysis with  $\mu$ PAD*

**Increase capacity for polarized neutron spectroscopy in Europe.**



*So far for spectroscopy, polarization analysis is not present in their day-1 scope and budget.*



CRG @





# GAPS

## Capacity for polarized neutron spectroscopy in Europe.

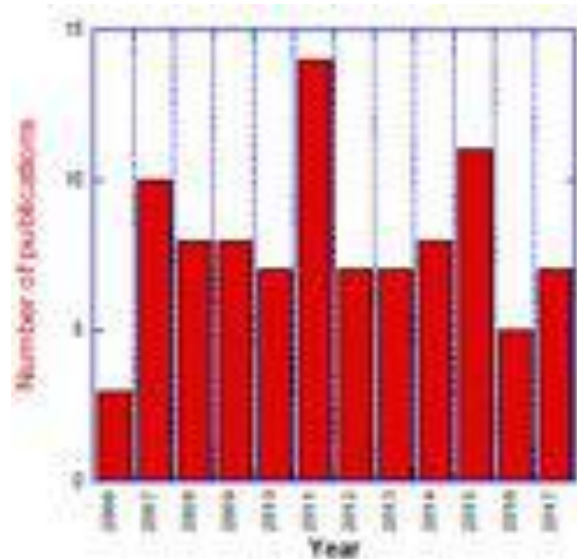
TAS fully equipped with polarization analysis in Europe

	NEUTRONS FOR SCIENCE	NEUTRONS FOR SCIENCE	Heinz Maier-Leibnitz Zentrum		Heinrich Heine Zentrum Berlin	PAUL SCHERRER INSTITUT
<b>Thermal TAS</b>	IN20	IN22	TRISP	<del>2T</del>	<del>FLEXX</del>	-
<b>Cold TAS</b>	THALES	IN12	PANDA	<del>4F1</del>		TASP
	} <i>Many options</i>		KOMPASS			<i>end 2019</i>

*different high magnetic field setups with/without dilution fridge insert*

*lattice dynamics studies with/without using spin-echo option,..)*

*Flatcone, + possible future multiplexing projects (MARMOT, BAMBUS)*



*4F1 + 4F2 publications record*

- 1 Science
- 4 Nature Pub. Group
- 14 PRL
- 40 PRB
- 1 PRX
- 4 EPJ

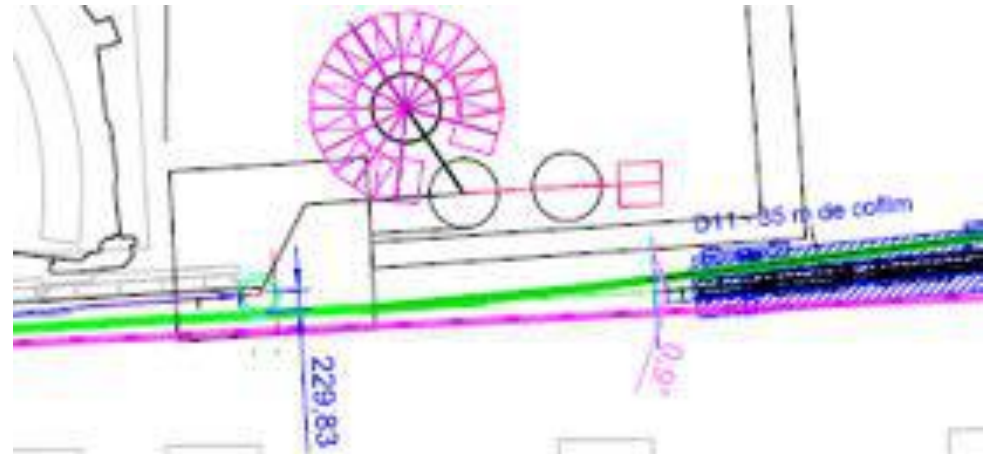
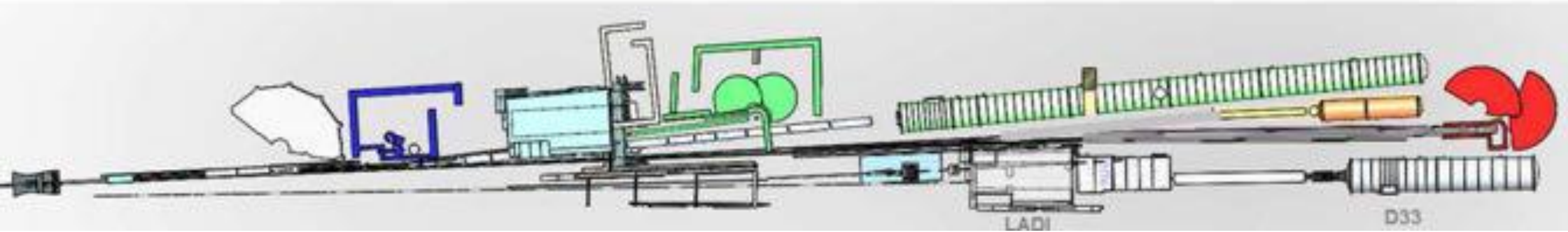


