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Спектрометры неупругого рассеяния в АНСТО

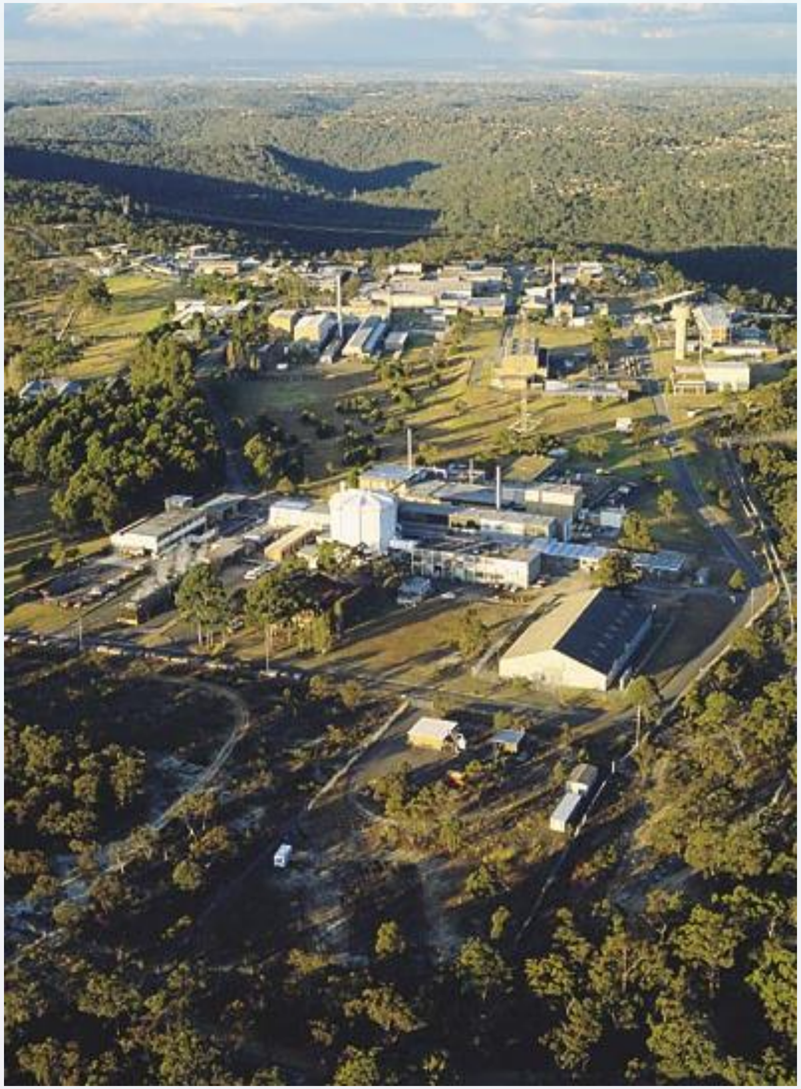
С.А. Данилкин

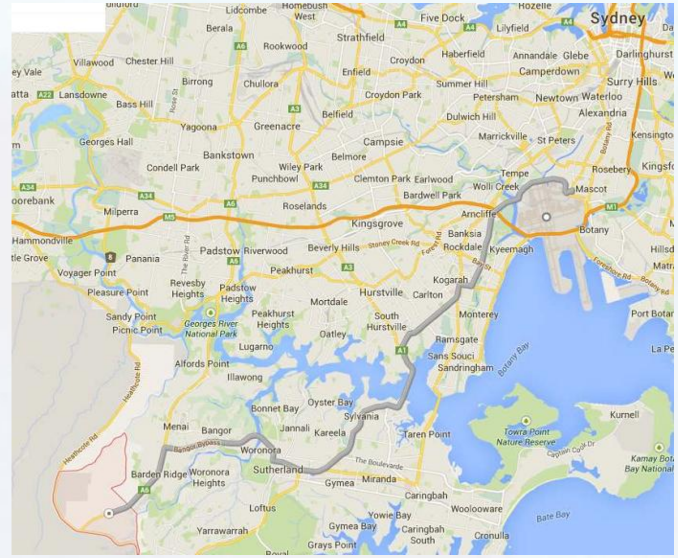
24 июня 2016, Гатчина

Outline

- “Old” HIFAR reactor and Instruments
- “New” Opal Reactor. Neutron Scattering Facility
- NGH: Neutron Guides and Instruments
- NGH Spectrometers: TOF “PELICAN” and Backscattering “EMU”
- RBH Spectrometers: TAIPAN (thermal TAS) and SIKA (cold TAS)
- Research Highlights
- Proposals / Publications / Statistics

The Australian Nuclear Science and Technology Organisation





Sydney airport – Lucas Heights
29.8 km 36 min

- *neutron beam and accelerator science*
- *radiopharmaceutical research and production*
- *nuclear waste handling and storage*
- *environmental research and monitoring*
- *neutron transmutation doping (Silicon)*

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The HIFAR Research Reactor (1956)

- Reactor Power =10-20 MW
- Fuel type 60% enriched UO_2
- Core ϕ=91cm h=60cm
- Neutron flux 1.4×10^{14} n/cm^2/s @ 10MW

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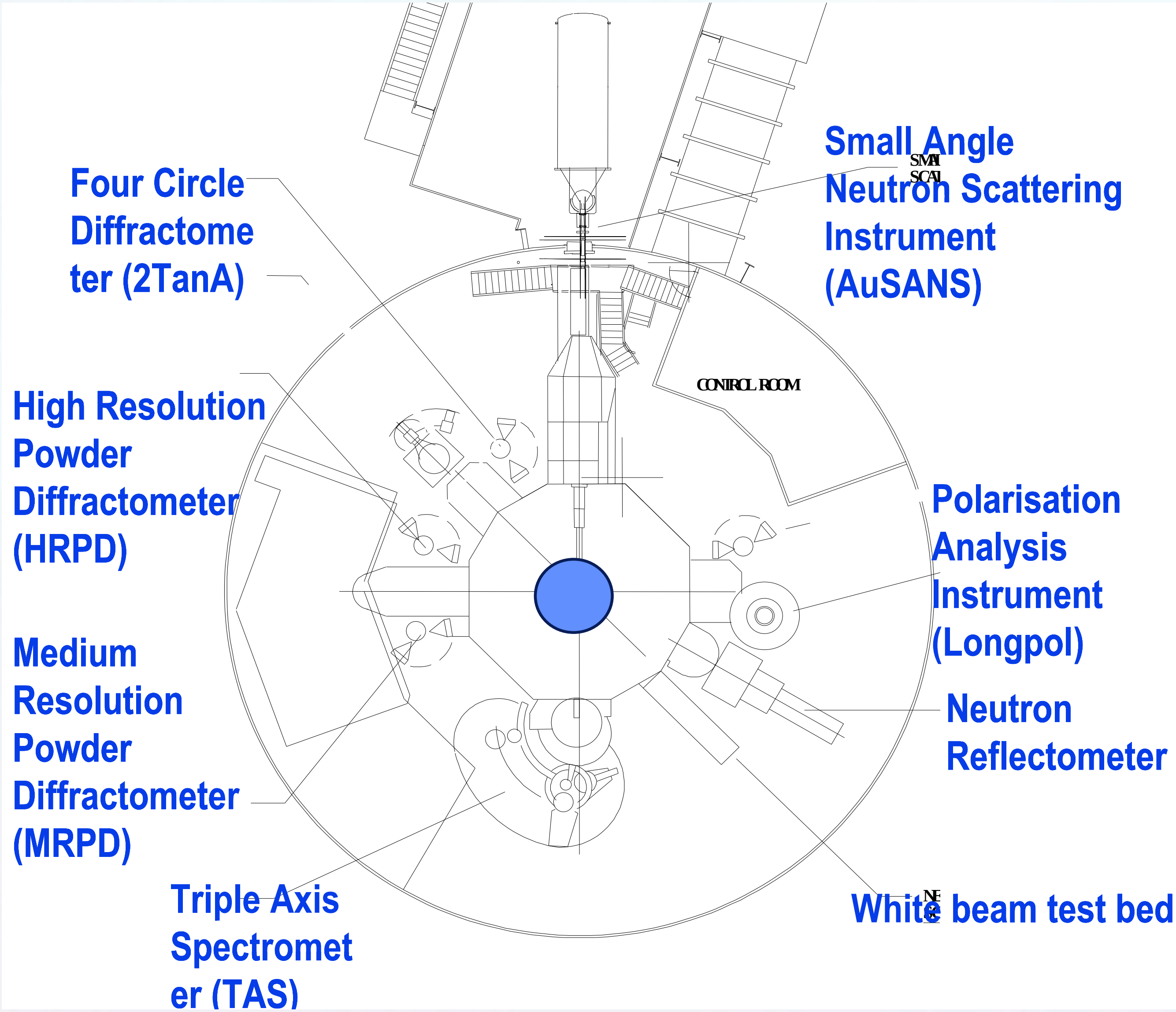
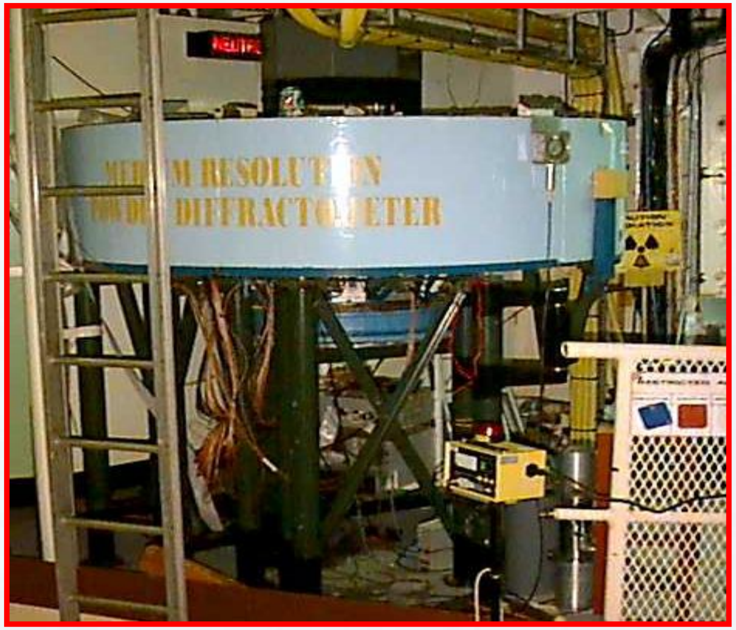
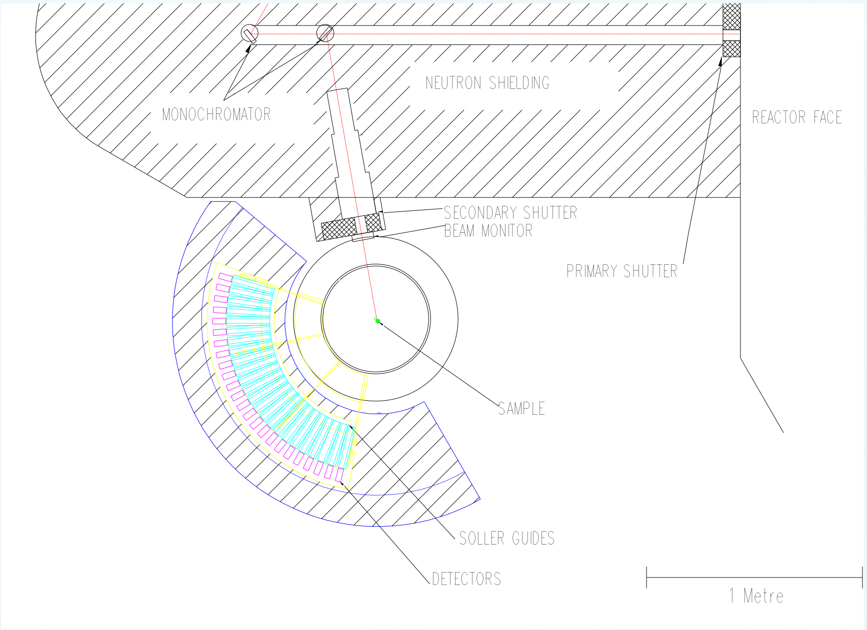
The HIFAR Research Reactor (1958-2006)



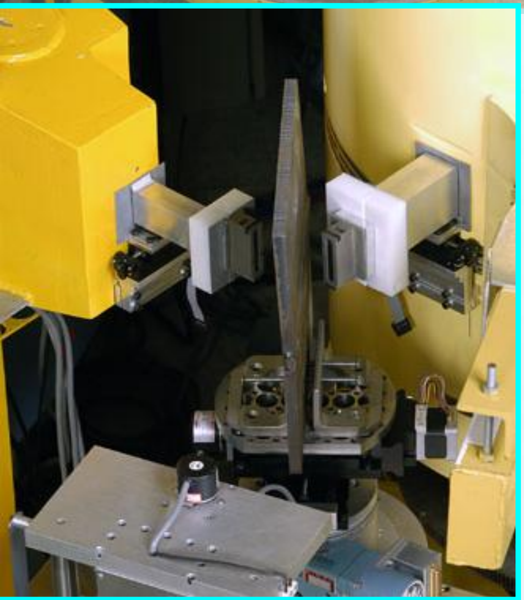
The Medium Resolution Powder Diffractometer (MRPD)

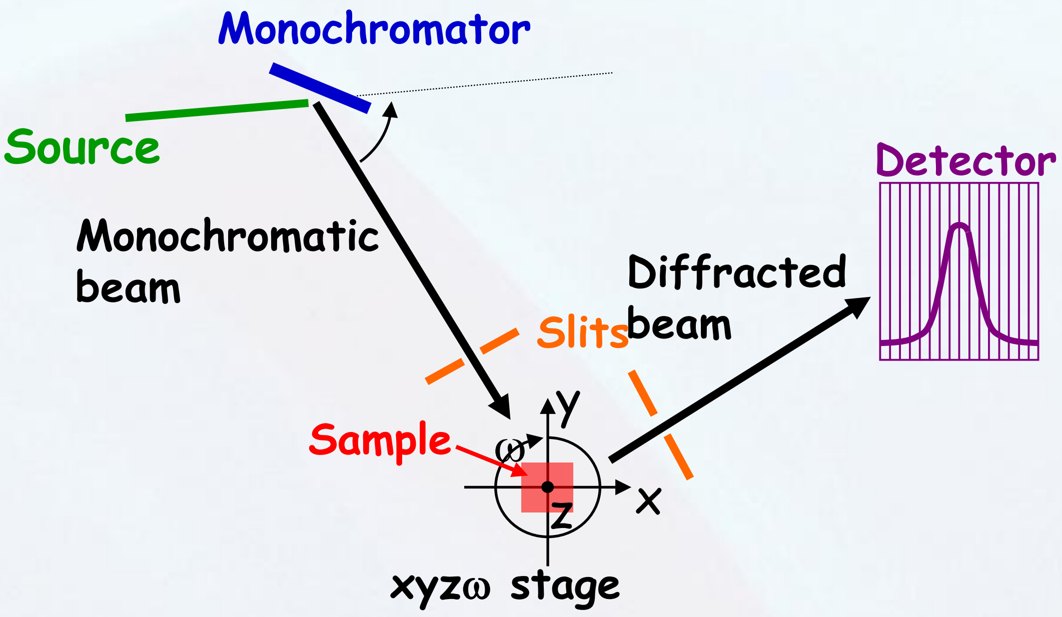




- Primary collimation α_1 = 0.45° or 0.25°
- Focusing monochromator: 8 x Germanium crystals (β~0.2°)
  l = 1.06, 1.21, 1.32, 1.66, 1.98, 2.61 or 5.0 Å
- Neutron flux = $4x10^5$ n/cm^2/sec at 1.66Å
- 32x ^{3}He Detectors with Soller collimators: α_3 = 0.35°
- Computer control of sample & detectors, data acquisition, temperature, pressure etc.,

The Australian Strain Scanner (TASS) in HIFAR





- Monochromator: 6 x Germanium crystals (115), 0.83 Å < l < 1.43 Å
- Neutron flux at sample ~10^6 n/cm^2/sec at 1.4 Å
- Samples stage –x,y,z translations, f ~35 mm, mass ~10 kg
- Gauge volume >1mm^3
- Detector 32 wire x ^{3}He PSD, spans 2.3º (0.07º per wire)
- Computer control of sample & detectors & data acquisition

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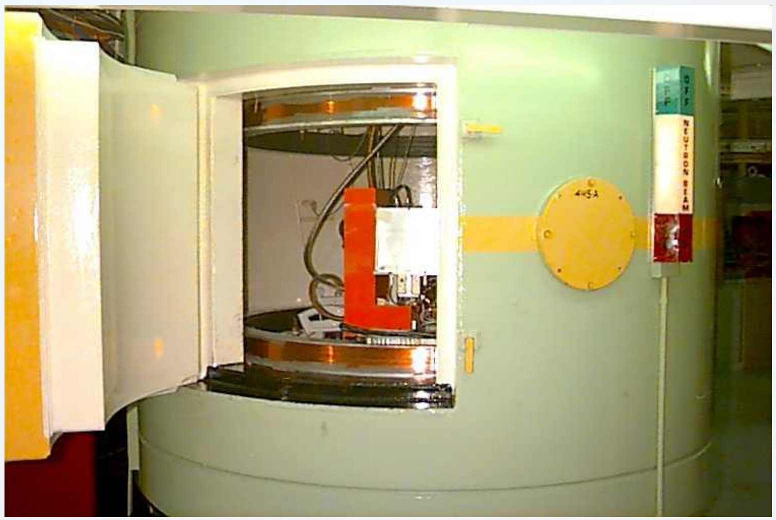
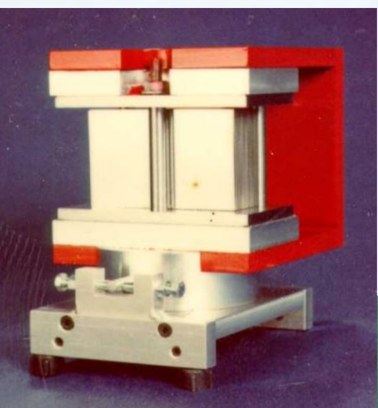
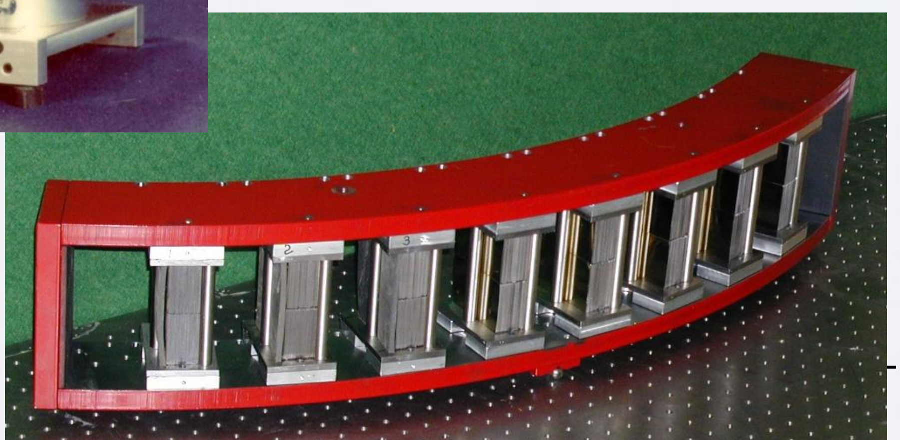
The HIFAR Polarization Analysis Spectrometer (Longpol)