# GAPS @ ILL 2023

Endurance 2: New Guide H15 (C. Dewurst/ILL) → 3 LLB/CRG  
Section GAPS 60x200 mm<sup>2</sup>

X	D <sub>11</sub>	R
G	D <sub>7</sub>	A+
A		MS
P		S
S		S

IN5    GAPS    X    T3    D7    @H141    D11    SAM    RAMSES



Limited space (**Compact instrument**)  
 → Double HOPG monochromators  
 as 4F1/4F2 @ LLB-Orphée

# MACS – NIST, 2008

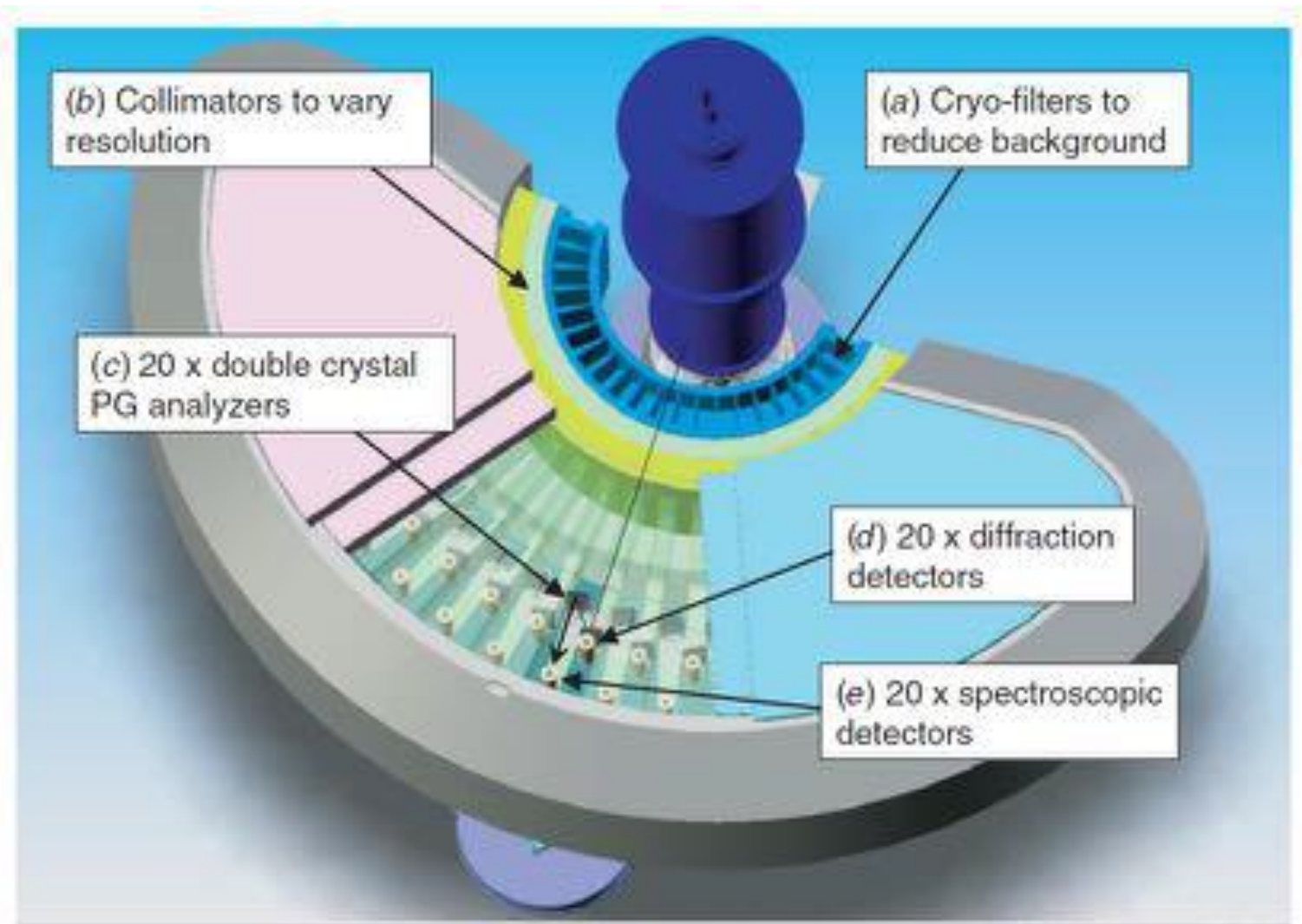
## Double PG analysers



9 PG002 crystals (6x2x0.2 cm)/ analyser

*J.A. Rodriguez et al*

[\*Meas. Sci. Technol.\* 19 034023 \(2008\)](#)

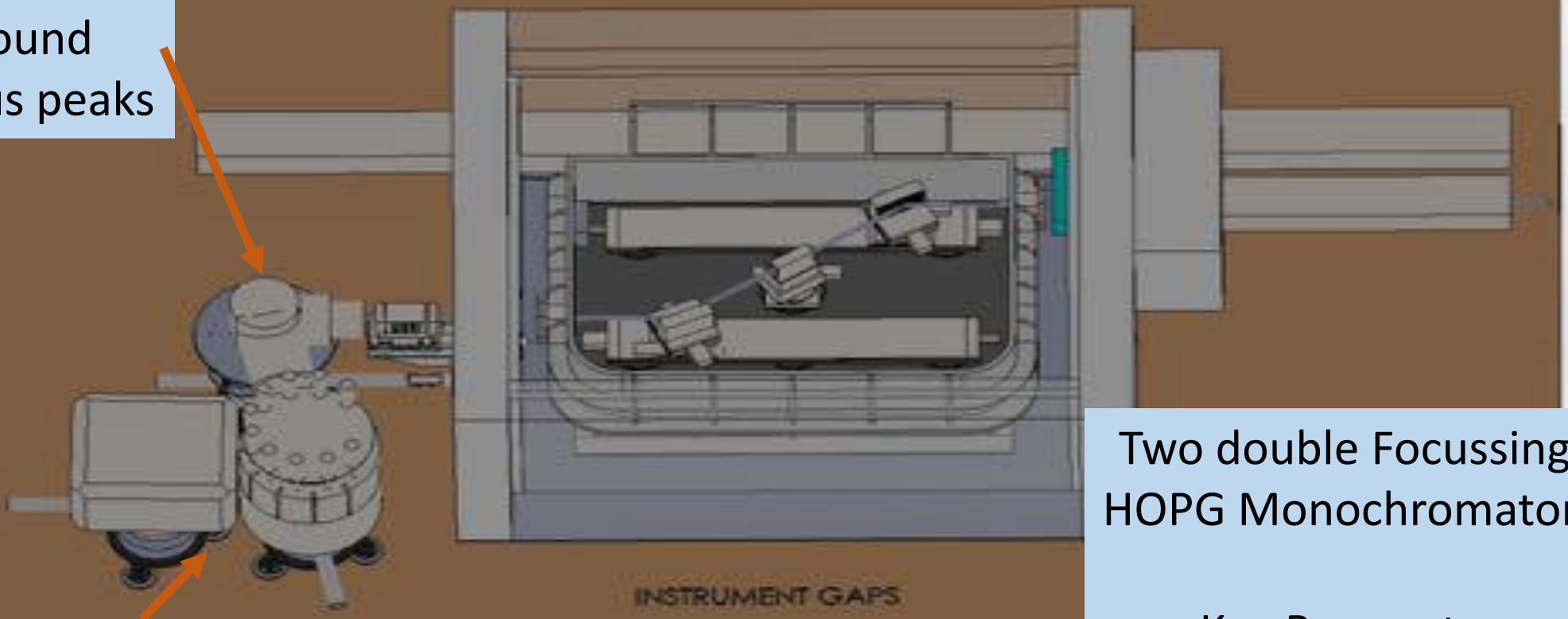


**Figure 2.** The detection system consists of 20 identical channels separated by  $8^\circ$  for a total  $152^\circ$  range of coverage in one setting. Each channel contains: (a) cooled Be, BeO or PG filter (b)  $36^\circ$ - $60^\circ$ - $90^\circ$  or open collimation. (c) Double crystal analyzer (d) diffraction detector (e) spectroscopic detector.