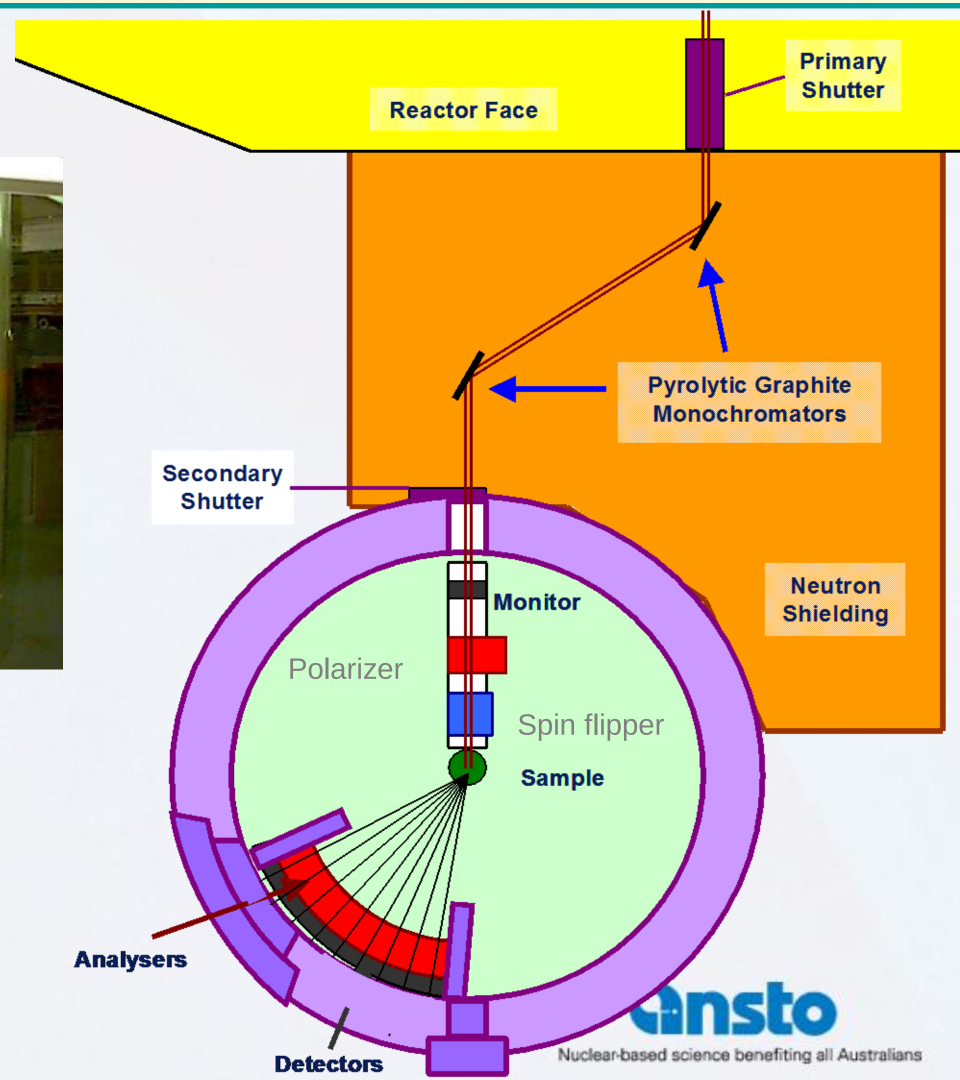
- The Longpol spectrometer uses supermirrors for Polarization Analysis.
- TOF energy analysis is also possible by pulsing the neutron spin flipper with a pseudo-random sequence

- Polarization efficiency ~96%.
- Energy resolution ~100 meV









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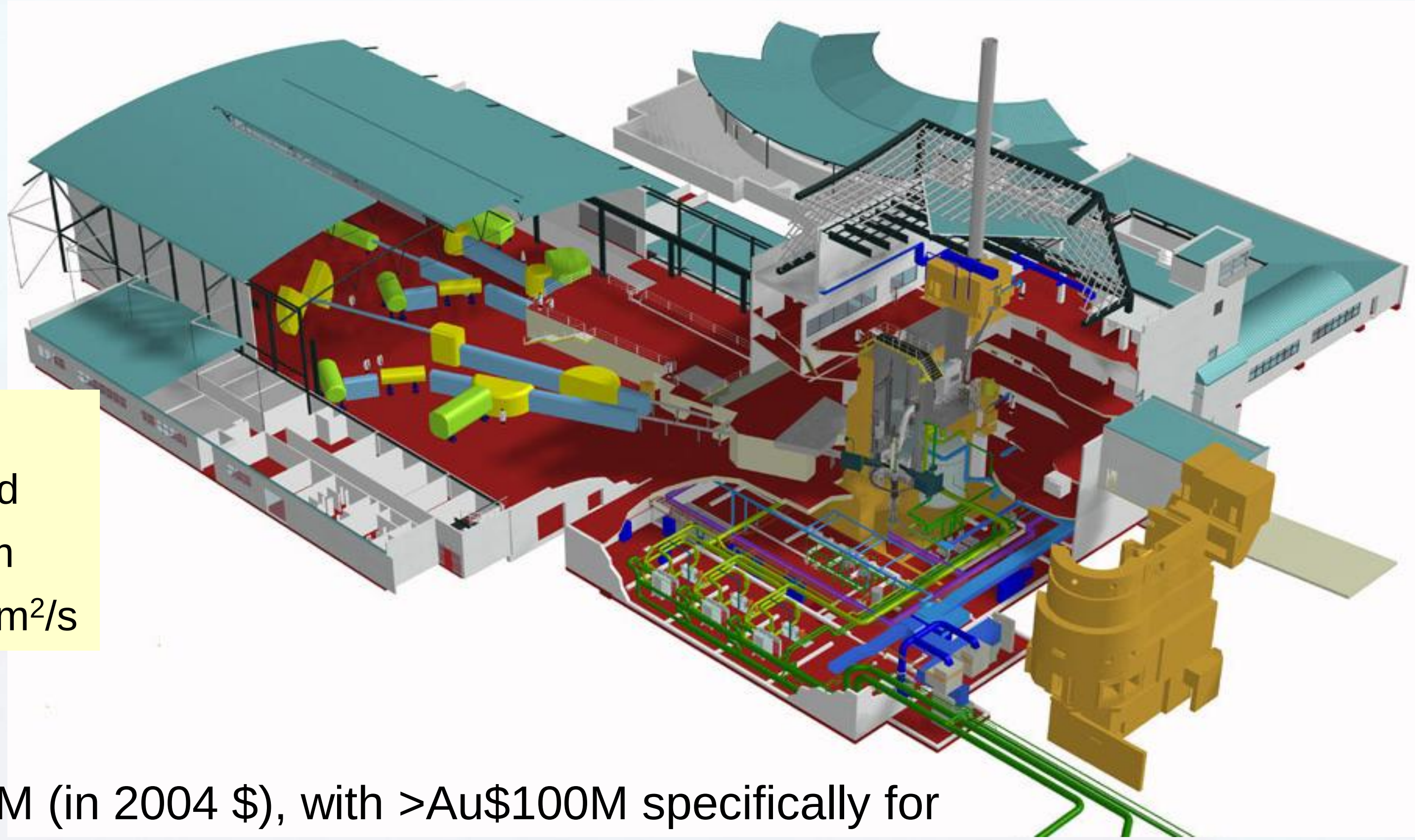
The New Research Reactor (2007)



- Reactor Power =20 MW
- Fuel type 19.7% enriched
- Core H=60cm x W=35cm
- Neutron flux 4 x 10^{14} n/cm^2/s

- Investment of >Au$350M (in 2004 $), with >Au$100M specifically for neutron beam research + enhanced capabilities for radioisotope production & Silicon transmutation
- Neutron scattering capability enhanced by ~100 times relative to HIFAR.
- Target performance for neutron scattering to rate with top 5 research reactors in the world.

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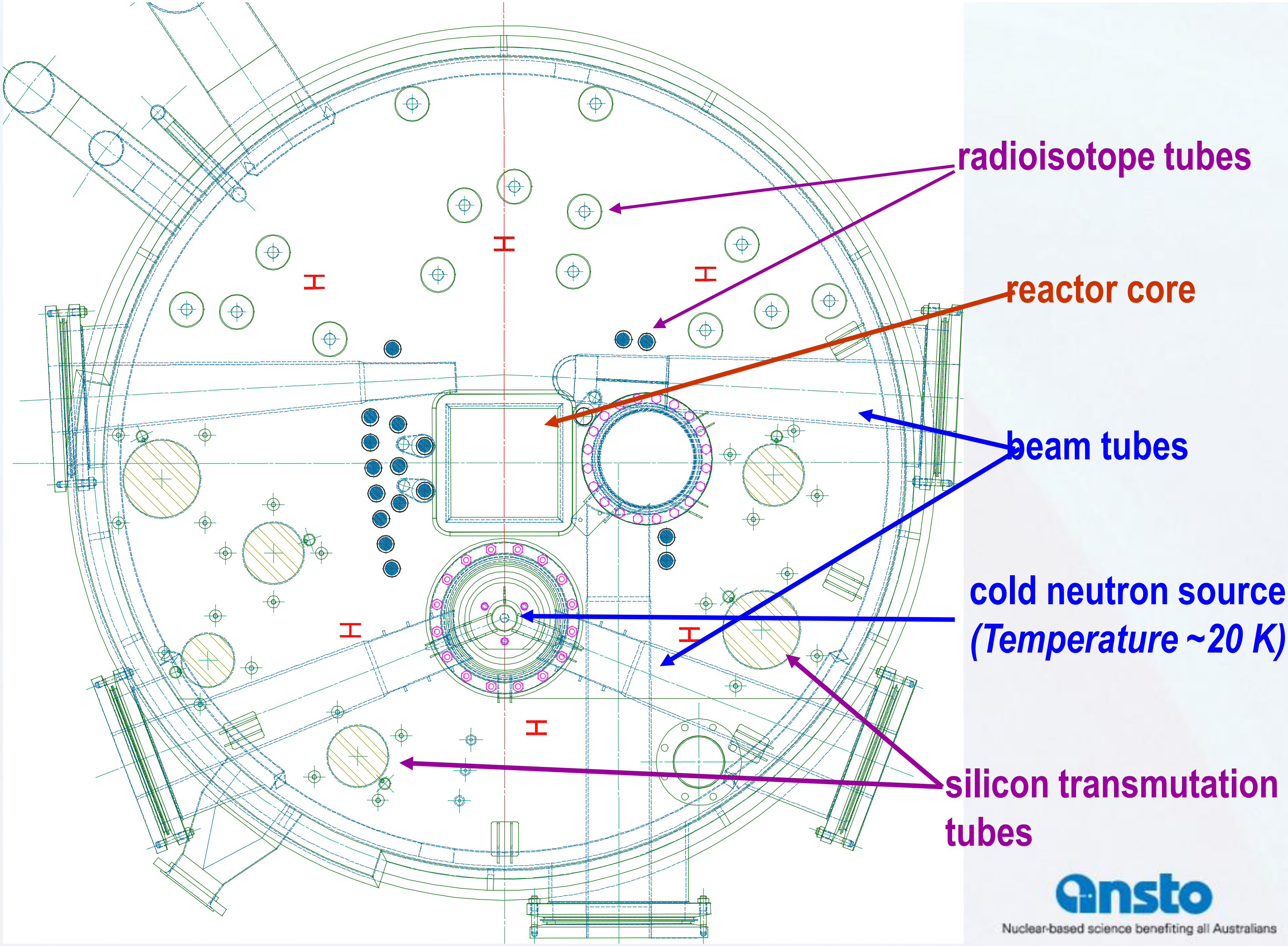
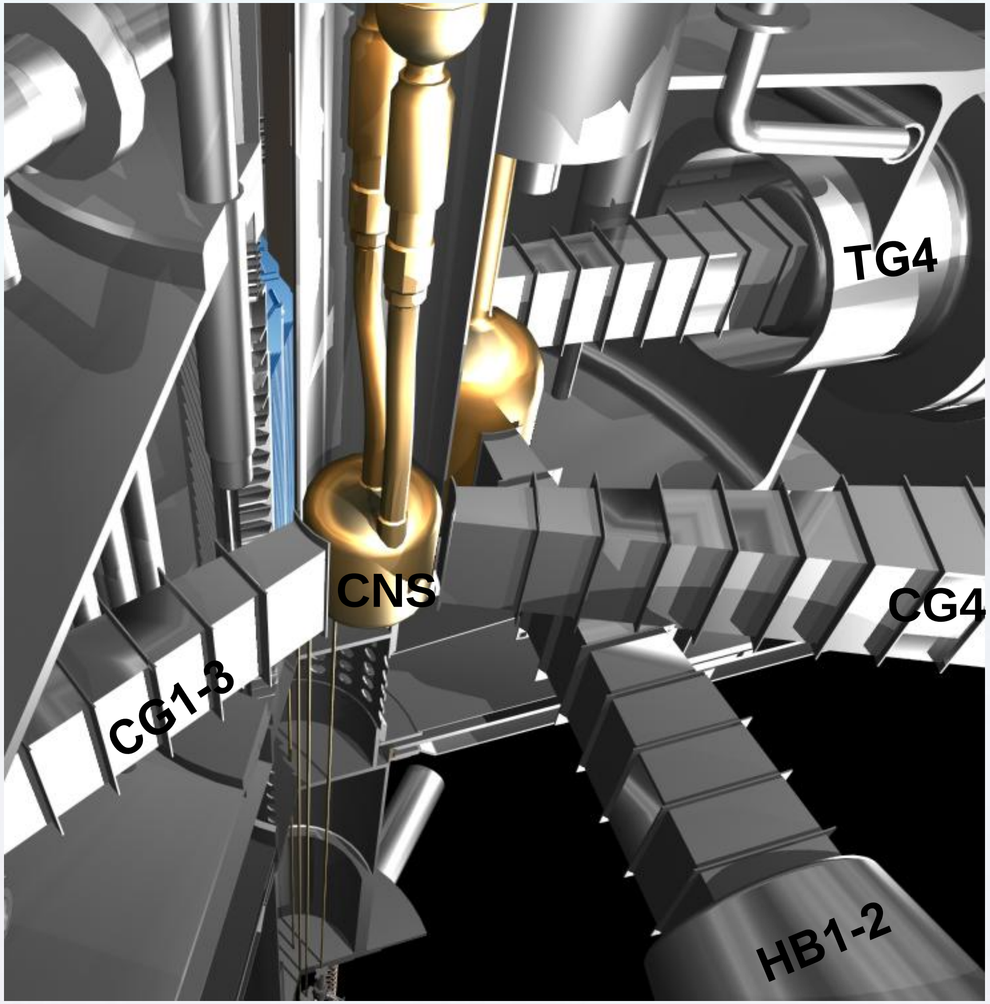
The reactor core, moderator and beam tubes



Inside the Moderator Tank



- Cold neutron source
- Two thermal beam assemblies
- Two cold beam assemblies
- Radio-pharmaceutical production ($^{99}Mo \rightarrow {}^{99m}Tc$, ^{131}I, ^{192}Ir etc.)
- NTD Silicon production (8”-10”)

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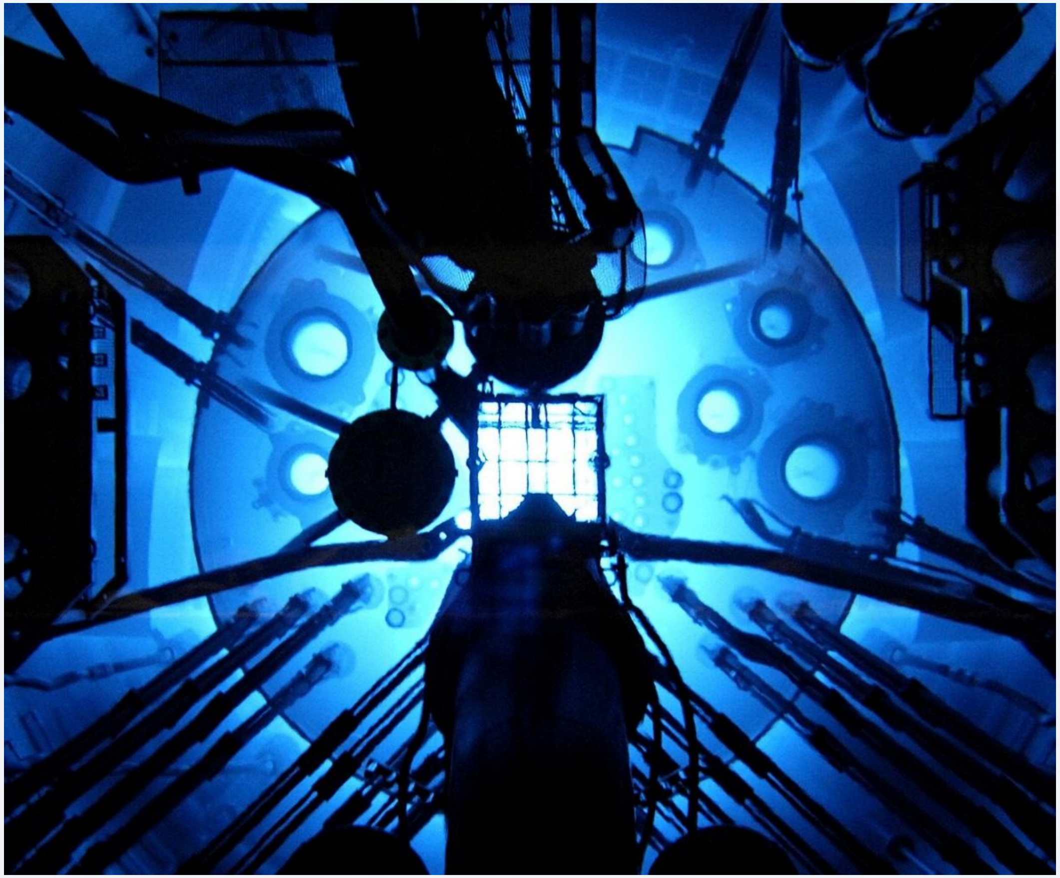
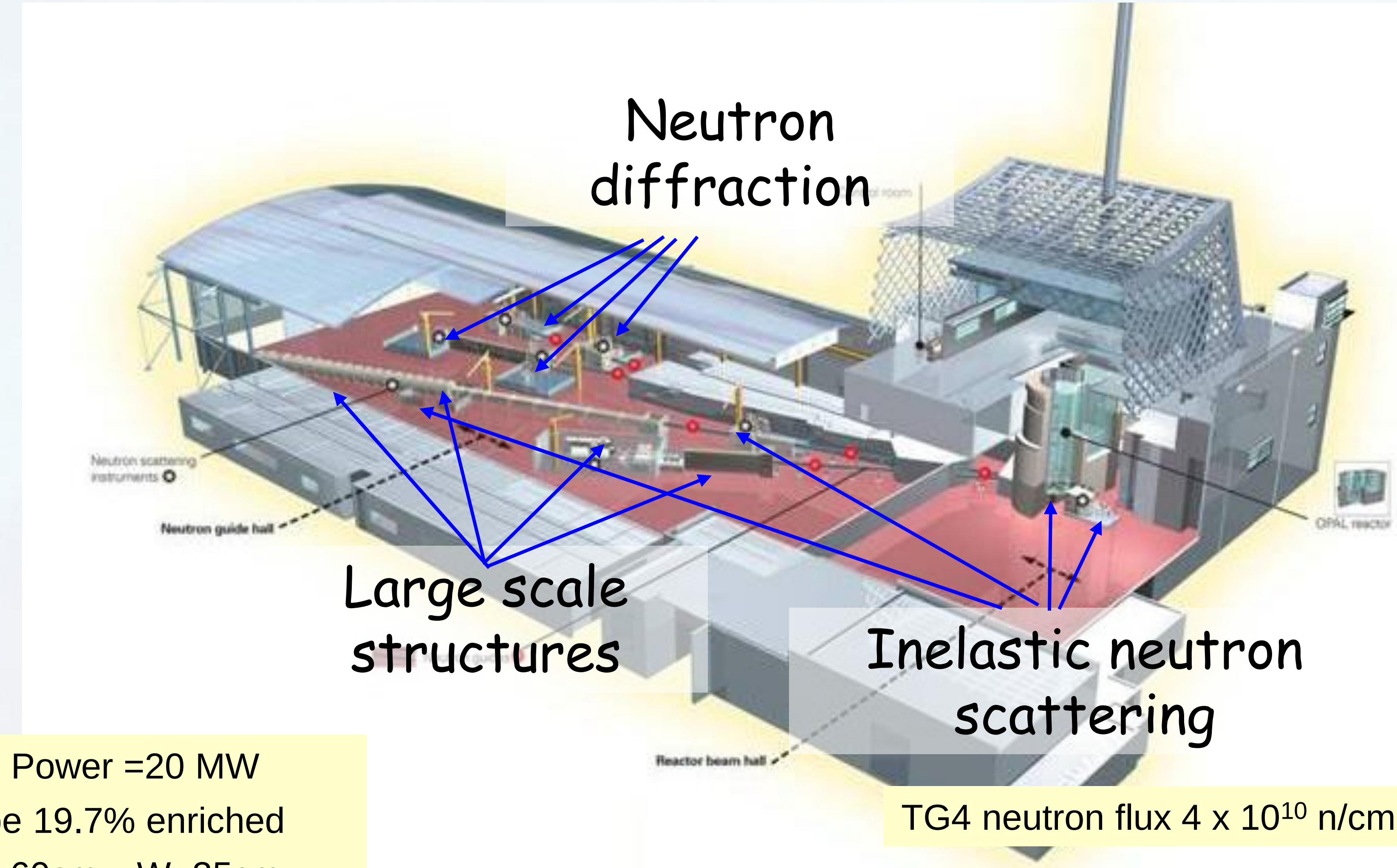
Inside the Moderator Tank



The OPAL Research Reactor (2007→)



- Reactor Power =20 MW
- Fuel type 19.7% enriched
- Core H=60cm x W=35cm
- Neutron flux 4 x 10^{14} n/cm^2/s

TG4 neutron flux 4 x 10^{10} n/cm^2/s

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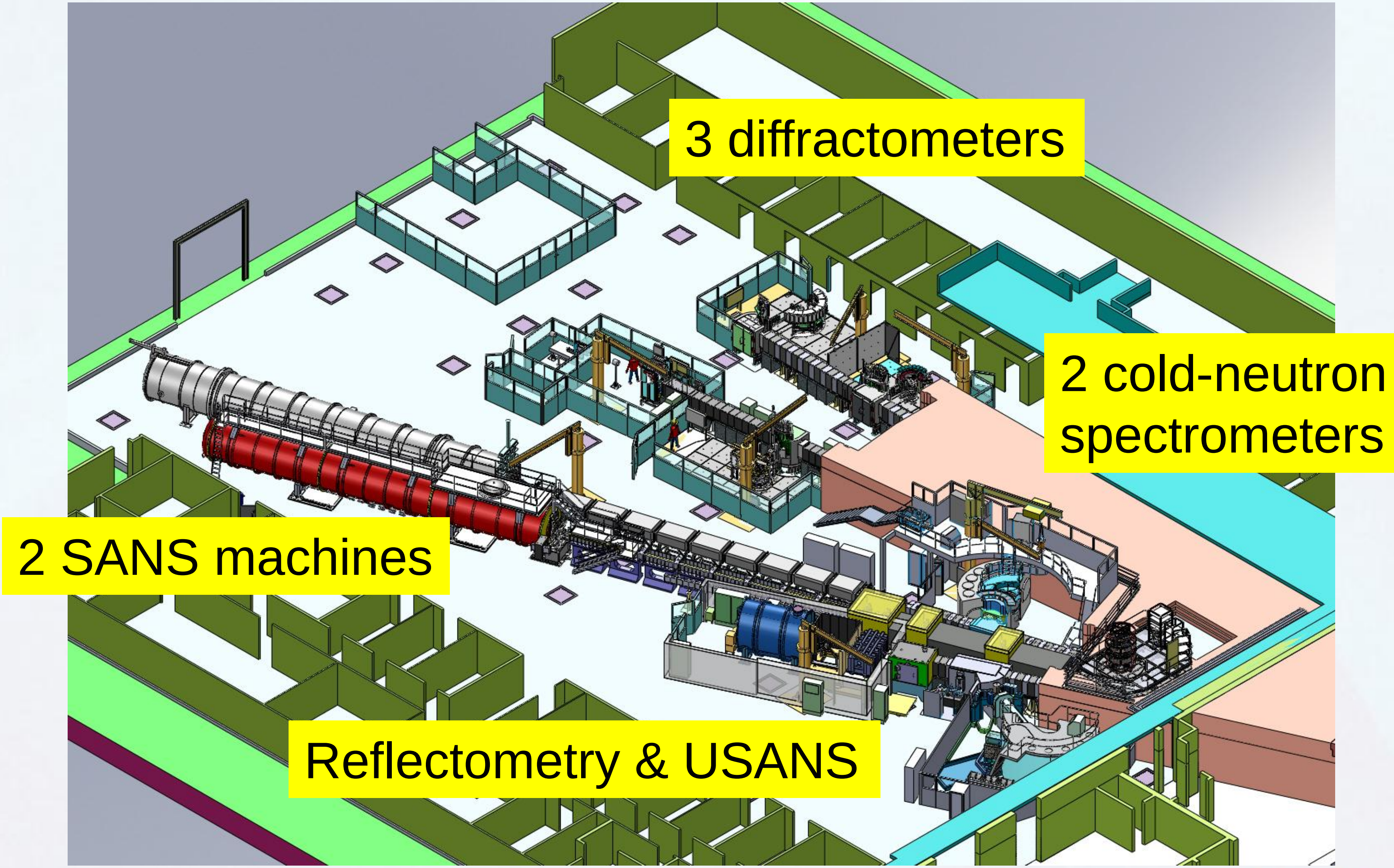
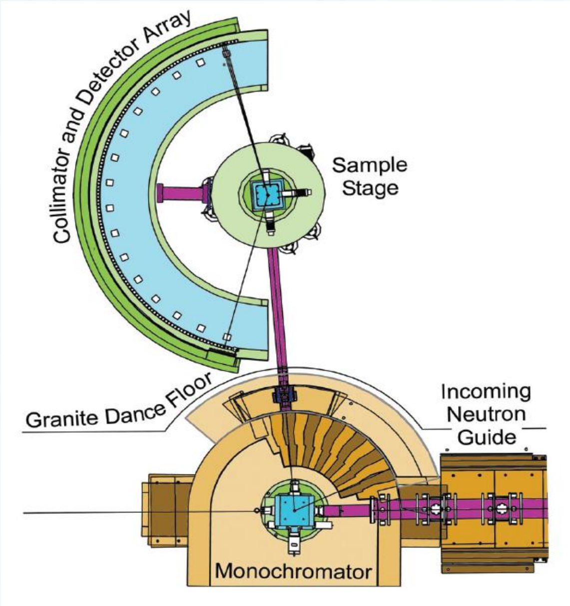
Neutron Scattering Instruments in NGH



"ECHIDNA" High-Resolution Powder Diffractometer

K.-D. Liss, B. A. Hunter, M. E. Hagen, T. J. Noakes and S. J. Kennedy, *Physica* B 385-386, 1010-1012 (2006).



Wavelength range: 1 – 3 Å
Range of momentum transfer: 0.35 – 12.5 $Å^{-1}$
Max. beam size: 20×50 mm^2
Flux at sample position: up to 10^7 $ncm^{-2}s^{-1}$
Monochromators: Ge (115), Ge(335)
Detector:
128 position sensitive detectors of Ø25 mm x 300 mm
128 collimators with 5' collimation, 15 mm x 300 mm (W x H)
Typical scan time: 2-3 hours

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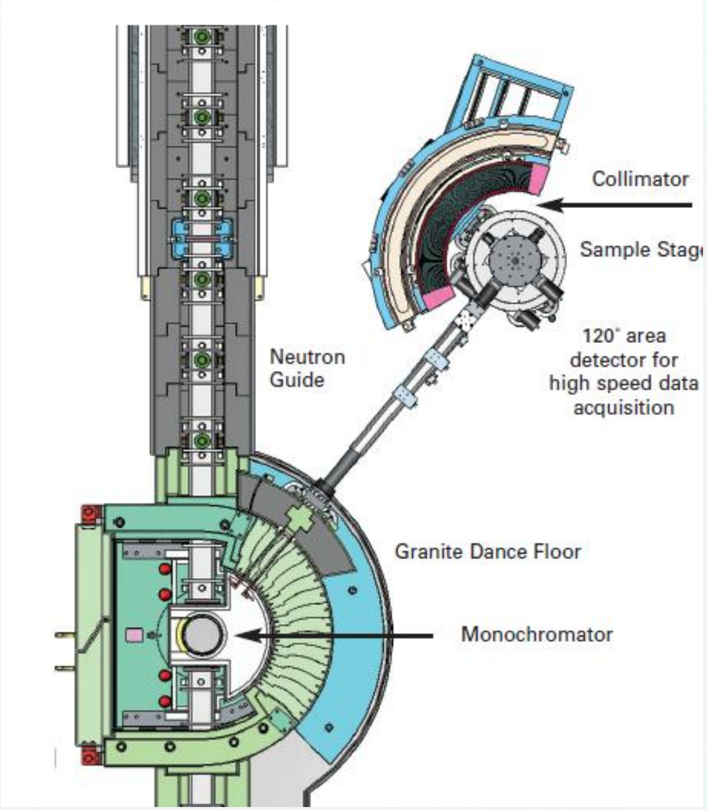
“WOMBAT” High-Intensity Powder Diffractometer

A. J. Studer, M. E. Hagen and T. J. Noakes, *Physica* B 385-386, 1013-1015 (2006)



> Wavelength ranges
  0.9 - 2.4 Å (Ge monochromator)
  2.4 - 5.8 Å (PG monochromator)
> Resolution $\Delta d/d > \sim 2 \times 10^{-3}$
> Beam size 20 mm (wide) x 60 mm (high)
> Sample weight ~10 mg to 10 g
> Typical sample size 1 cm^3
> 1s acquisition for 10 mm^3 (15 min for 1 mm^3) in one shot irreversible experiments
> Estimated flux at sample position $>10^8$ $ncm^{-2}s^{-1}$
> Detector area: continuous detection over 120° x 200 mm high

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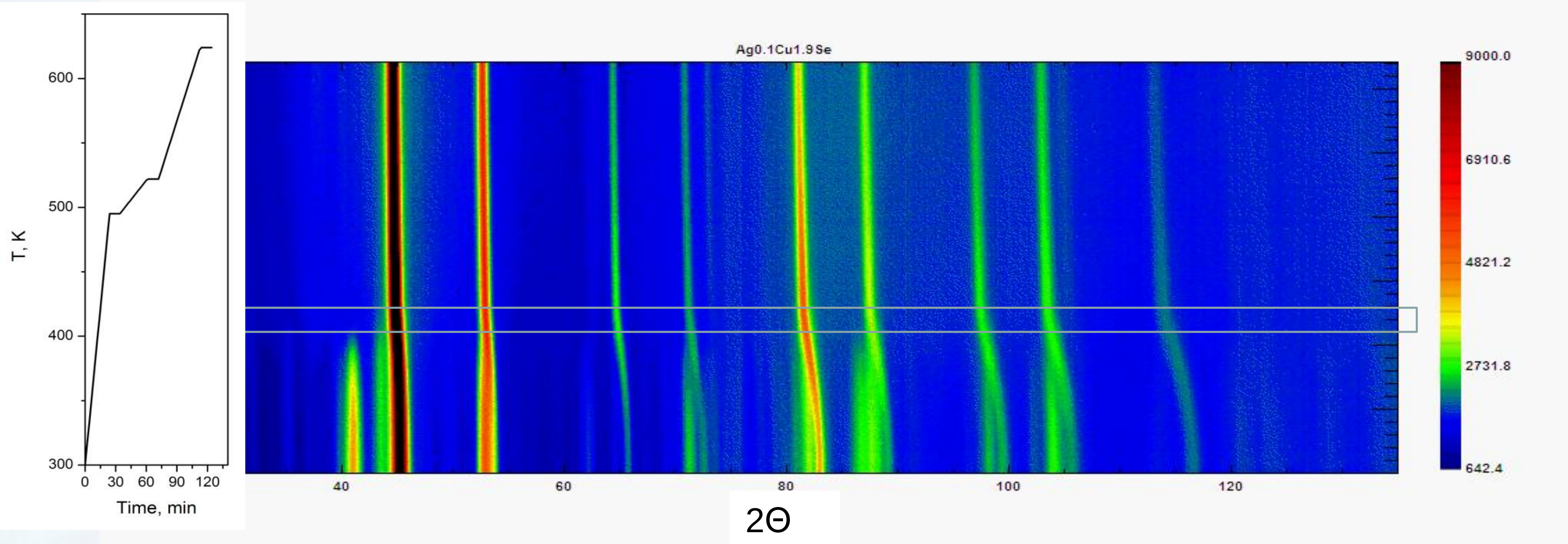
Neutron Diffraction: $Ag_{0.1}Cu_{1.9}Se$



Wombat diffractometer @ ANSTO

ΔT=1K, time/pattern = 1 min

“Koala” Laue Diffractometer

A. J. Edwards, *Aust. J. Chem*. **64**, 869–872 (2011)

Single-crystal neutron diffraction studies complement X-ray crystallography by revealing the precise positions of light atoms such as hydrogen, which cannot be determined by X-ray methods.

> Fast data collection: one structure per day for larger unit cells
> Small samples: ~ 0.1 mm^3 or less with slower data collection
> Solid angle for quasi-Laue diffractometer about 3π
> Neutron wavelength is peaked at 1.4 Å
> Routine for crystals with primitive cell up to 20 $Å^3$
> Sample environment: 6 K to 800 K (standard), gas-environment (hydrogen, oxygen, inert), electric fields

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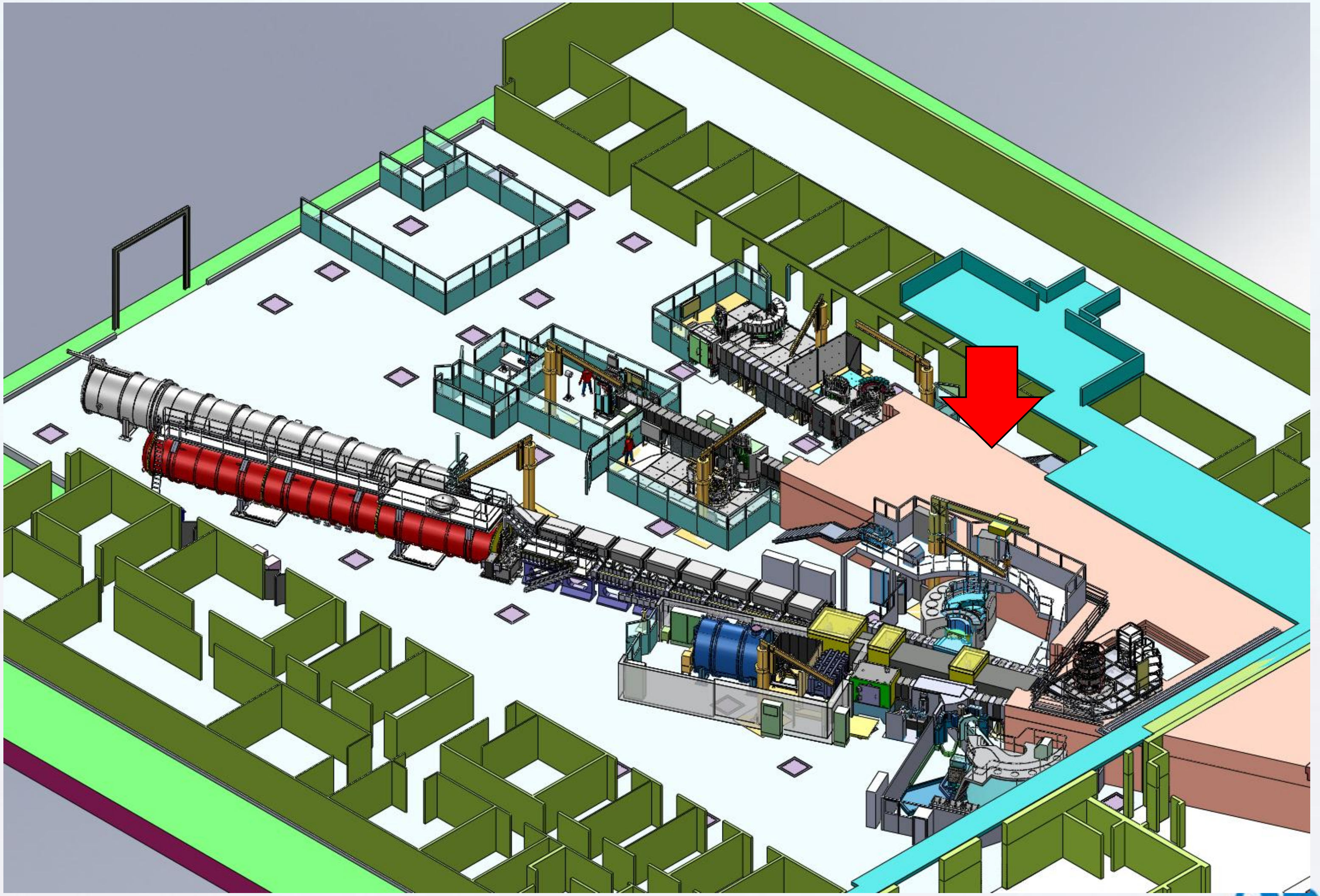
TOF Spectrometer “PELICAN”

D. H. Yu, R. A. Mole, T. Noakes, S. J. Kennedy and R. A. Robinson, *J. Phys. Soc. Japan* **82** SA027 (2013).



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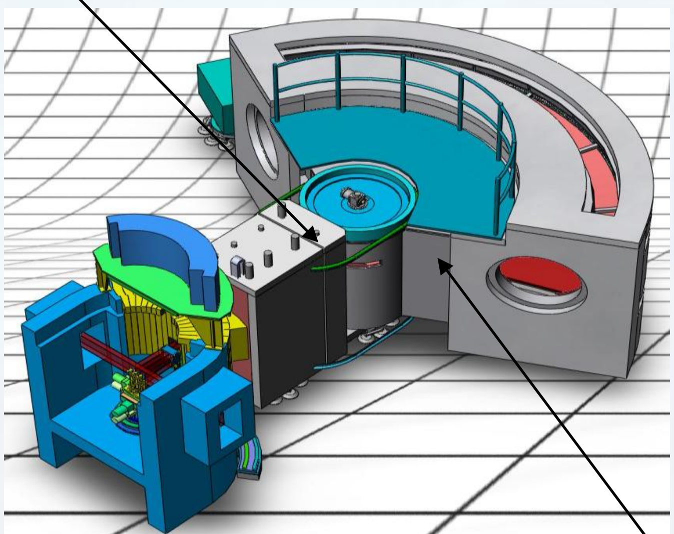
TOF Spectrometer “PELICAN”

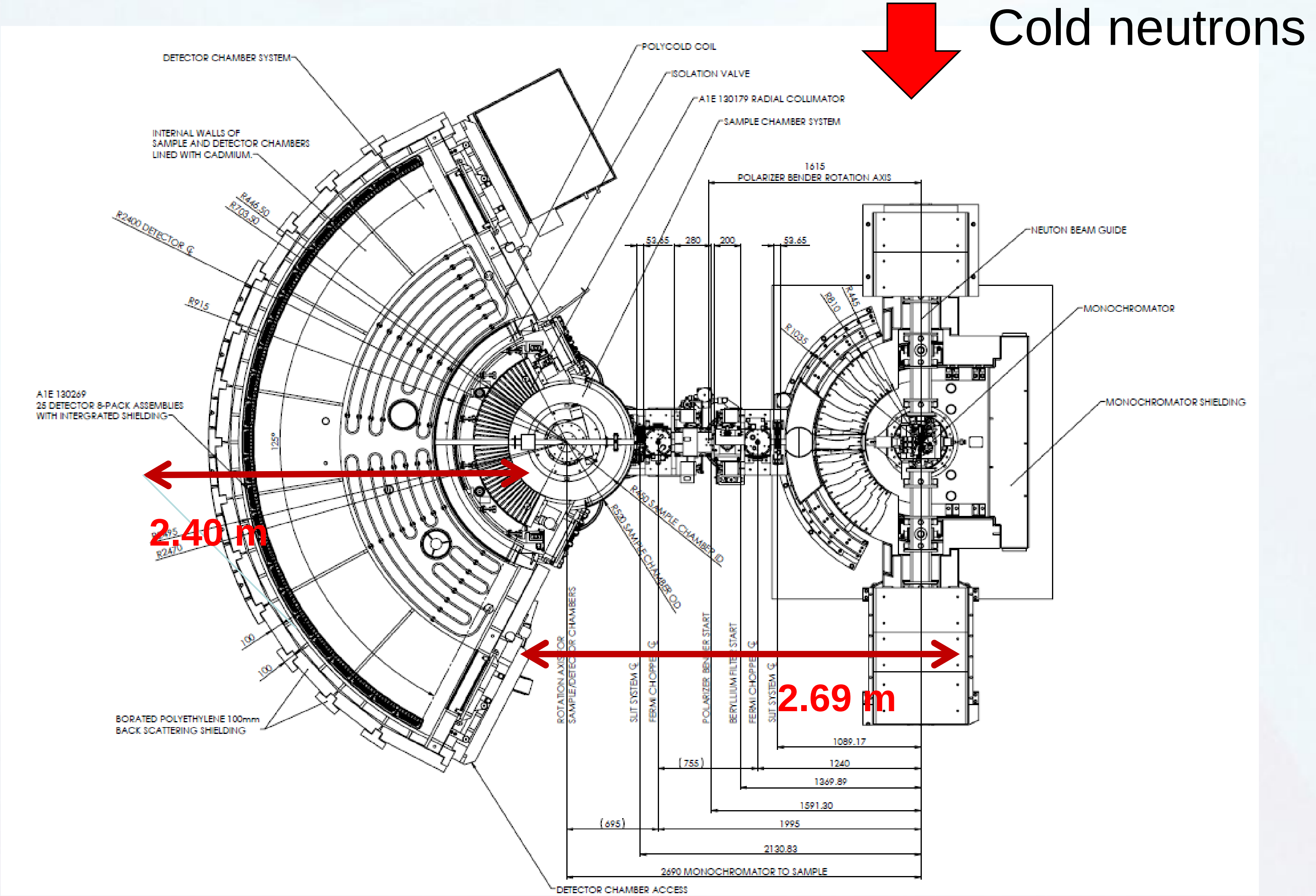


• Crystal field excitation, **phonon density of states**, short range order, **atomic diffusion**, atomic confinement, magnetic excitation in H-T_c superconductors, novel magnetic, **thermo electrical** and piezoelectric **materials**.