# GAPS @ ILL 2023

- Fixed sample Table
- Less Background
- Less spurious peaks



Secondary Spectrometer  
In-kind LLB 4F1/4F2  
Including polarisation

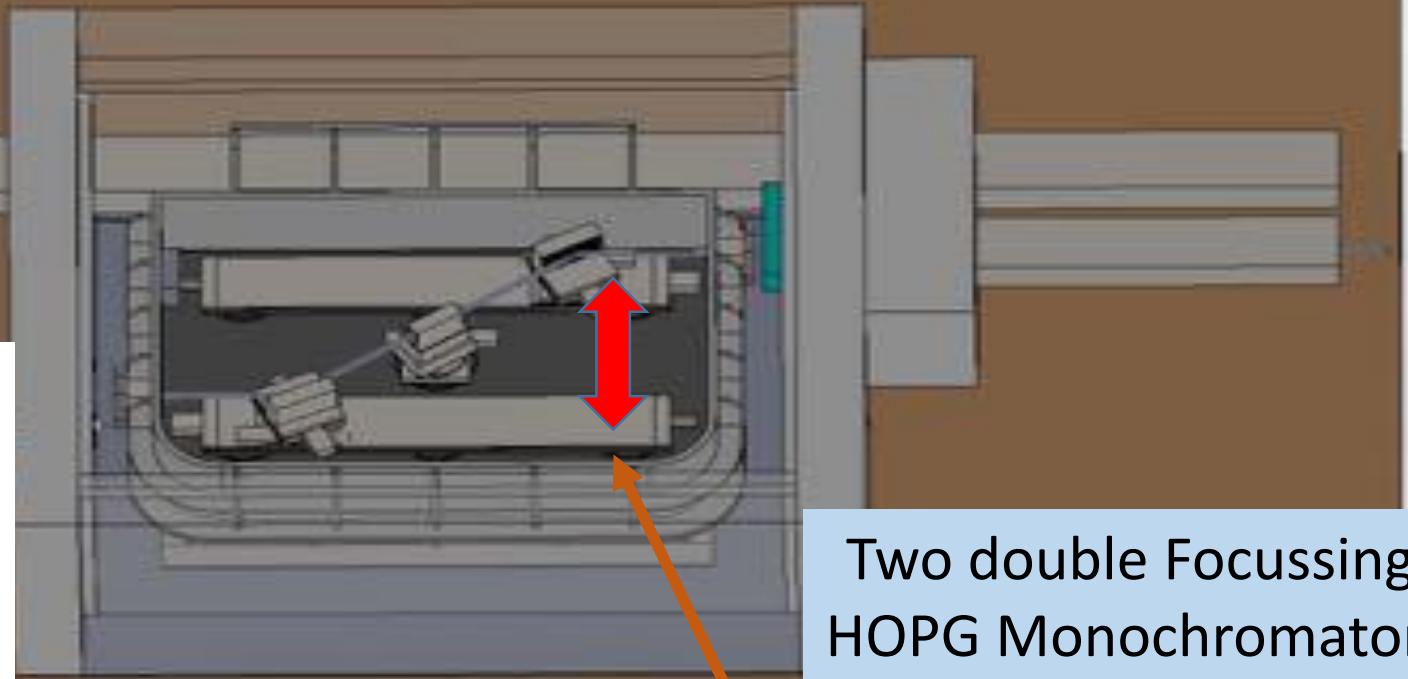
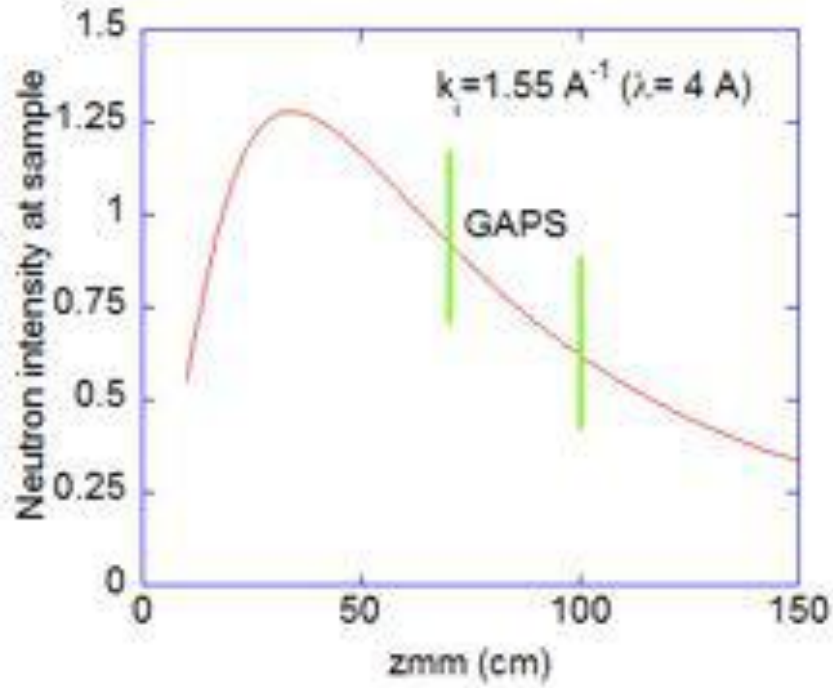
Two double Focussing  
HOPG Monochromators

Key Parameter  
Distance between  
Both Monochromators



# GAPS @ ILL 2023

- Fixed sample Table
- Less Background
- Less spurious peaks



Two double Focussing  
HOPG Monochromators

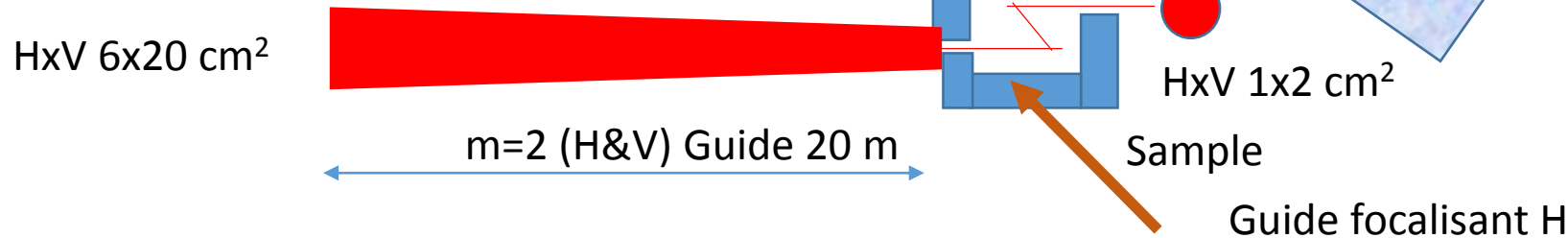
Key Parameter  
Distance between  
Both Monochromators