• Molecular dynamics and diffusion in molecular magnets, hydrogen-bonding and storage systems, catalytic materials, cement, soils and rocks.

• Dynamics of protein structures, hydration process and ion diffusion through membranes biological samples.

Instrument Layout



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“Pelican” Specifications

Monochromator	**Wavelength**: 2.4 x10^{-10} m - 6.3 x10^{-10} m, (14.2 meV - 2.1 meV), HOPG **Resolution**: 50 µeV to 350 µeV (~2.5% of incident energy) **Q range**: 0.08 A^{-1} - 4.5 A^{-1} **Q resolution**: 0.05 A^{-1} **Solid angle**: 0.8 srad (non-pol), 5 m^2 detector coverage
Sample area	**Neutron flux at sample**: > 2.0x10^5 n/cm^2/s at 4.0 x10^{-10}m (tof) **Sample size**: 1.25cm diameter and 8cm high **Sample type**: Powder, liquid, glass, single crystals etc.
Detector	PSD He^3 detectors

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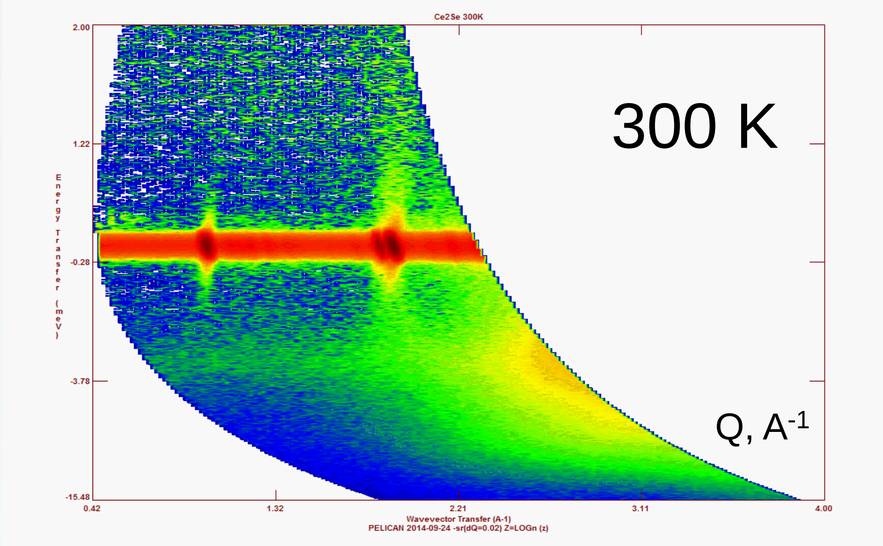
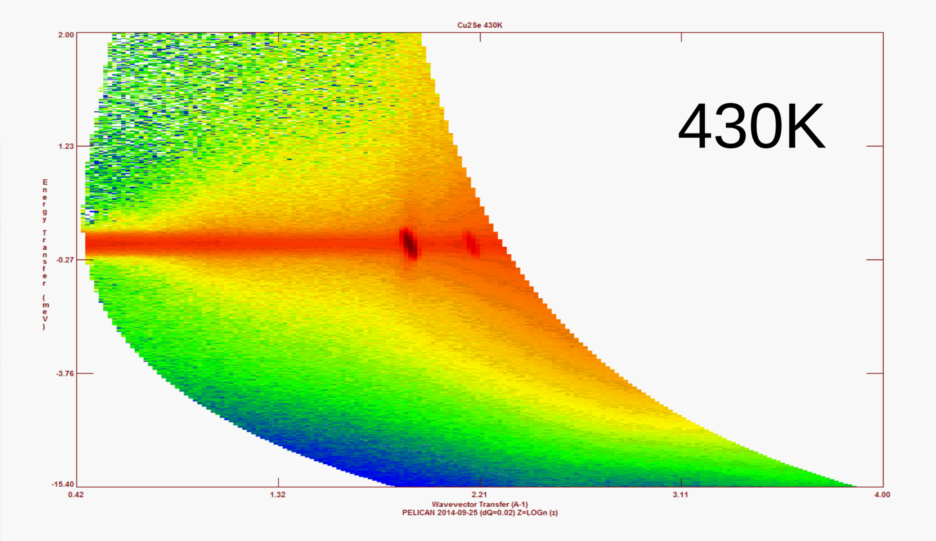
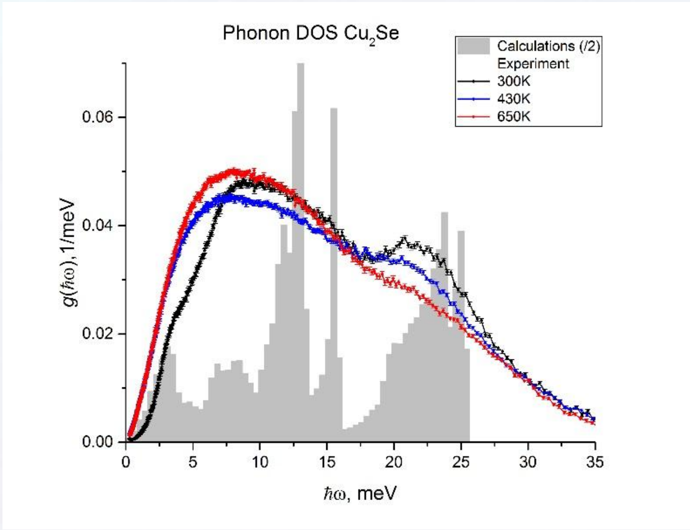
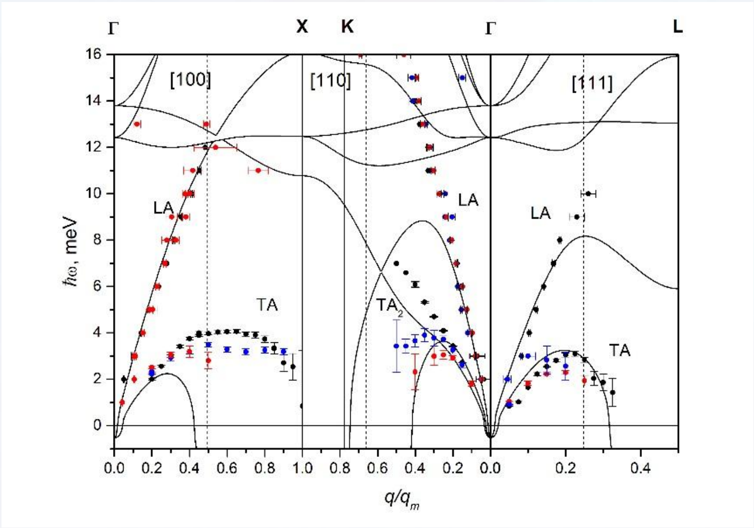
Lattice Dynamics of $Cu_{2-x}Se$ superionic conductors

Energy transfer, meV









VDOS (Pelican)

Phonon dispersion (Taipan)

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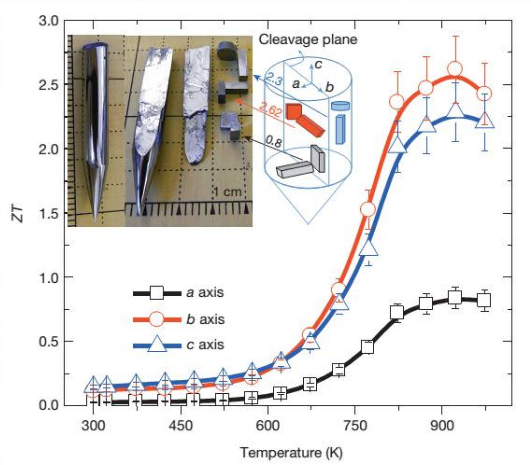
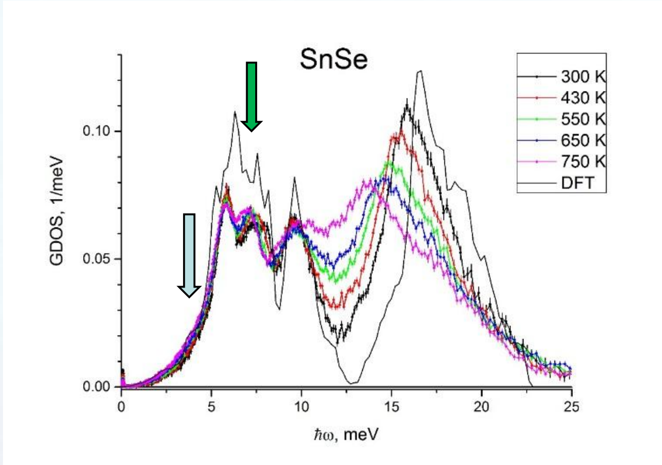
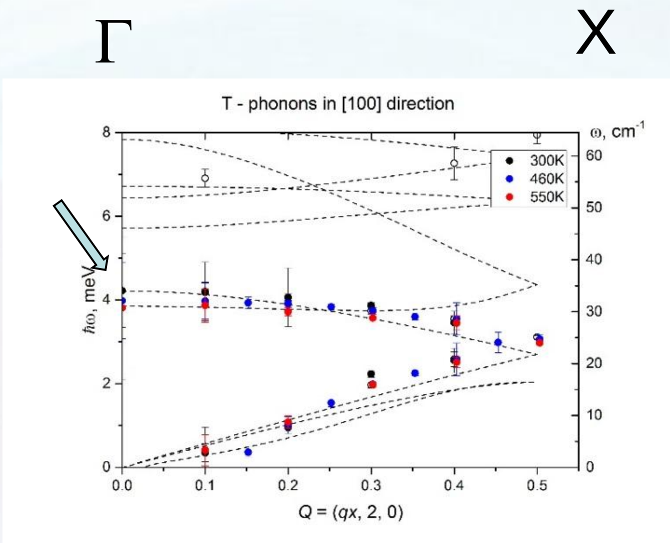
Lattice Dynamics of SnSe

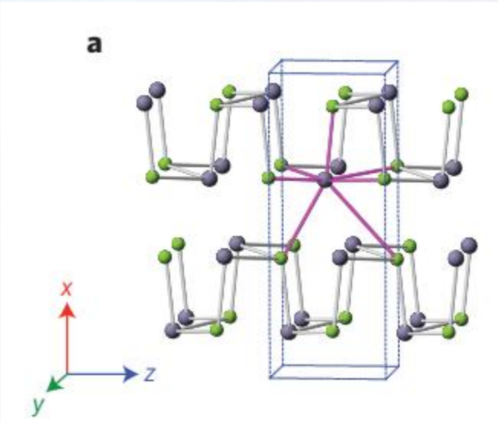


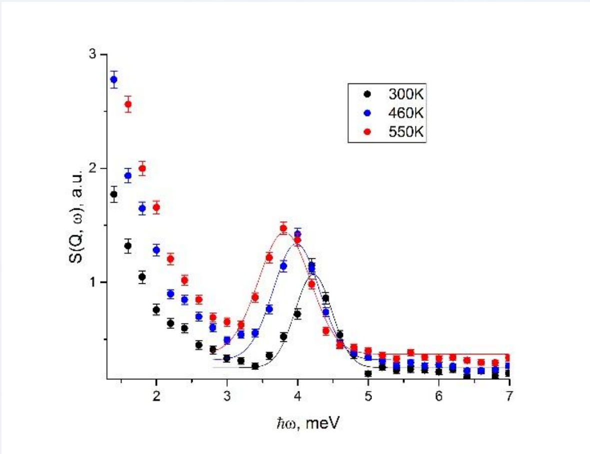
Zhao *et al.*,, 2014
doi:10.1038/nature1318

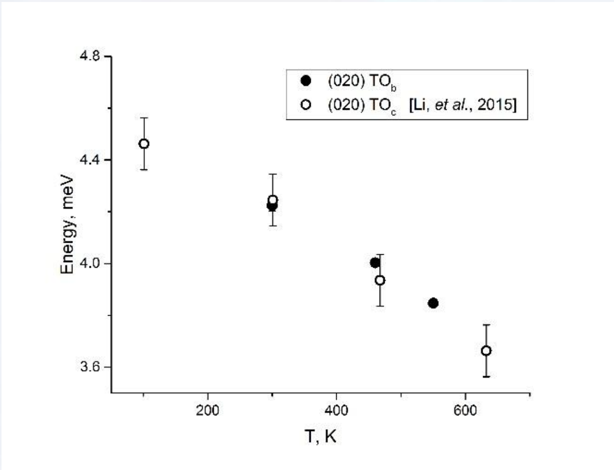


VDOS (Pelican)









Phonon dispersion (Taipan)

a = 11.49 Å, b = 4.44 Å, c = 4.135 Å

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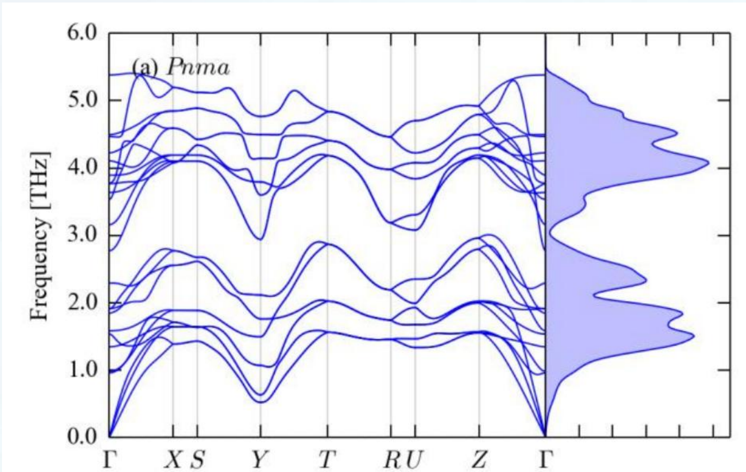
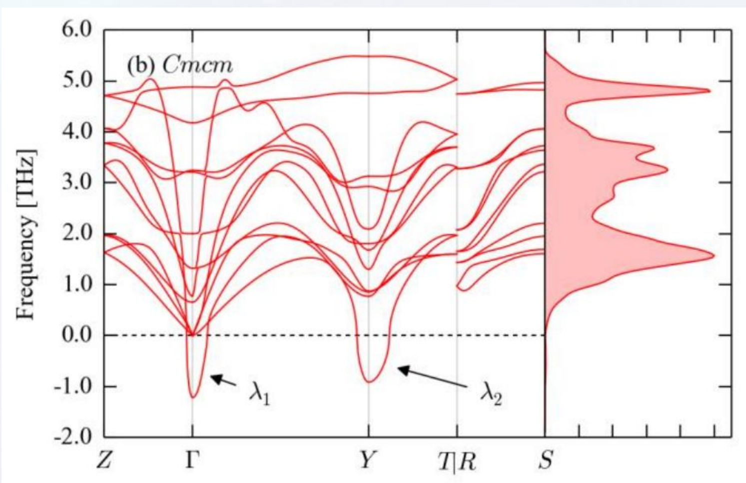
Cmcm – *Pnma* phase transition

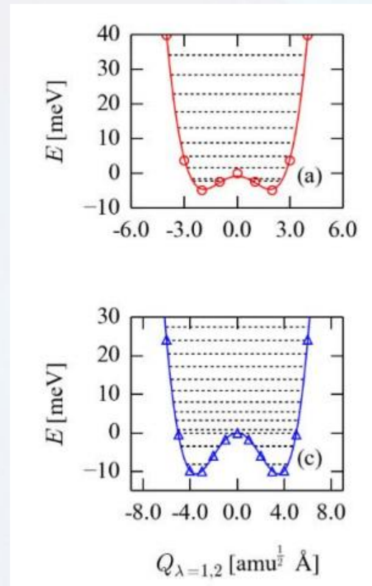


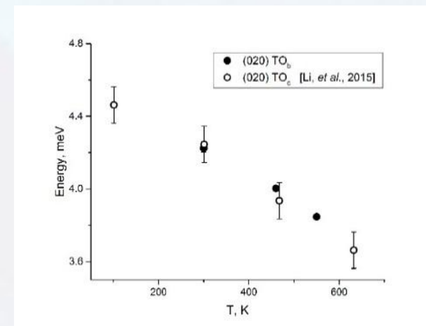


SnSe phonon dispersion and DOS

Skelton et al., arXiv:1602.03762 [cond-mat] (2016)

λ_1 (Γ) and λ_2 (Y) modes in *Cmcm* correspond to symmetry-breaking displacive instabilities

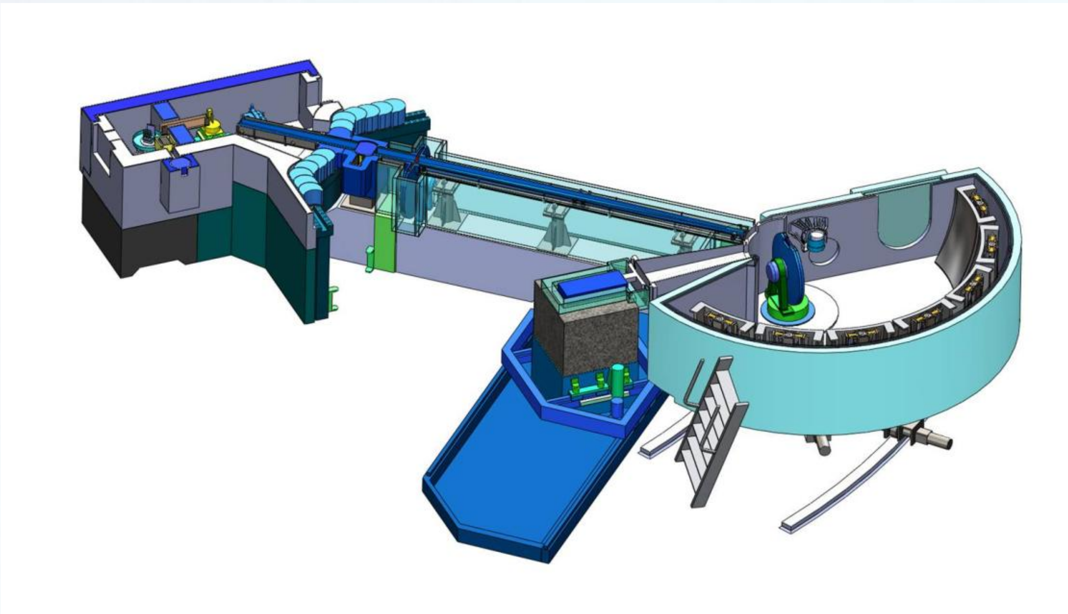




Double-well potential of Γ and Y modes
Eigenvectors along *c* and *b*

“Emu” - High-Resolution Backscattering Spectrometer

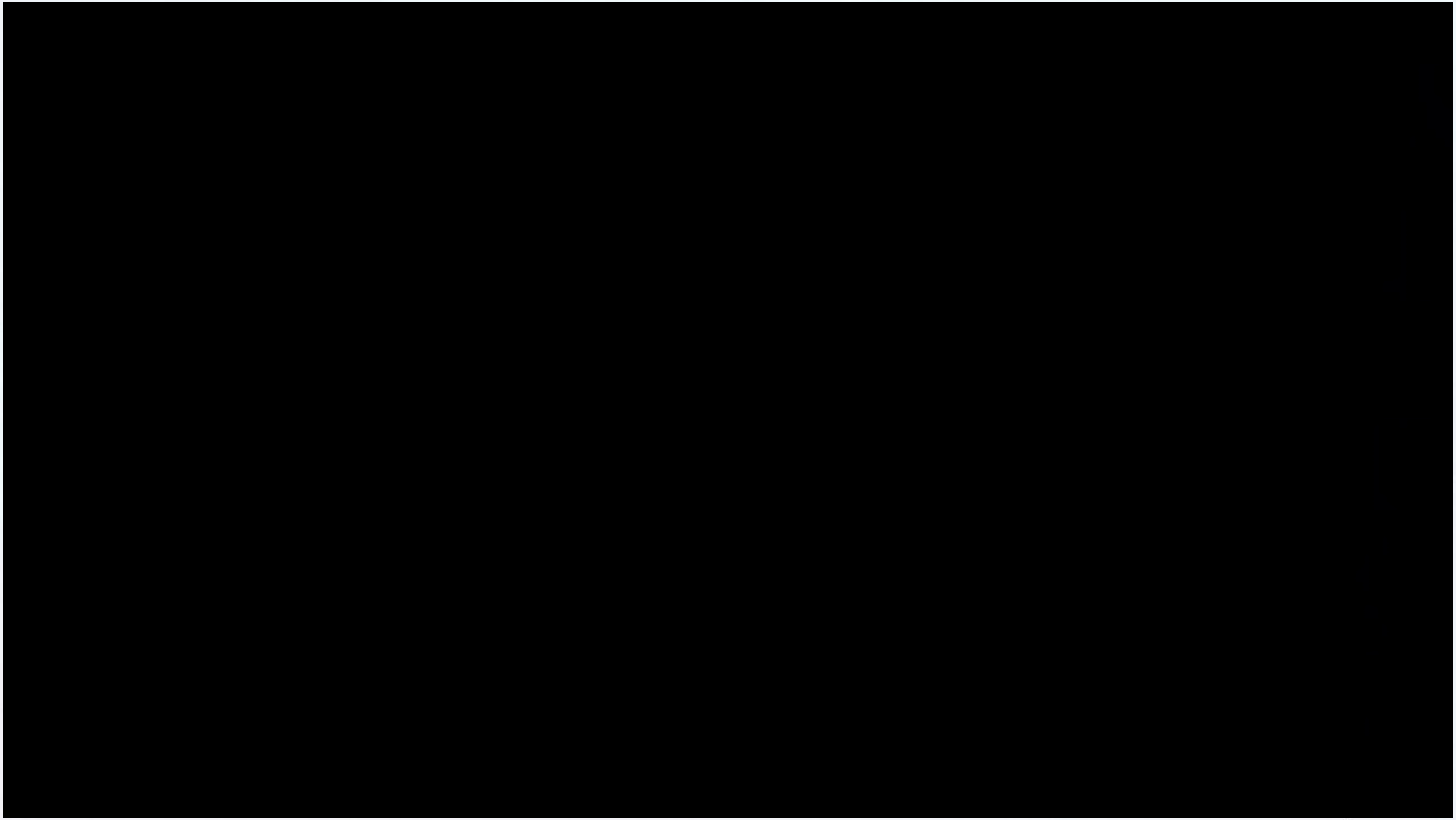
Nicolas R. de Souza, Alice Klapproth & Gail N. Iles, Neutron News 27 (2016) 20



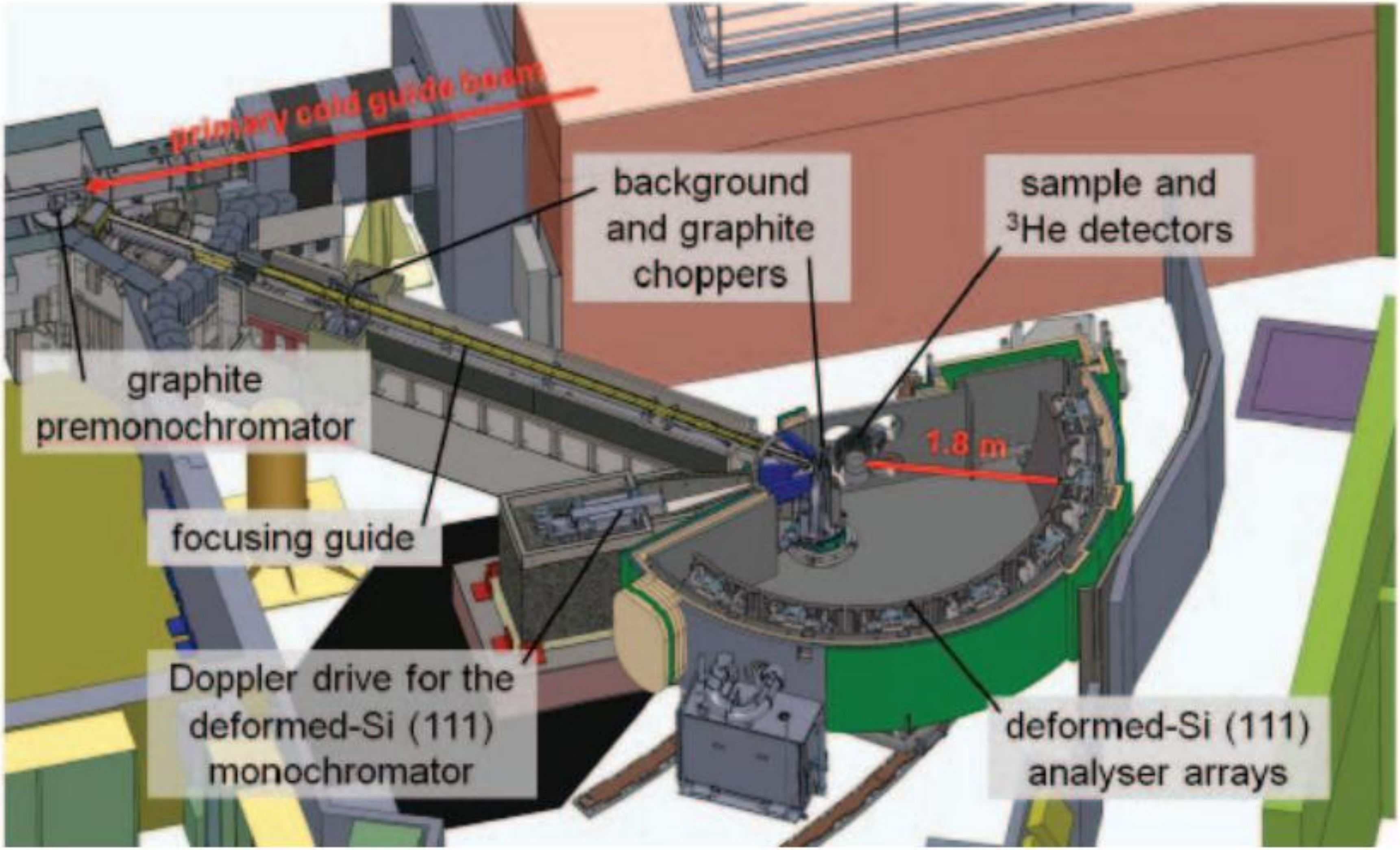
EMU delivers a constant full-width half maximum resolution of ~1.1 μeV at the elastic line, for a total energy transfer range of ±28 μeV, across an elastic momentum transfer range spanning from ~0.1 to 1.95 $Å^{-1}$.

“Emu” - High-Resolution Backscattering Spectrometer

Nicolas R. de Souza, Alice Klapproth & Gail N. Iles, Neutron News 27 (2016) 20

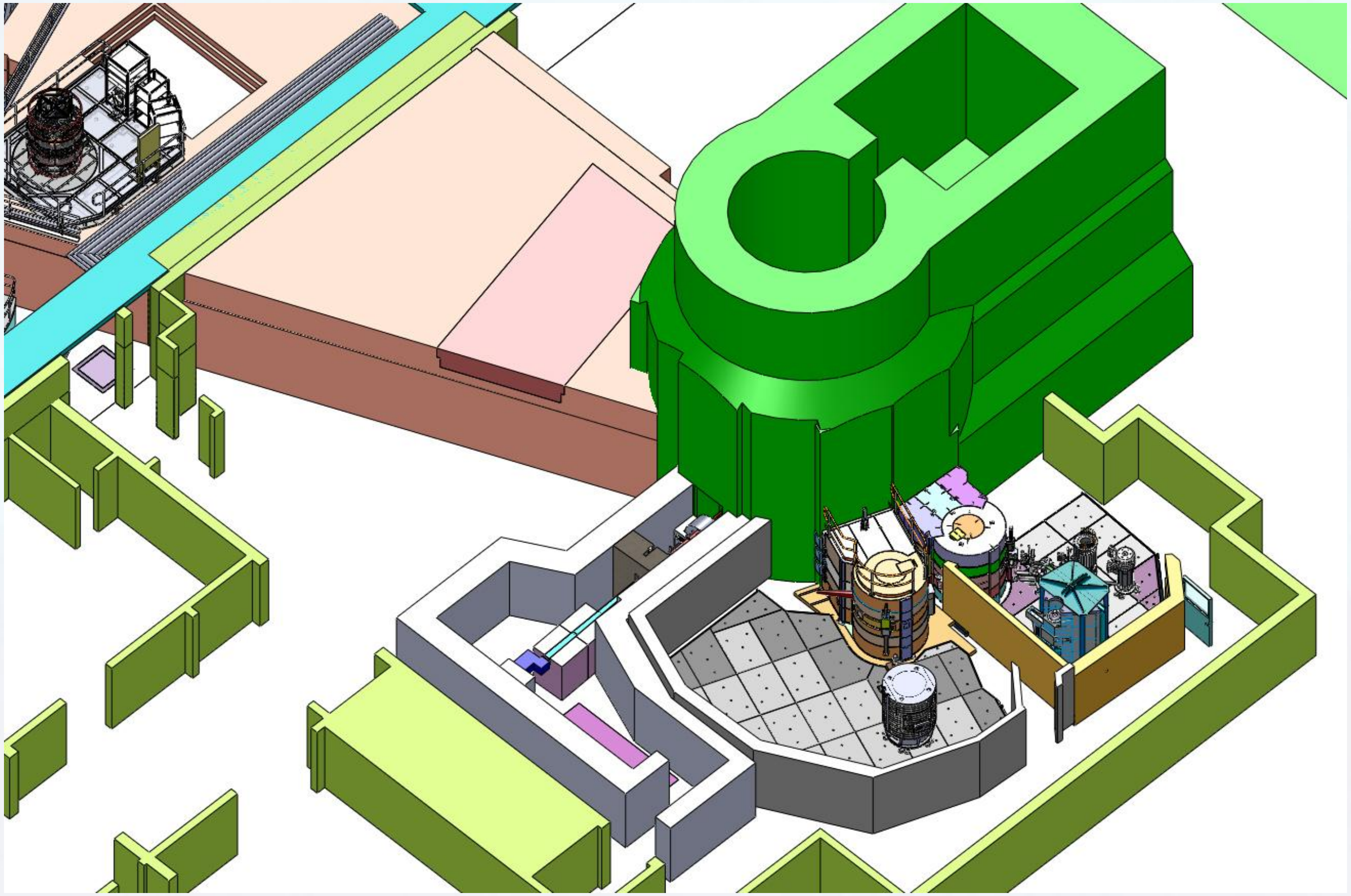


“Emu” - High-Resolution Backscattering Spectrometer



Nicolas R. de Souza, Alice Klapproth & Gail N. Iles, Neutron News 27 (2016) 20

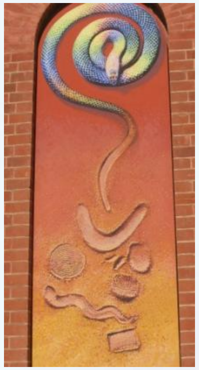
Neutron Scattering Instruments in RBH

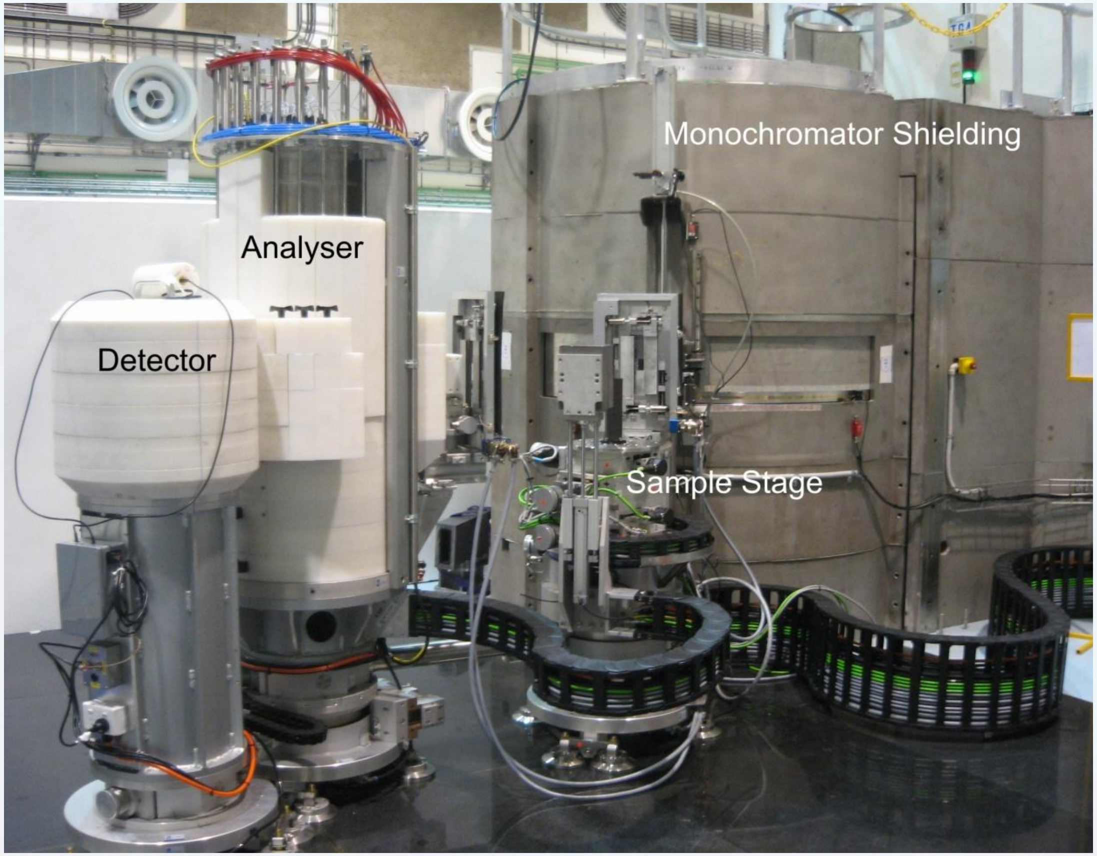


Cold TAS (left) and Thermal TAS TAIPAN (right) in RBH

Triple-axis spectrometer "TAIPAN"

S. Danilkin, G. Horton, R. Moore, G. Braoudakis, M. Hagen, J. of Neutron Research, 15 (2007) 55.





- Thermal neutron beam
- Double-focusing monochromator and analyser
- Single detector
- Polarisation analysis capability

Operational Licence: October 2010

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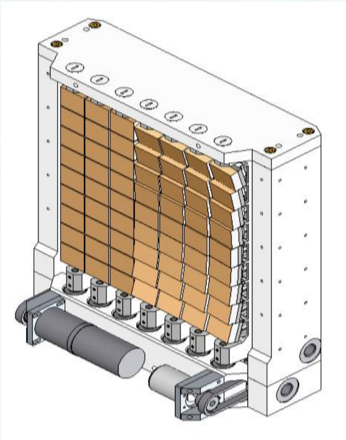
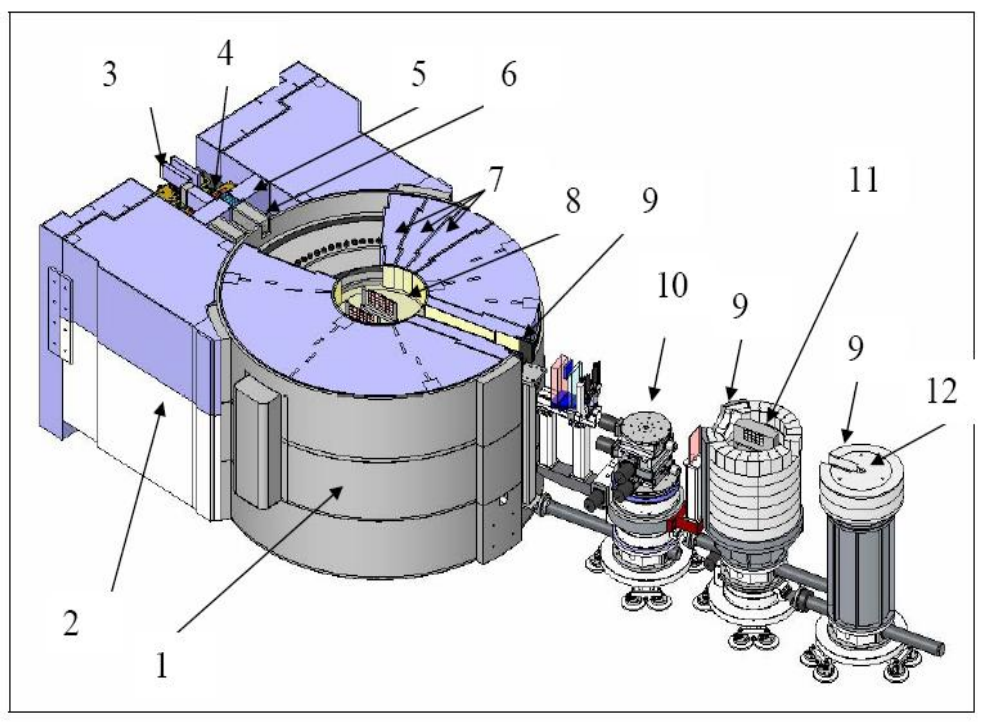
Layout of TAS TAIPAN