# World Class instrument

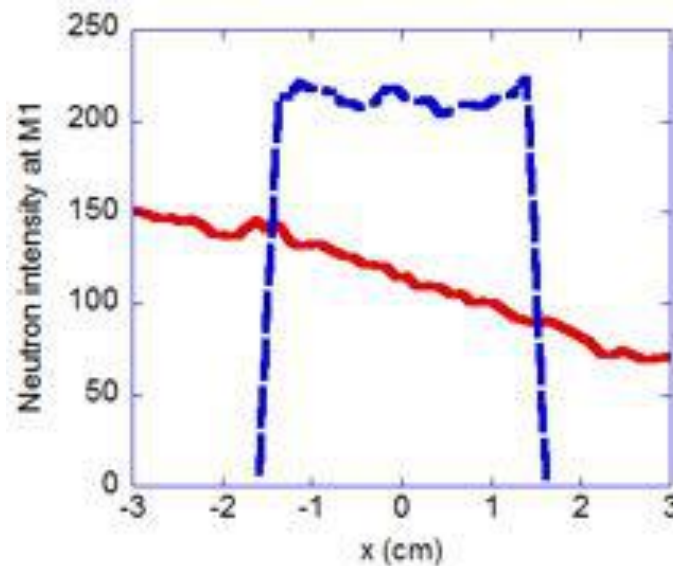
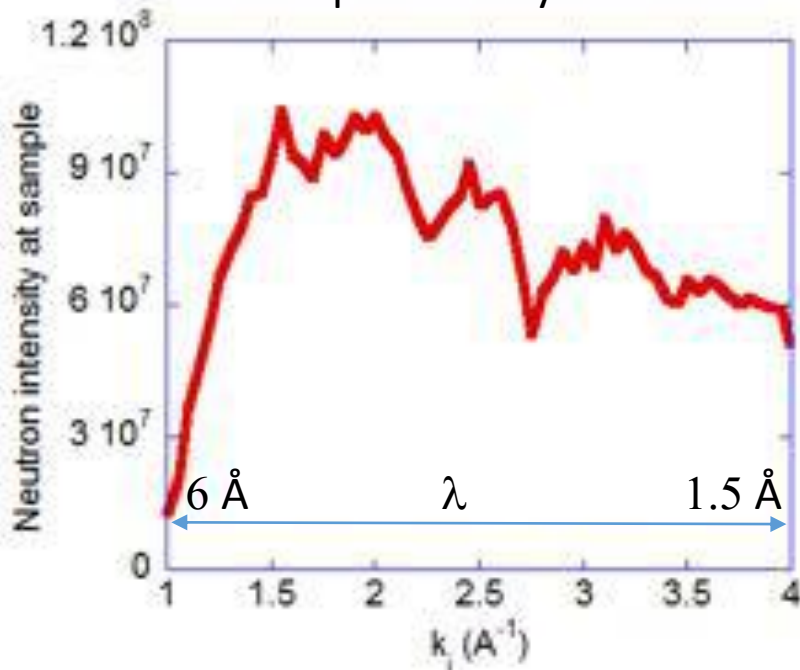
# GAPS

Instrument simulation:

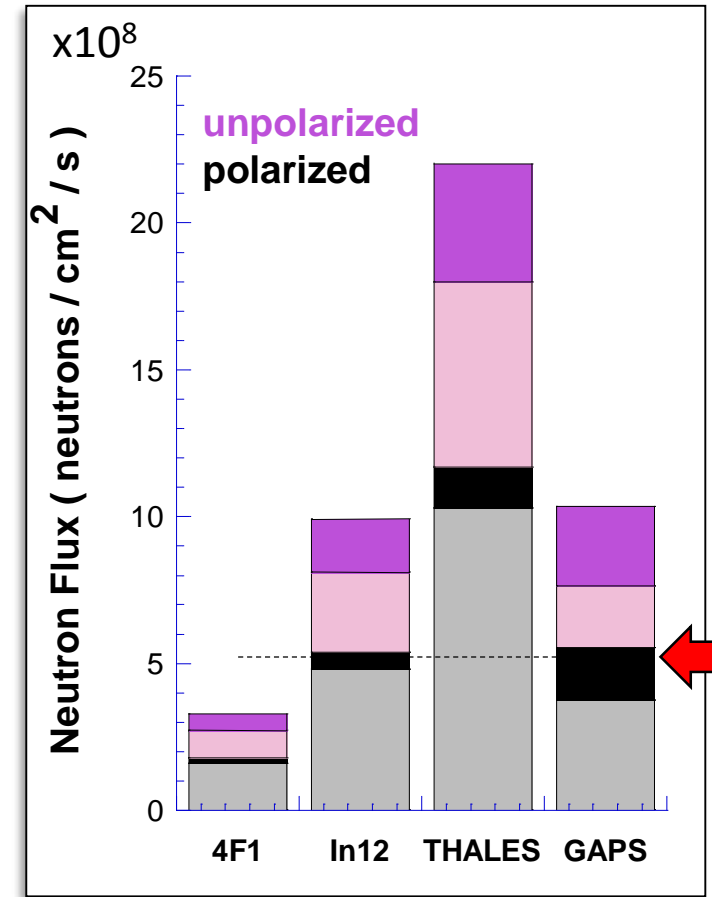
- Analytic calculations: Cooper-Nathans/Popovici  
Beam geometries & sizes B. Hennion (SFN 2010)
- Monte-carlo calculations McStas