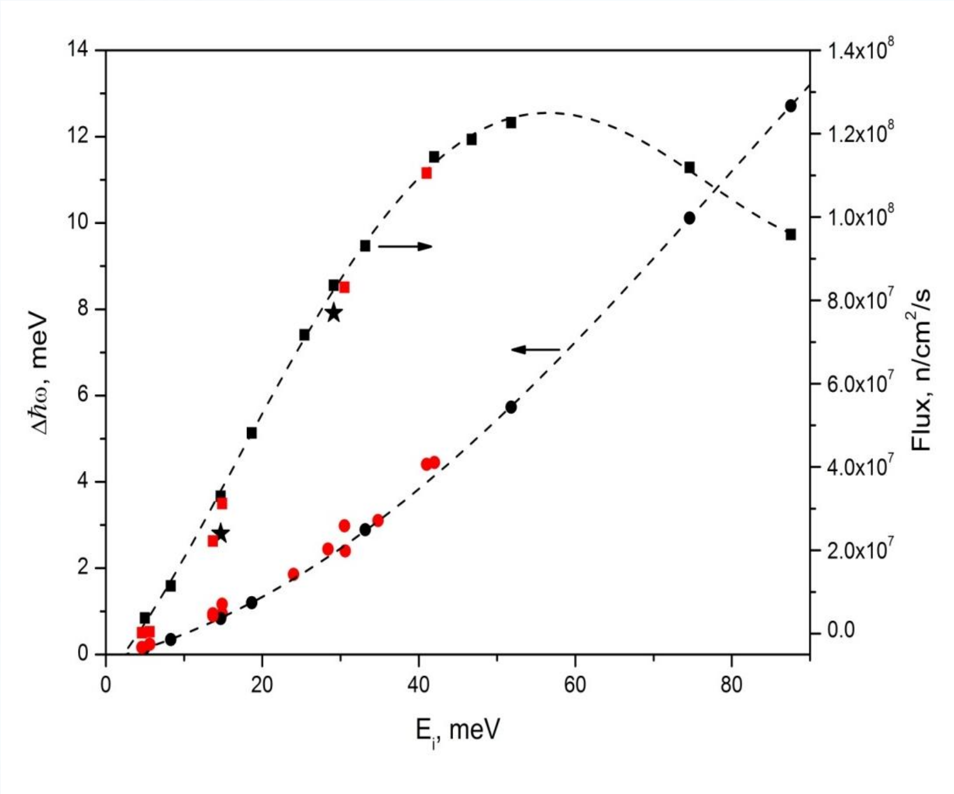


(1) monochromator shielding
(2) ancillary shielding
(3) virtual source
(4) secondary beam shutter
(5) sapphire filter
(6) pre-monochromator collimators
(7) mobile wedges
(8) monochromator
(9) collimators
(10) sample stage
(11) analyser stage
(12) detector stage

Taipan Specifications

Size of beam at reactor face	50 × 175 mm^2 (W×H)
Horizontal virtual source aperture	(0 - 65) × 200 mm^2
Monochromator	HOPG (002) 24′ and Cu (200) 20′, Double-focusing; 200 × 200 mm^2
Monochromator, take-off angle	$16° \leq 2\theta_M \leq 85°$
Sample table	Non-magnetic double goniometer, on air-pads, maximum central weight 5 kN,
Sample scattering angle	$-145° \leq 2\theta_S \leq 115°$
Analyser	HOPG (002) 24′ Double-focusing; 160 × 140 mm^2
Analyser scattering angle	$-110° \leq 2\theta_A \leq 110°$
Detector	∅25 mm ^3He detector (focused analyser);
	∅50 mm ^3He detector (collimator)
Distance, Source – Monochromator	6500 mm
Distance, Reactor Face – Monochromator	2000 mm
Distance Monochromator – Sample	1750 - 2000 mm
Distance Sample – Analyser; Analyser – Detector	810 - 1125 mm
Pre-monochromator collimators	15′, 30′, Open; 90 × 185 mm^2 (W×H)
Post-monochromator collimators	10′, 20′, 40′, 60′, 80′; 50 × 130 mm^2 (W×H)
Pre-analyser and pre-detector, collimators	20′, 40′, 60′, 150′, Open; 50 × 130 mm^2 (W×H)
Polarisation	Polarized 3He spin filters

Neutron flux and resolution of TAS TAIPAN



Neutron Incident energy, E_i (meV)

■ - calculated neutron flux at the sample position from HOPG (002) monochromator (McSTAS);

★ - neutron flux (gold foils) from vertically focused HOPG (002) monochromator; with PG filter for E_i =14.8meV and corrected for second order contamination for E_i= 30.6 meV;

■ - neutron flux (vanadium) of monochromatic neutrons from vertically focused HOPG (002) monochromator and with PG filter;

●- calculated FWHM of resolution function at sample position for HOPG monochromator (McSTAS);

● - measured FWHM of vanadium elastic peak for vertically focussed HOPG (002) monochromator and collimation 40´ before and after sample.

S. A. Danilkin; M. Yethiraj, Neutron News, 20 (2009) 37.

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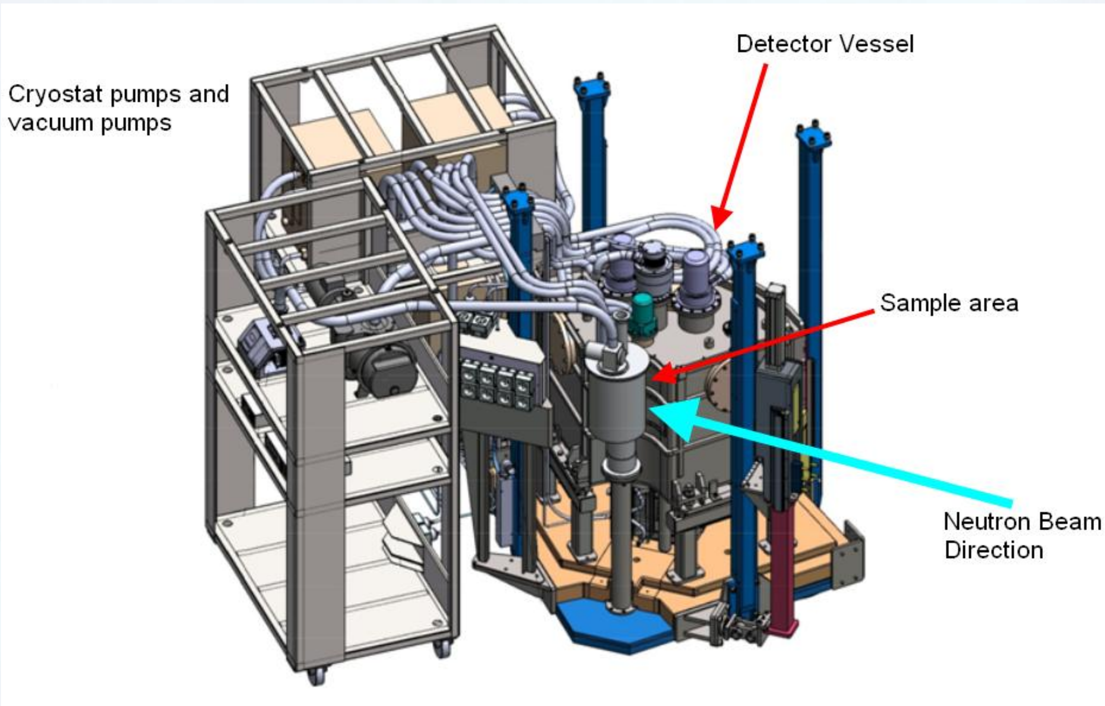
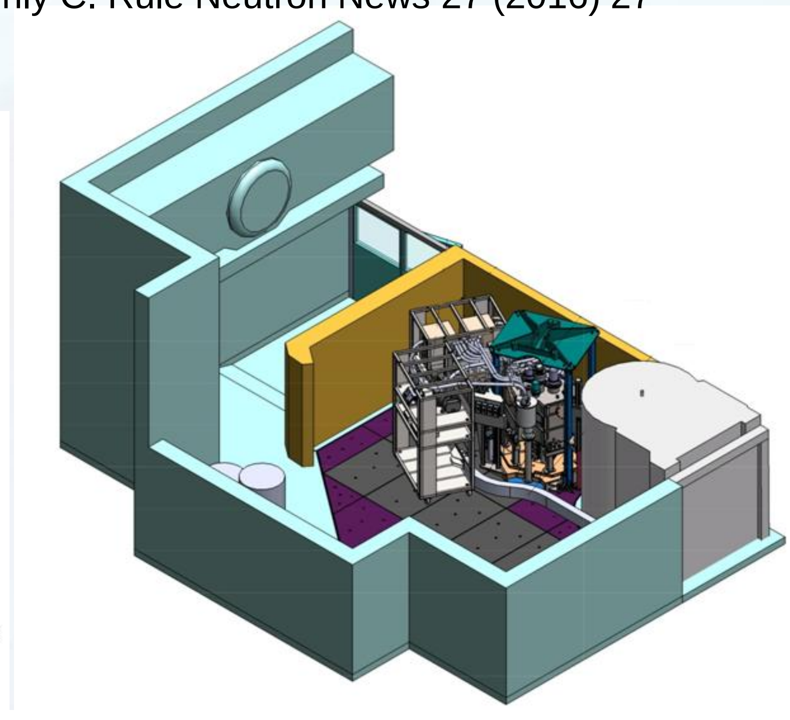
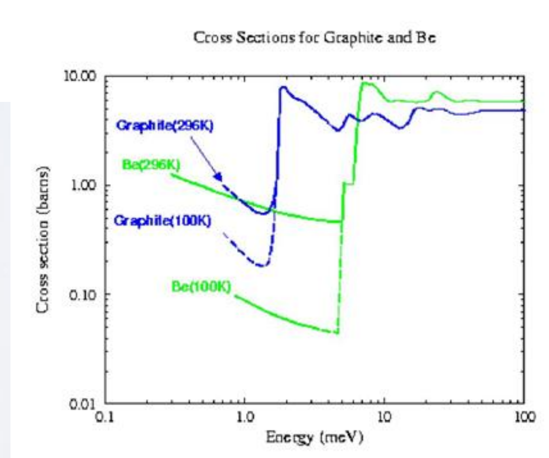
Be Filter Analyser / Detector

Anton P. J. Stampfl, Andrew Eltobaji, Frank Darmann & Kirrily C. Rule Neutron News 27 (2016) 27







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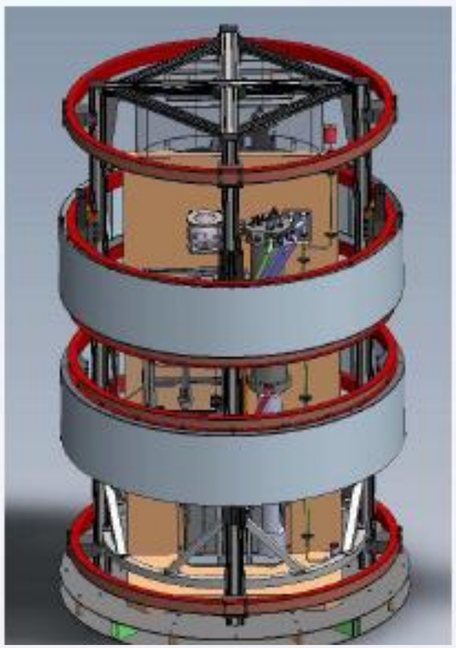
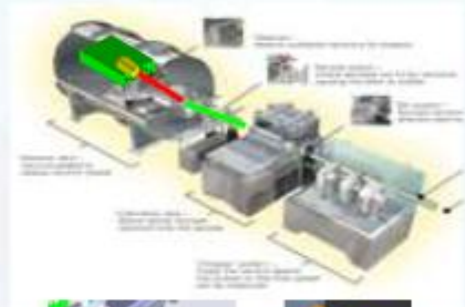
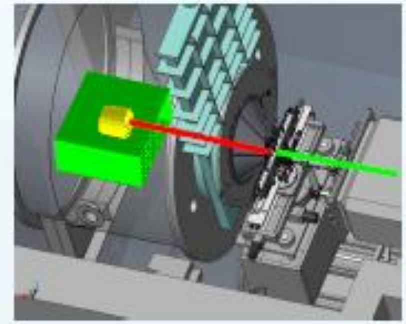
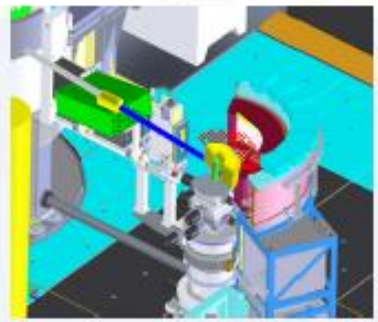
Polarised ^{3}He Setup for 6 ANSTO Instruments

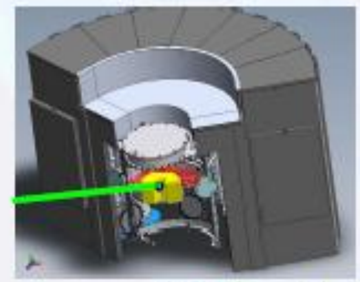
To facilitate the use of polarised neutrons in scattering works, ANSTO will acquire a ^{3}He polarising station and instrument equipment (silicon spin filter cell, "magic box", wide-angle analyser cell, "Pastis" coils, "local filling" setup, transporter, etc.)

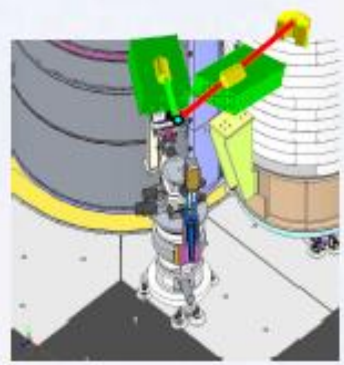


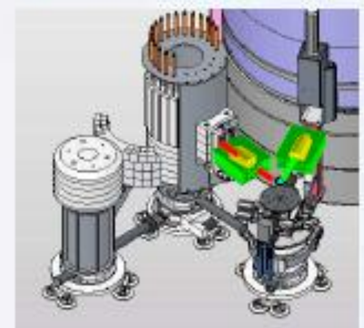




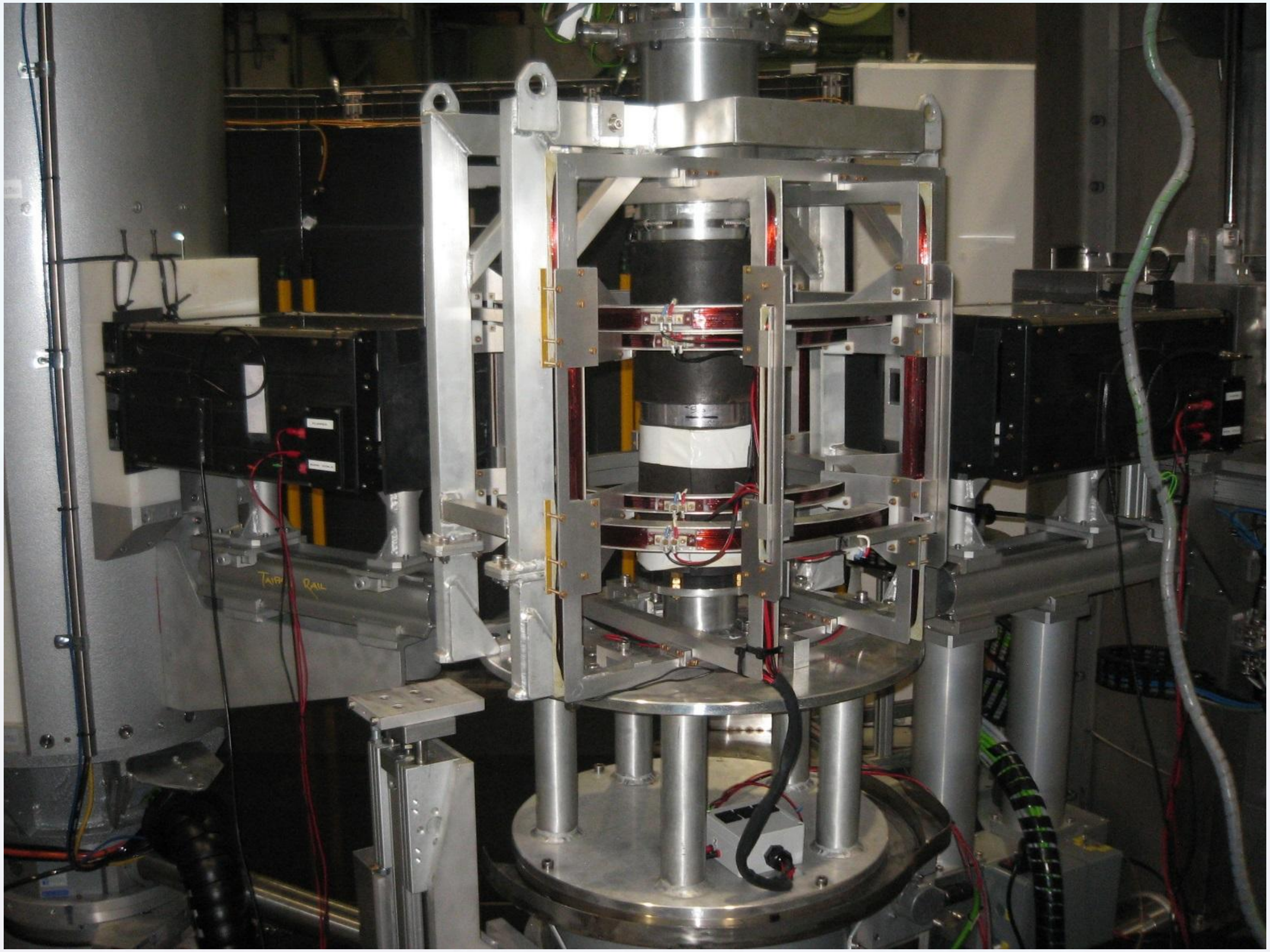








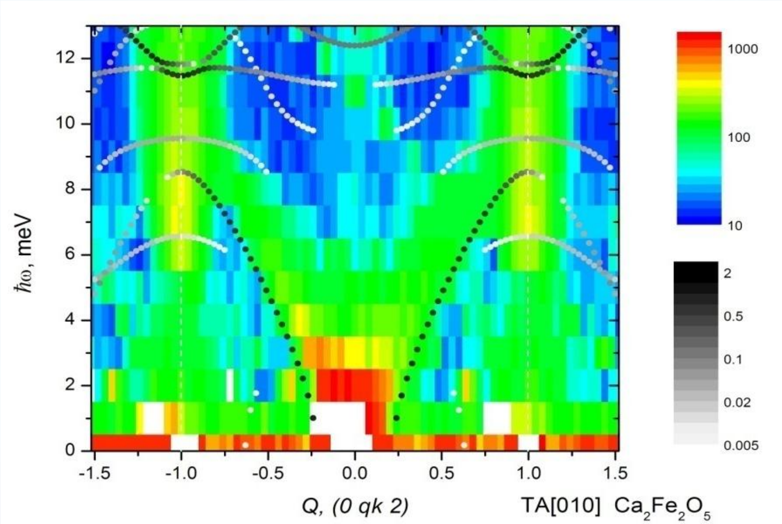
Polarisation setup at TAIPAN

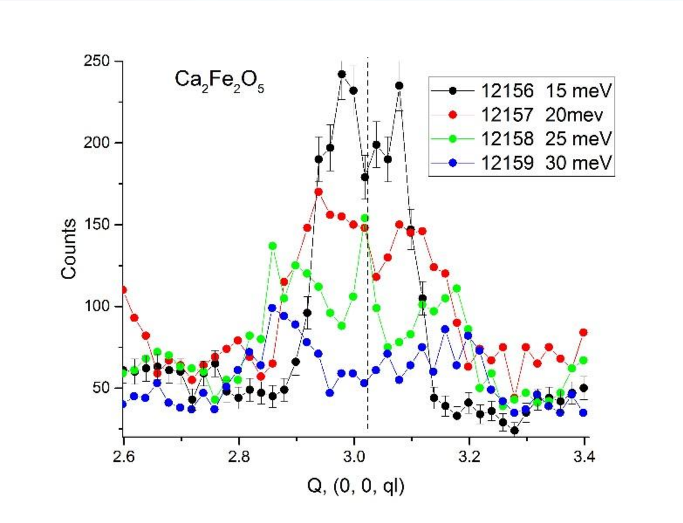


Magnons in $Ca_2Fe_2O_5$

Magnetic reflections (0 -1 2) and (0 1 2)

↓ ↓





Phonon transverse [010] mode

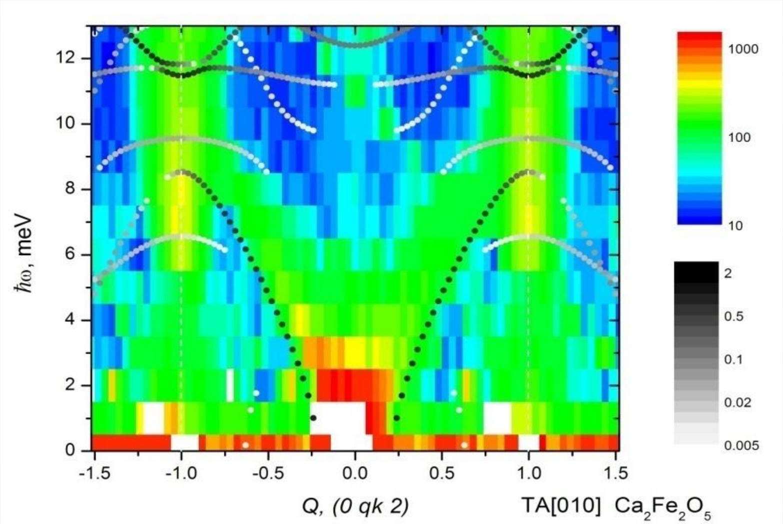
$\boldsymbol{q}$ = (0, ξ, 0) $\boldsymbol{e}$ = (0, 0, 1)