McStas preliminary results



- Diffraction with polarization (FR from 30 to 80) → P ~ 0.93-0.97
- Cold neutron from 2 to 35 meV ( $k_i = 1$  to  $4 \text{ \AA}^{-1}$ )
- Complement IN12/Thales

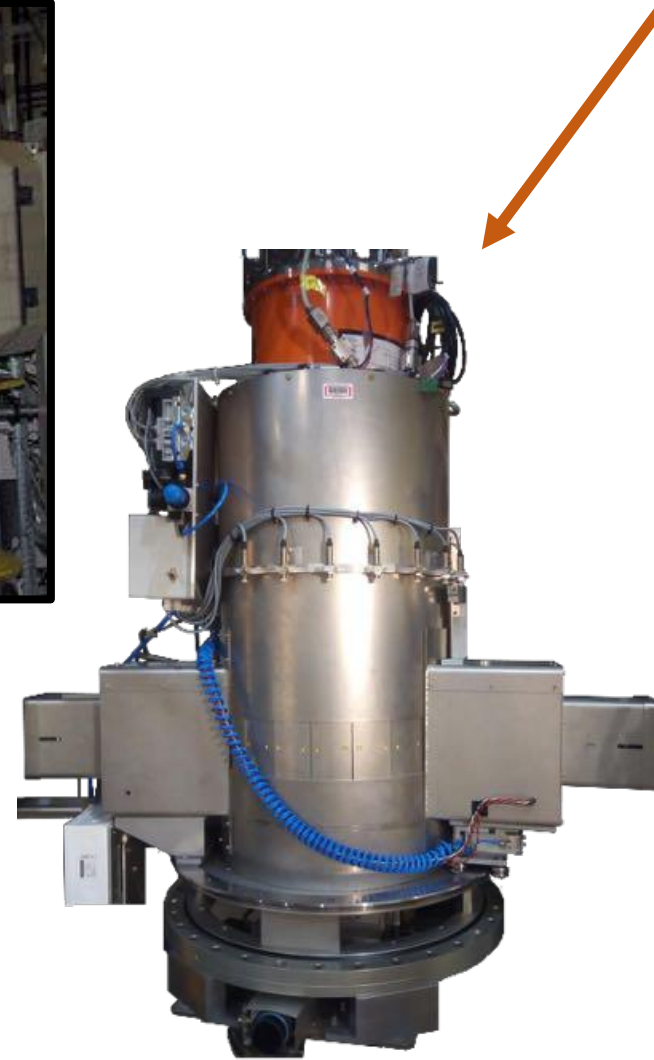
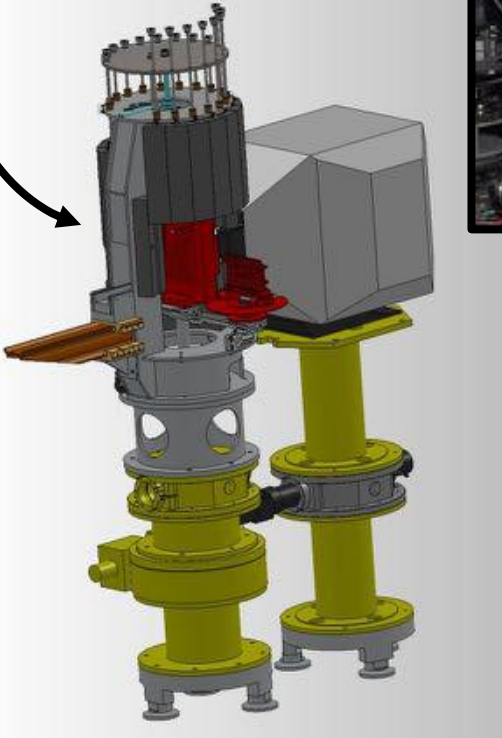


# In kind from 4F1/4F2@LLB: full polarization analysis (polarimetry with $\mu$ PAD)



3 Heusler Analyzers  
High flipping ratio  
& High intensity

+  
Benders (sur  $k_i$ )  
+  
PG analysers  
+  
Be/PG filters



+  
Sample  
Environments

- 4K Cryogenerators & Cryostats
- 2 Dilution Fridge (100 mK)
- Vertical magnet 10T

*S. Klimko, F. Maignen (2017)*

## Primary spectrometer

(1) Double monochromator ~400 k€

(2) Casemate ~500 k€\*

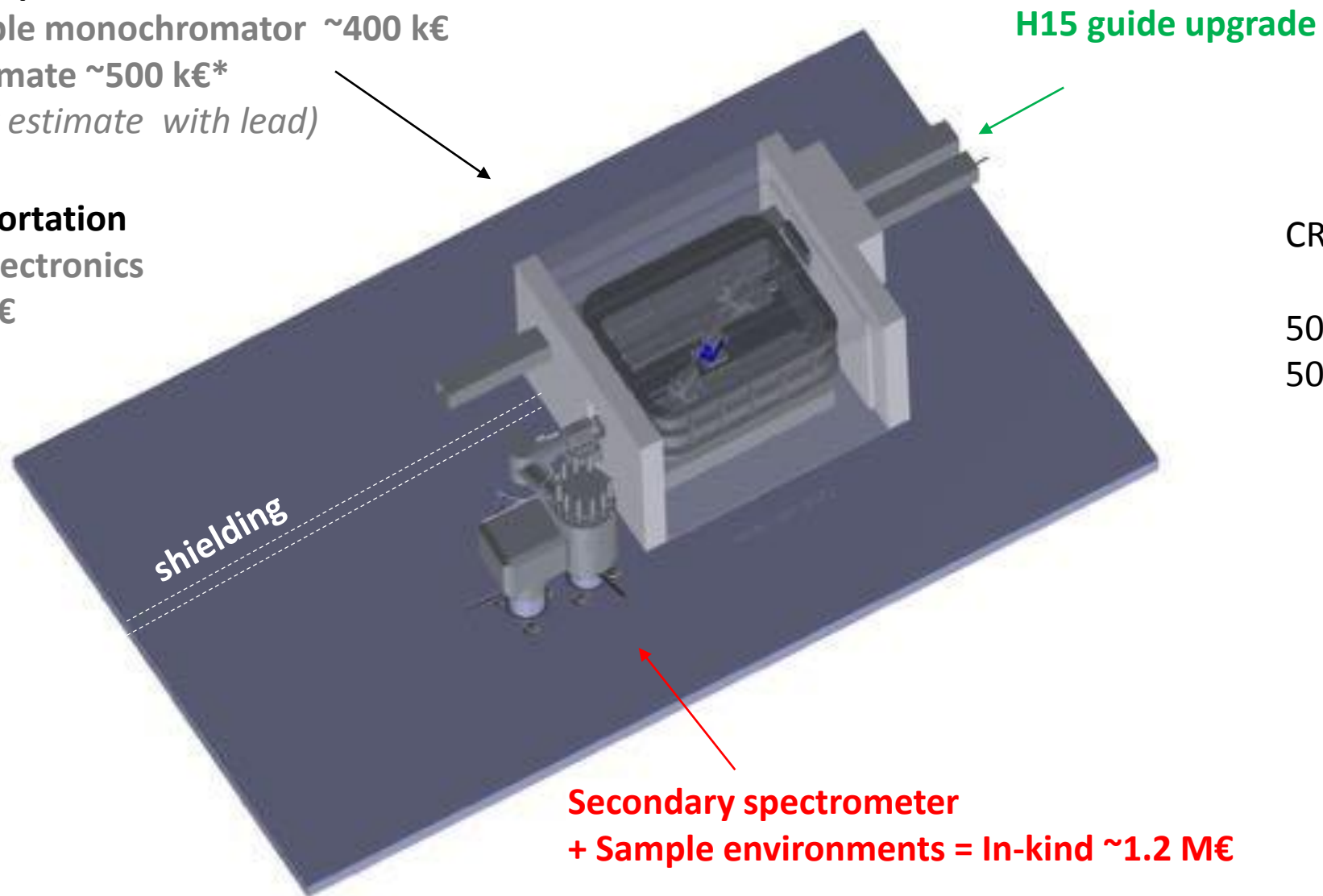
(\* upper estimate with lead)

## Transportation

+ ILL electronics

~100 k€

Total: 1M€



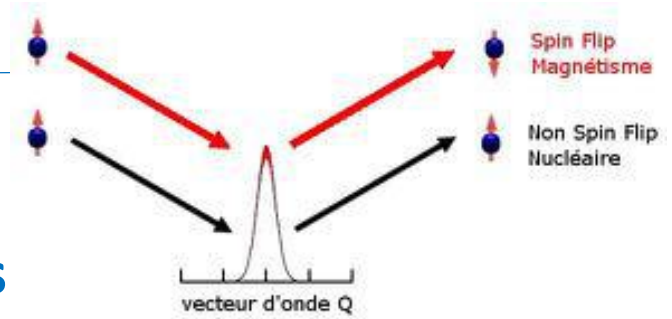
CRG type A:

50% France

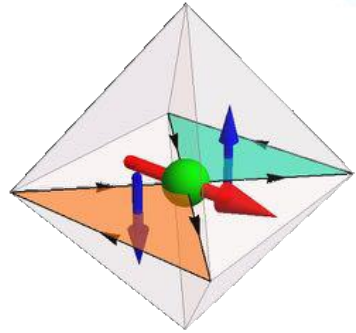
50% ILL



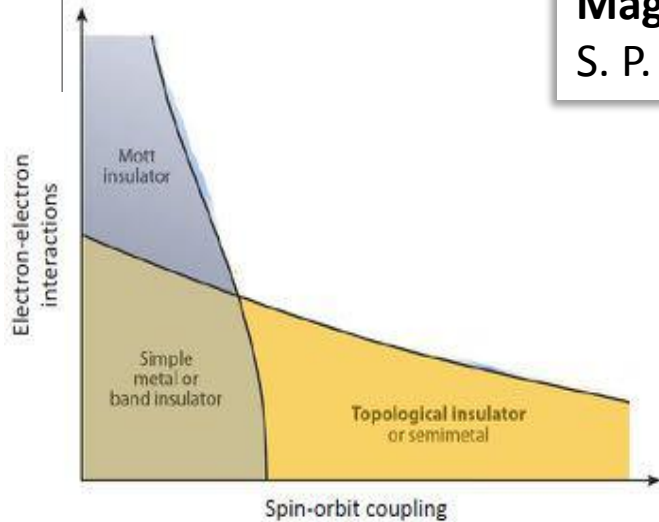
# GAPS



## Search for Intra-Unit Cell Magnetic orders



Loop current



**Magnetic Ordering and SpinWaves in Na0.82CoO2**

S. P. Bayrakci, PRL (2005) – 4F1

**Magnetic Order in the Pseudogap Phase of High-TC Superconductors**

B. Fauqué et al, PRL (2006) – 4F1

**Unusual magnetic order in the pseudogap region of the superconductor HgBa2CuO4+δ**

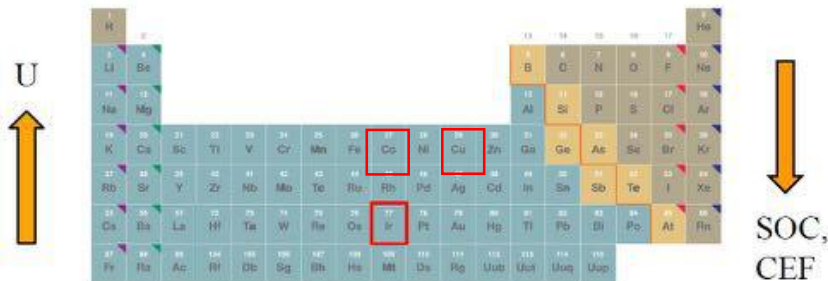
Y. Li et al, Nature (2008) – 4F1

**Hidden magnetic excitation in the pseudogap phase of a high-Tc superconductor**

Y. Li et al, Nature (2010) – IN20

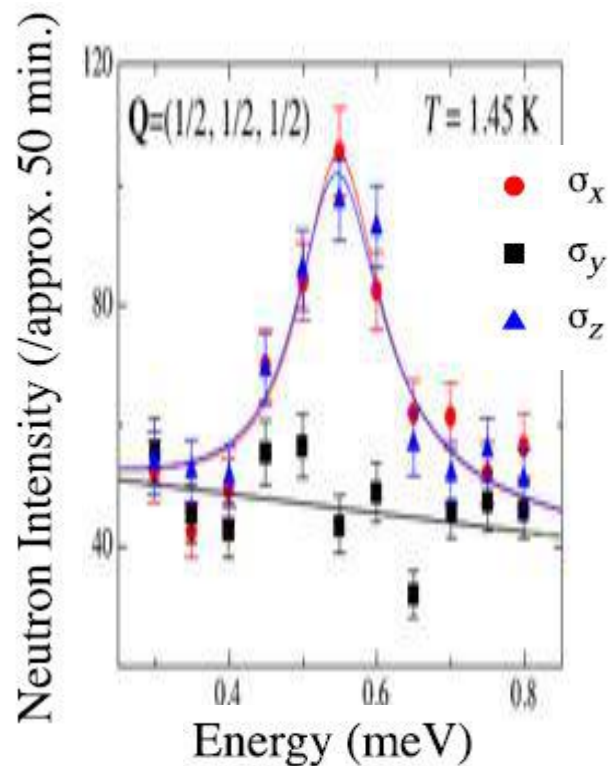
**Time-reversal symmetry breaking hidden order in Sr2(Ir,Rh)O4**

J. Jeong et al. Nat. Comm. (2017) – 4F1



High Flipping ratio

## Probing the spin-space anisotropy of collective magnetic modes in unconventional superconductors



*Ising Spin Resonance in CeCoIn5*

**Polarized neutron scattering studies of magnetic excitations in electron-overdoped superconducting BaFe<sub>1.85</sub>Ni<sub>0.15</sub>As<sub>2</sub>**  
M.Liu et al, PRB (2012) – IN20

**Splitting of Resonance Excitations in Nearly Optimally Doped Ba(Fe<sub>0.94</sub>Co<sub>0.06</sub>)<sub>2</sub>As<sub>2</sub>: An Inelastic Neutron Scattering Study with Polarization Analysis**  
P. Steffens et al, PRL (2013) – IN20

**Ising Incommensurate Spin Resonance of CeCoIn<sub>5</sub>: A Dynamical Precursor of the Q Phase**  
S. Raymond et al., PRL (2015) – IN12

**Prominent Role of Spin-Orbit Coupling in FeSe Revealed by Inelastic Neutron Scattering**  
Mingwei Ma et al, PRX (2017) – 4F1

High  
intensity

- 2 instruments for the spectroscopic communities in five years
- Complementary with direct TOF instruments:



### BIFROST@ ESS

Very efficient parametric studies on spallation source

### GAPS @ ILL

Powerful and dedicated polarized neutron beam

For the long run (post 2030):

- Triple axis « Farm » at ESS (A. Hiess):  → 

« many » TAS-like spectrometers (back end) sharing guide system (front end)  
with different fonctionnalités (polarization, cold, thermal,  
High magnetic field, small samples....)