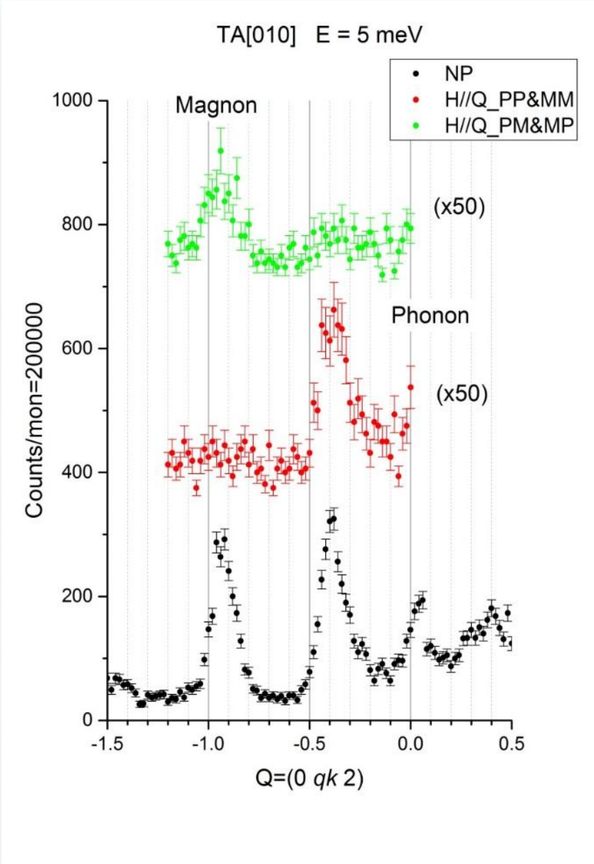
Magnons in (003) BZ

Magnons in $Ca_2Fe_2O_5$

Magnetic reflections (0 -1 2) and (0 1 2)

↓ ↓

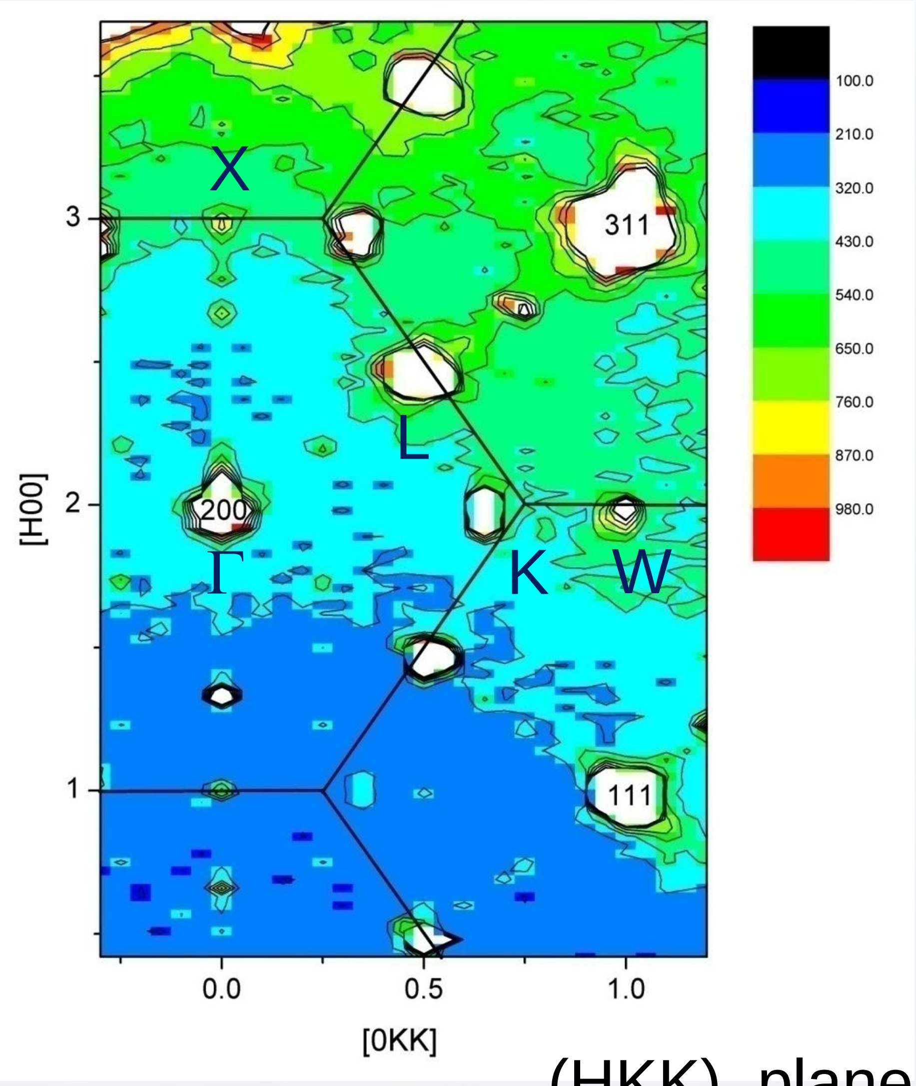




Phonon transverse [010] mode

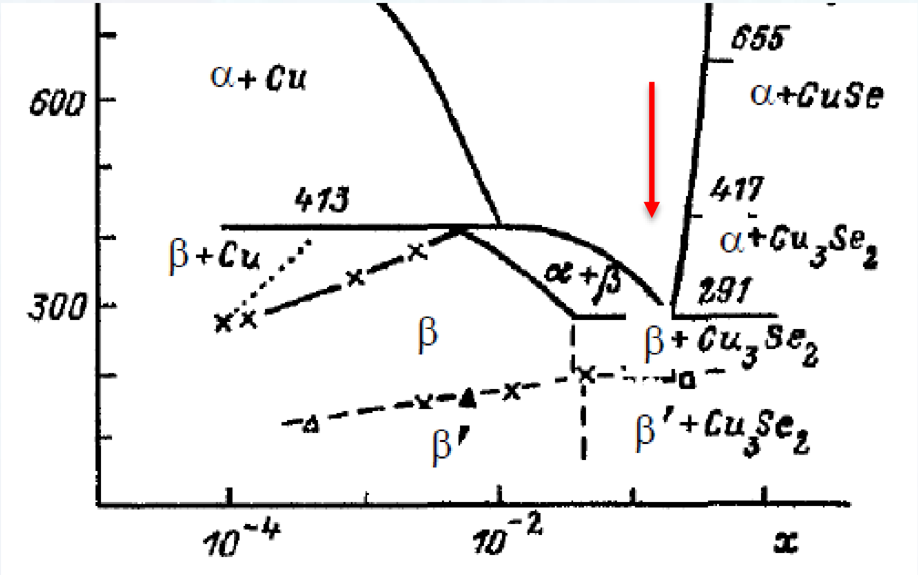
$\boldsymbol{q} = (0, \xi, 0)$ $\boldsymbol{e} = (0, 0, 1)$

Ordering in Superionic High-T α-phase at RT



(HKK) plane

α- $Cu_{1.8}Se$ @ RT



q = 1/8 [1, 1, 1]
q = 1/3 [2, 2, 0]

Kashida (1988)

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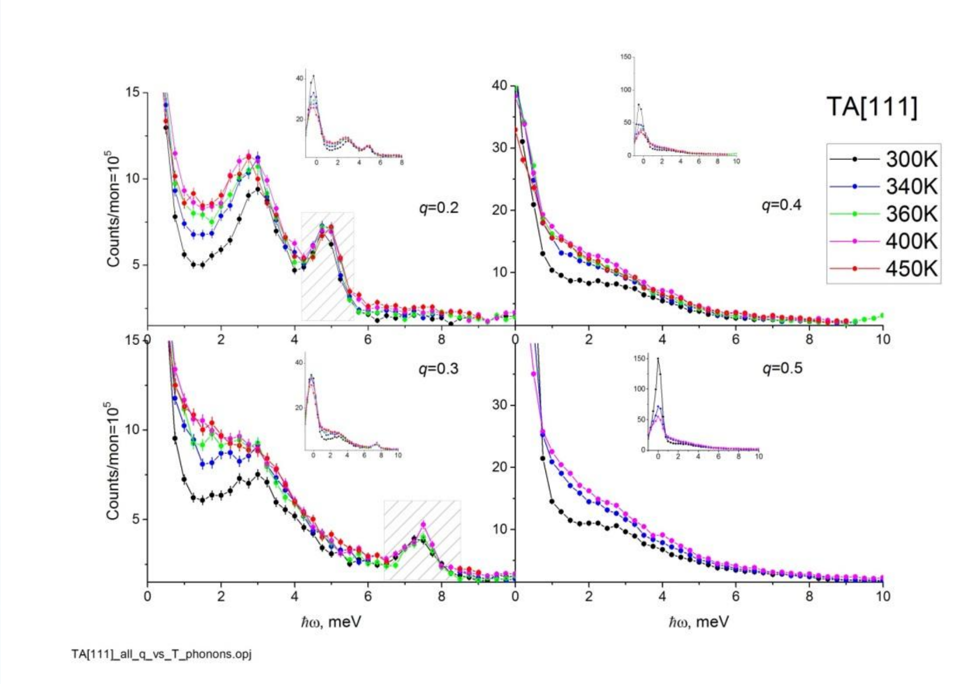
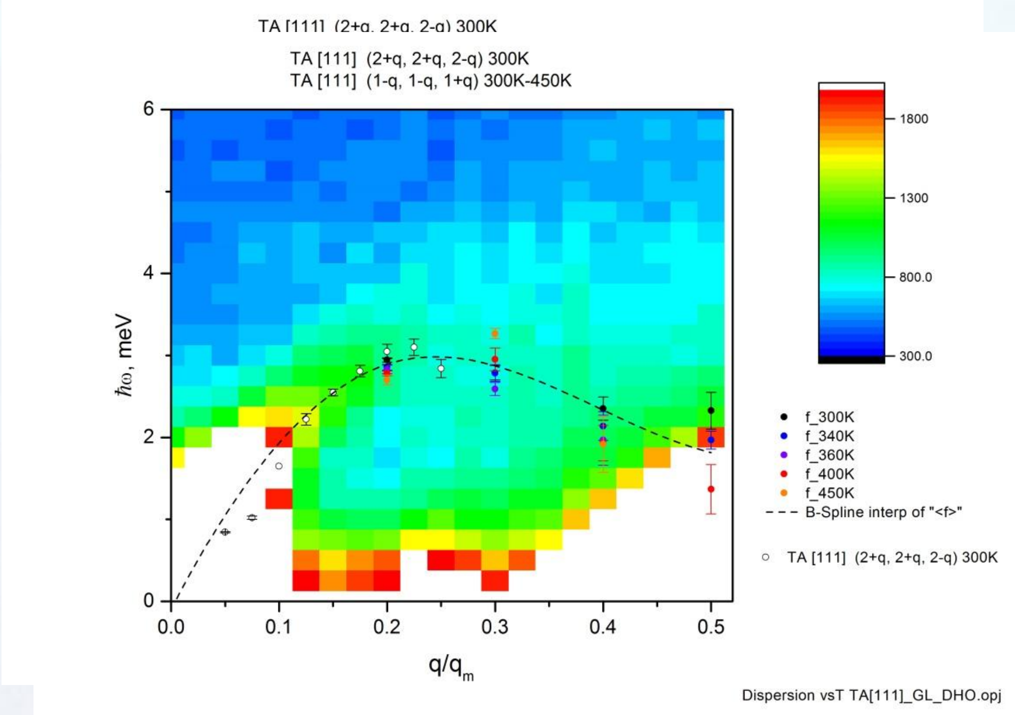
Phonons *vs.* T in $Cu_{1.85}Se$





TA [111] one-phonon peaks in $Cu_{1.85}Se$

2nd order phase transition with formation of large ordered structures at LT
Superstructure and BZ folding in HT phase
Strong phonon damping at $q/q_m \geq 0.5$

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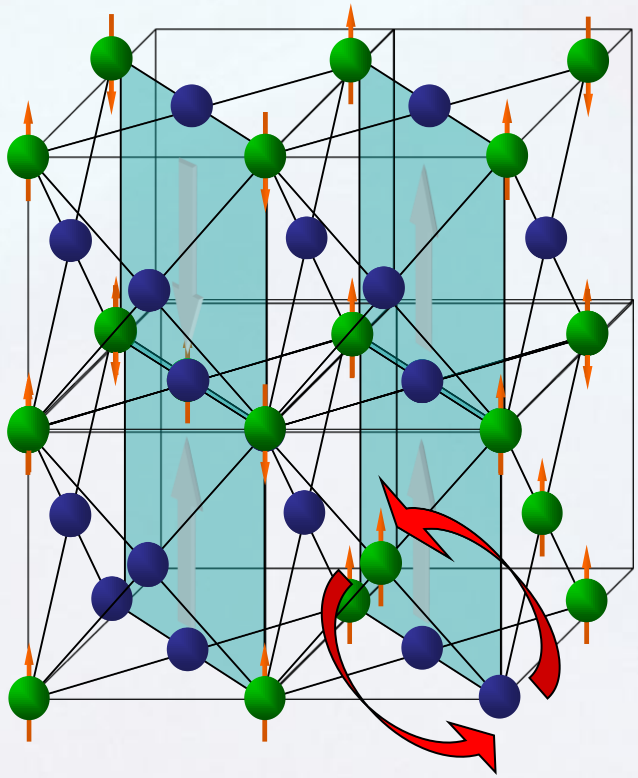
Chemical Order/Disorder in $FePt_3$ Thin Films: FM/AFM Interfaces

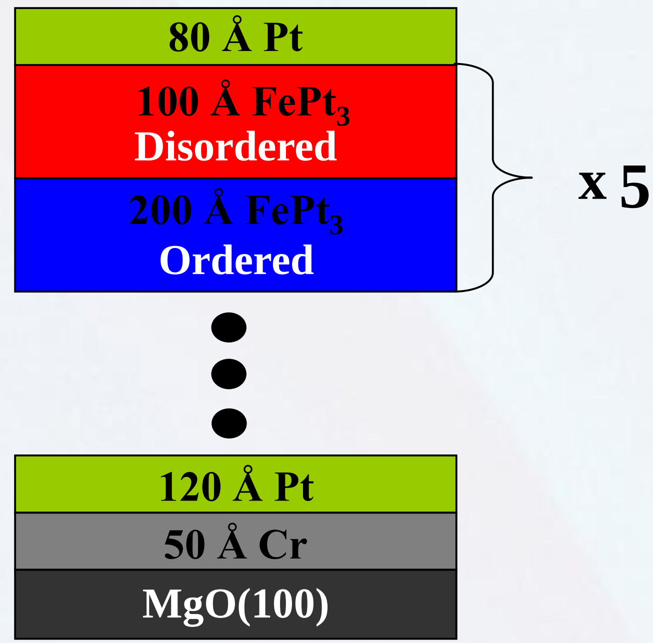
Creation of AFM/FM superlattice by modulation of substrate temperature during growth

Chem. order:
AFM

Chem. disorder:
FM

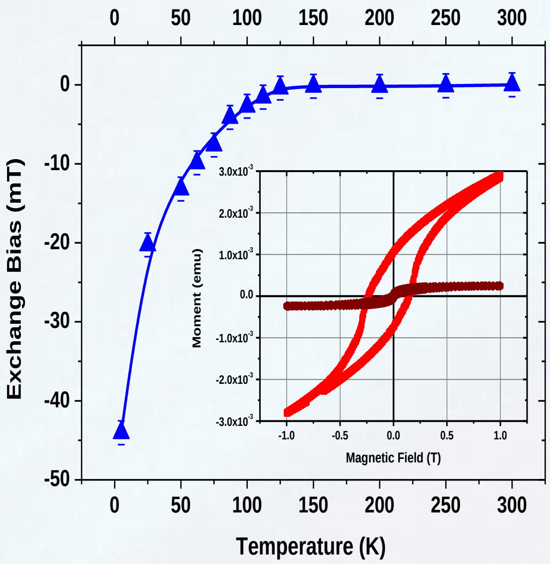


Chemical order modulation

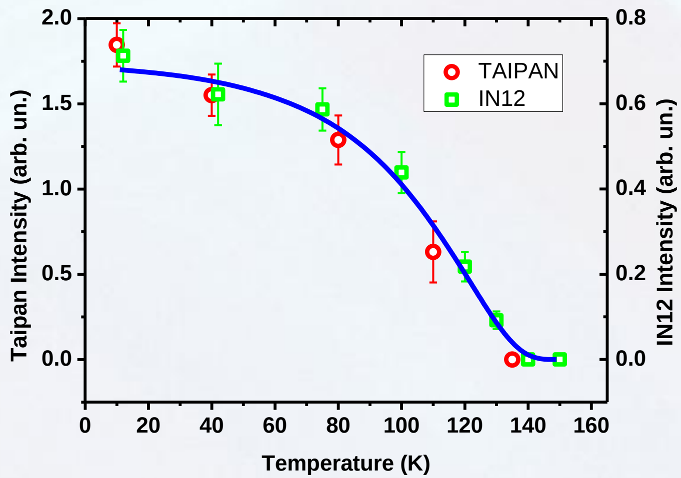


T. Saerbeck, F. Klose, D. Lott, G.J. Mankey, Z. Lu, P.R. LeClair, W. Schmidt, A.P.J. Stampfl, S. Danilkin, M. Yethiraj and A. Schreyer
Phys. Rev. B 82 (2010) 134409

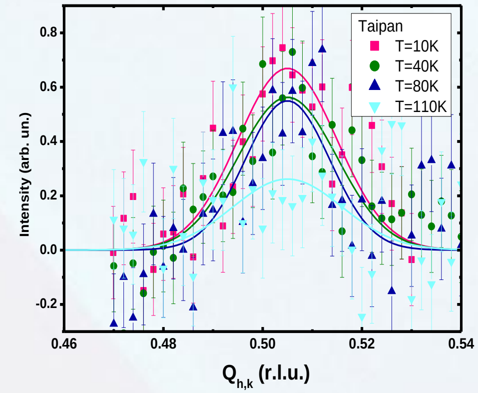
Chemical Order/Disorder in $FePt_3$ Thin Films: FM/AFM Interfaces

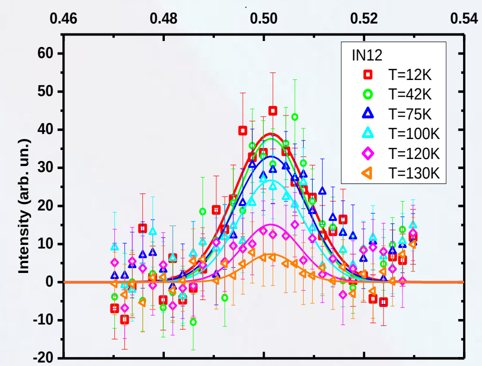


Exchange Bias Field *vs.* T
Onset agrees with T_N

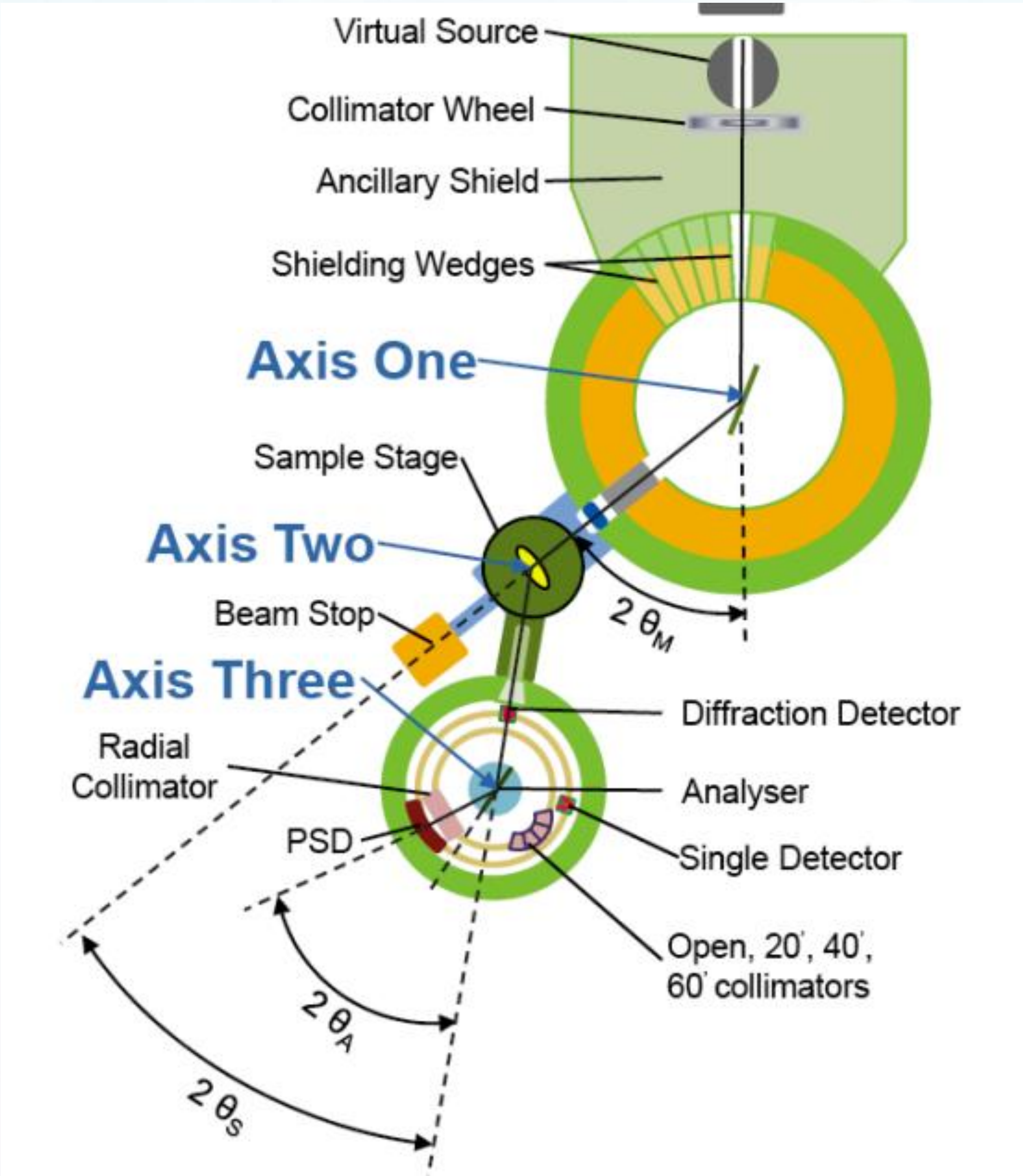


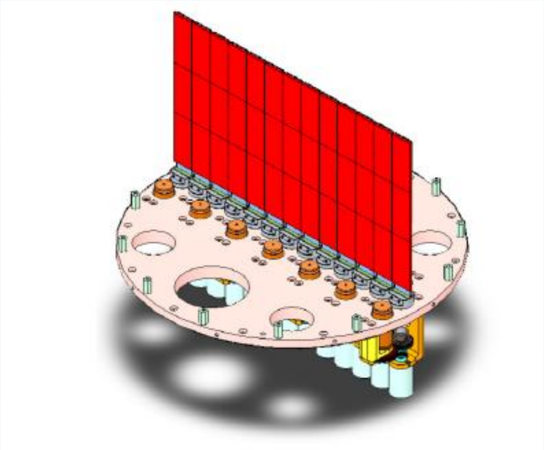
Integrated AFM peak intensity *vs.* T
AFM ordering along (½ ½ 0)





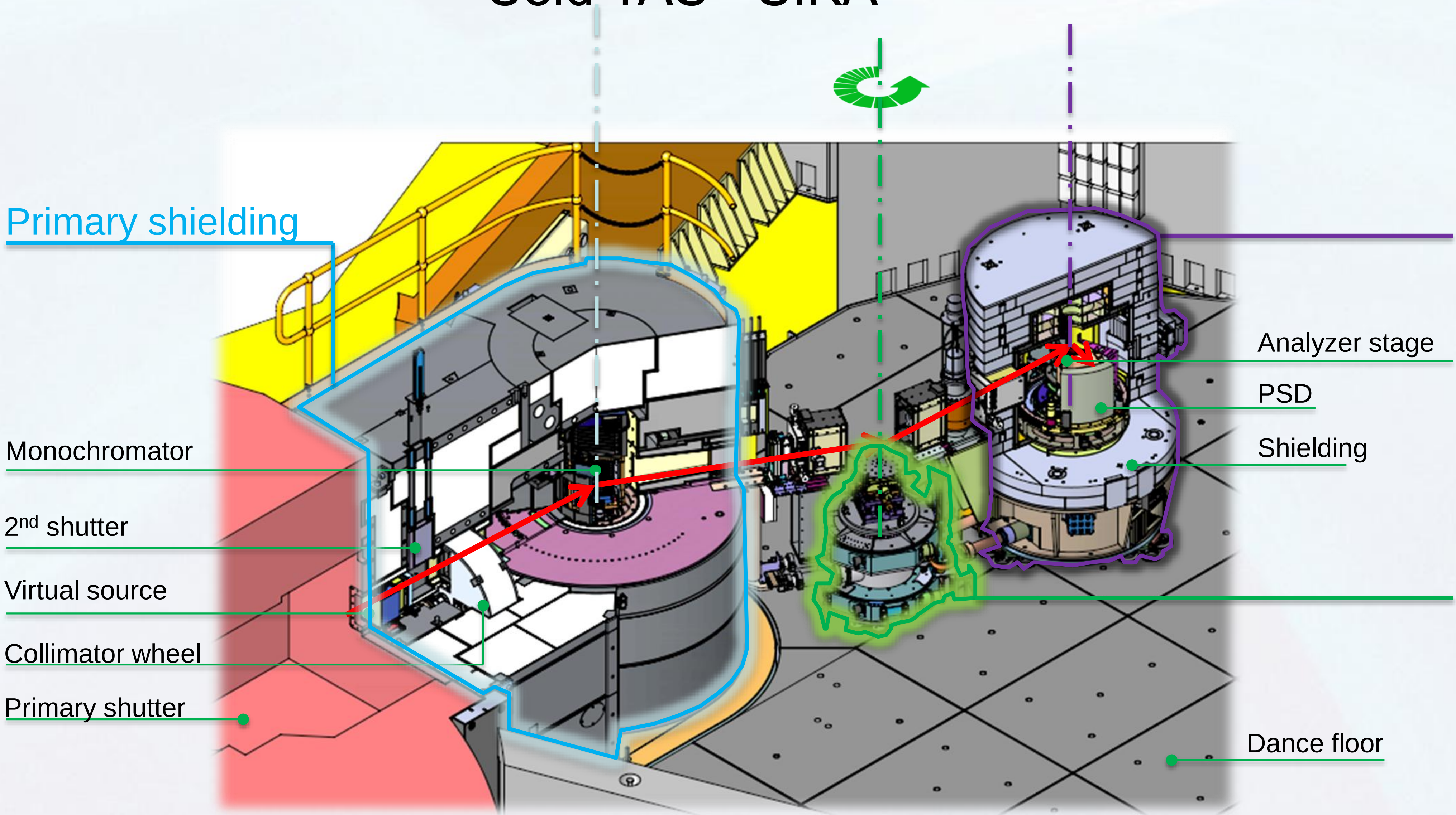
Cold TAS “SIKA”





Analyzer Stage with 13 independent PG blades
Multi-Q Constant E_f mode

Cold TAS "SIKA"



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Cold TAS “SIKA”

SIKA Specification:

Monochromator PG 002
Analyzer PG 002
Take-off angle 2θM 30~120 (1.08~3.6A-1)
Analyzer angle 2θA 35~120 (1.08~3.05A-1)
Pre-monochramator collimator:……open, 20’, 40’, 60’
Pre-sample collimator:………………open, 20’, 40’, 60’
Pre-analyzer radial collimator:…..………………40’, 80’
Pre-detector radial collimator:…. ………………40’, 80’
Incident Energy:……………………………2.6~28meV
Energy Transfer:…………………………..……0~15meV
Beam filters Be cooled (10cm) (E_i < 5 meV)
PG (8cm) (E_i = 13.7 and 14.7 meV)
Sapphire (8cm) (E_i > 15meV)

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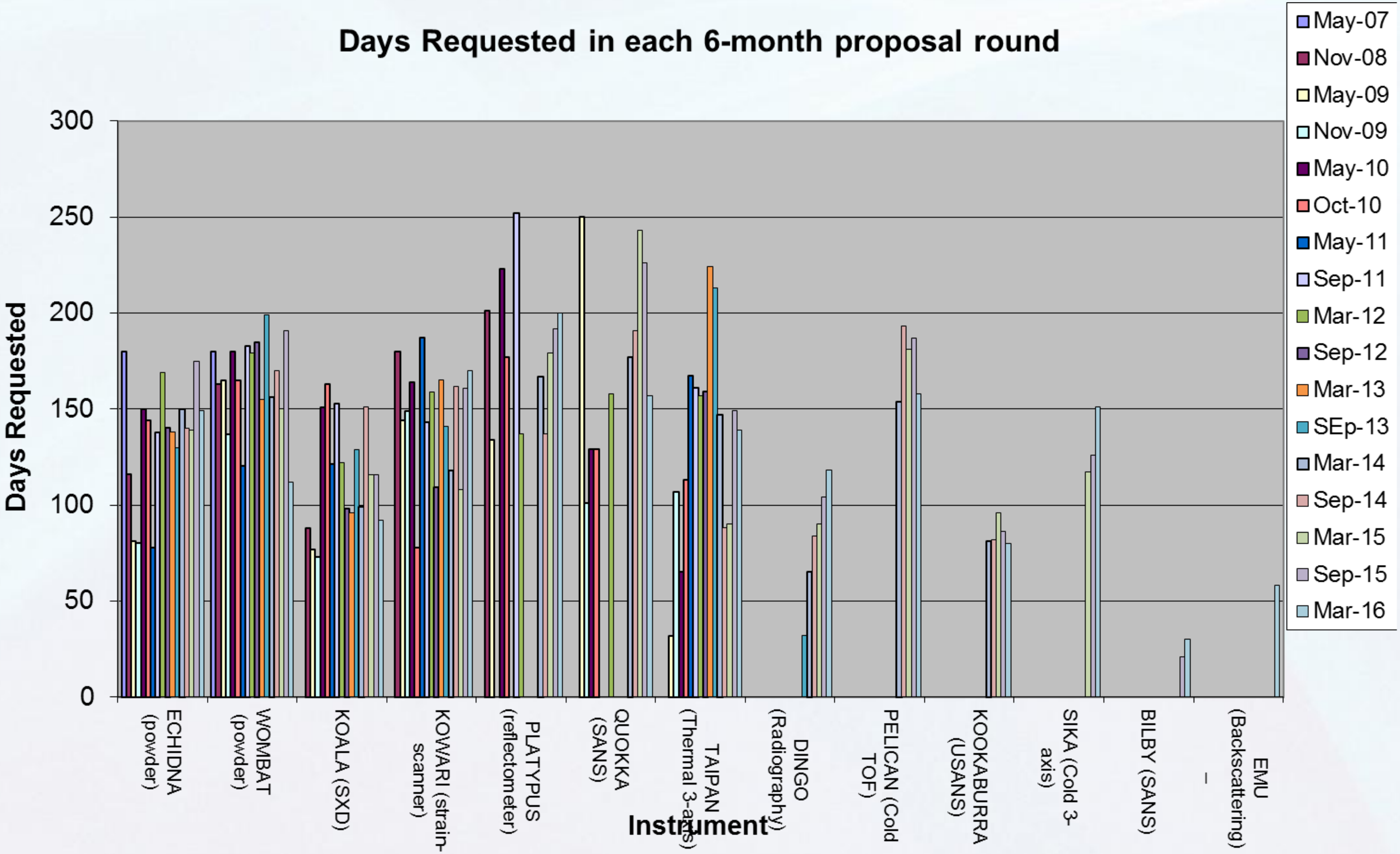

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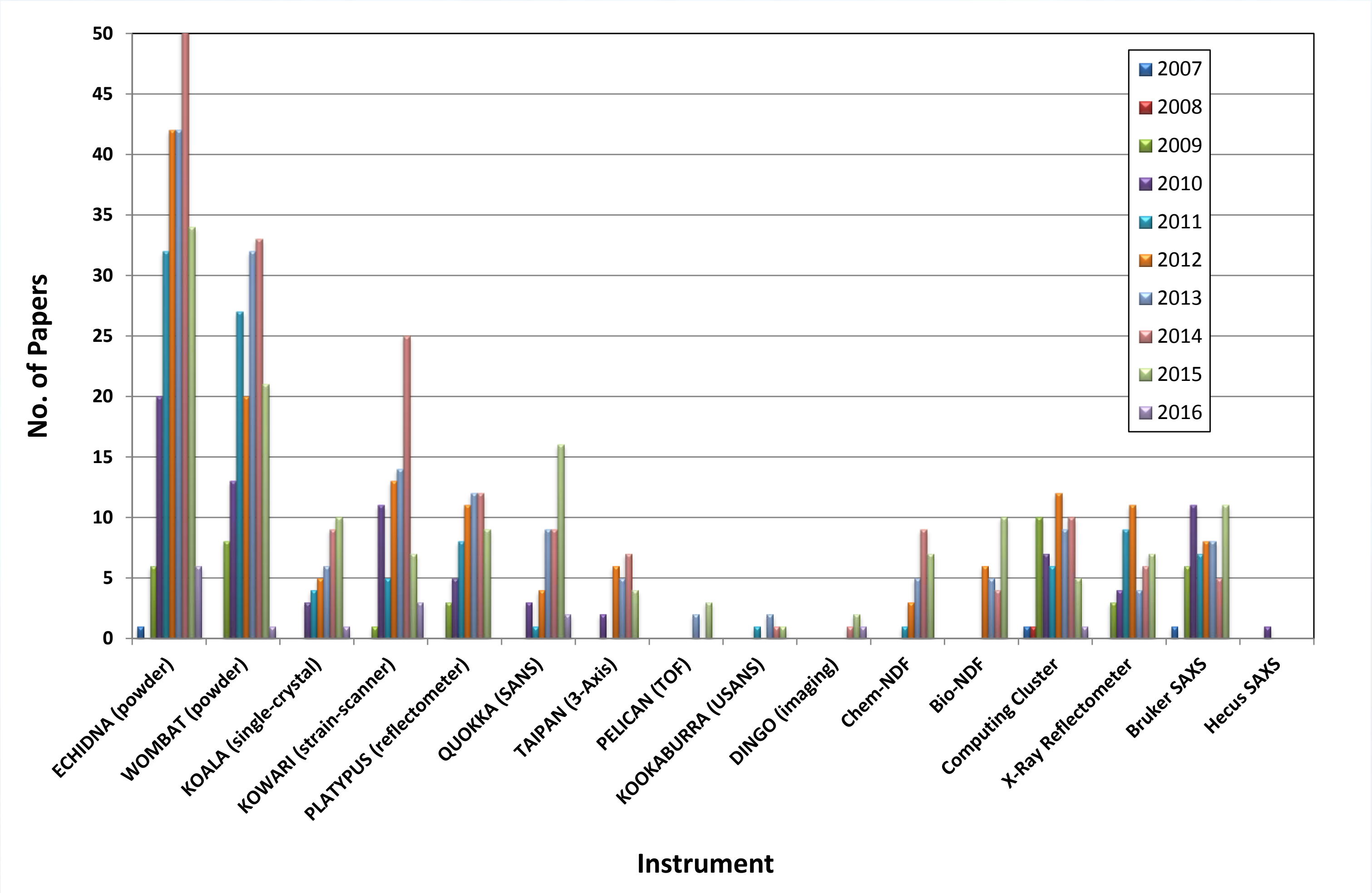
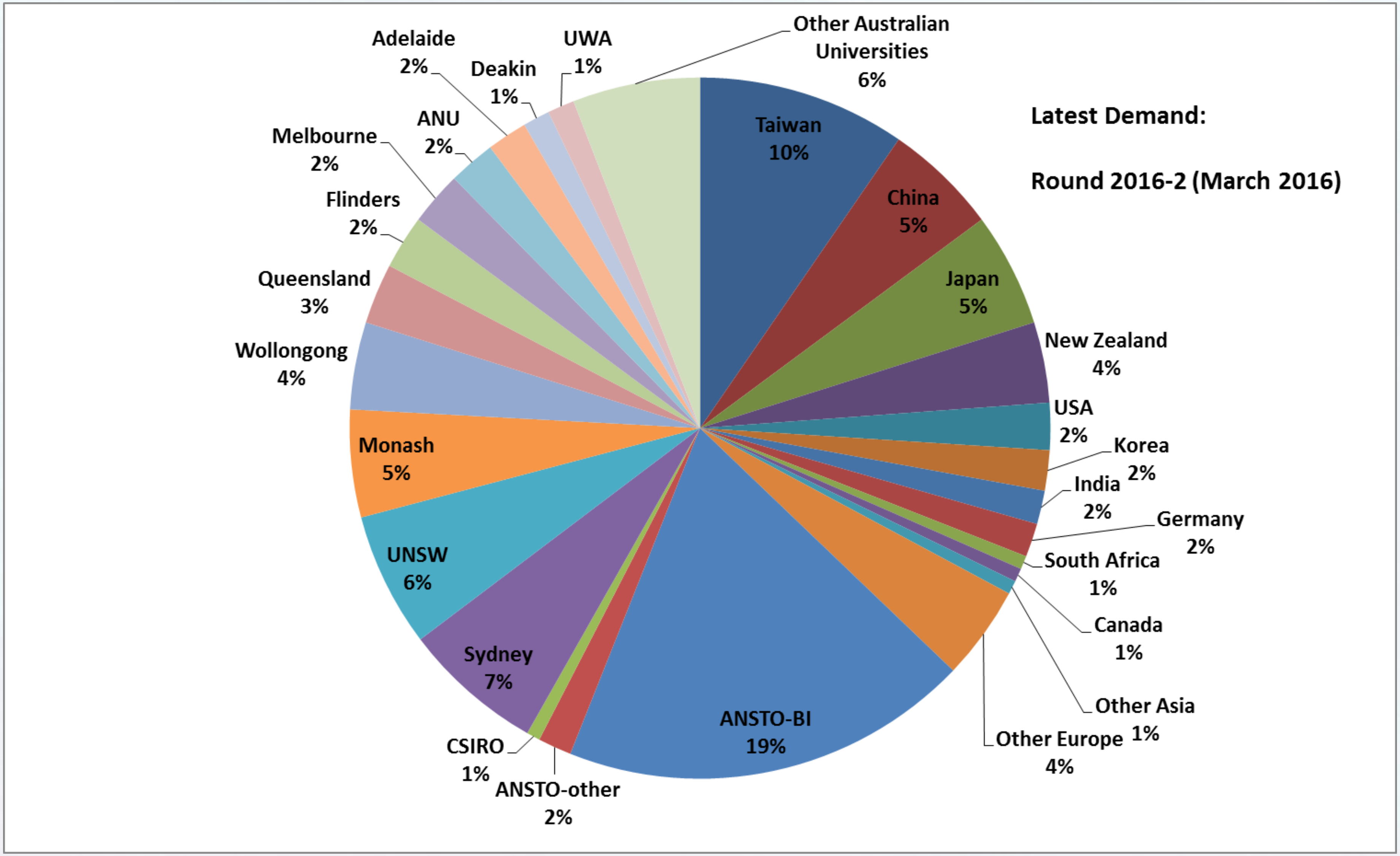
Publications from OPAL





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Australian Government

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