Presenting Diffraction & Imaging Division

- **PhD (2004 – 2007):** *'Magnetic and structural properties of thin films and nanoparticles studied by scattering methods'*, **University of Aachen / Research Center of Jülich**

- **PostDoc (2007 – 2010):** *Condensed Matter Physics & Materials Science Department at* **Brookhaven National Laboratory**, *Supervisor: Prof. M. Aronson*

- **Instrument Scientist (2011 - 2016):** *Spallation Neutron Source at* **Oak Ridge National Laboratory**, *NOMAD diffractometer*

- **Lead Instrument Scientist (2016 -):** *Jülich Center for Neutron Scattering at* **Research Center of Jülich**, *DREAM diffractometer*

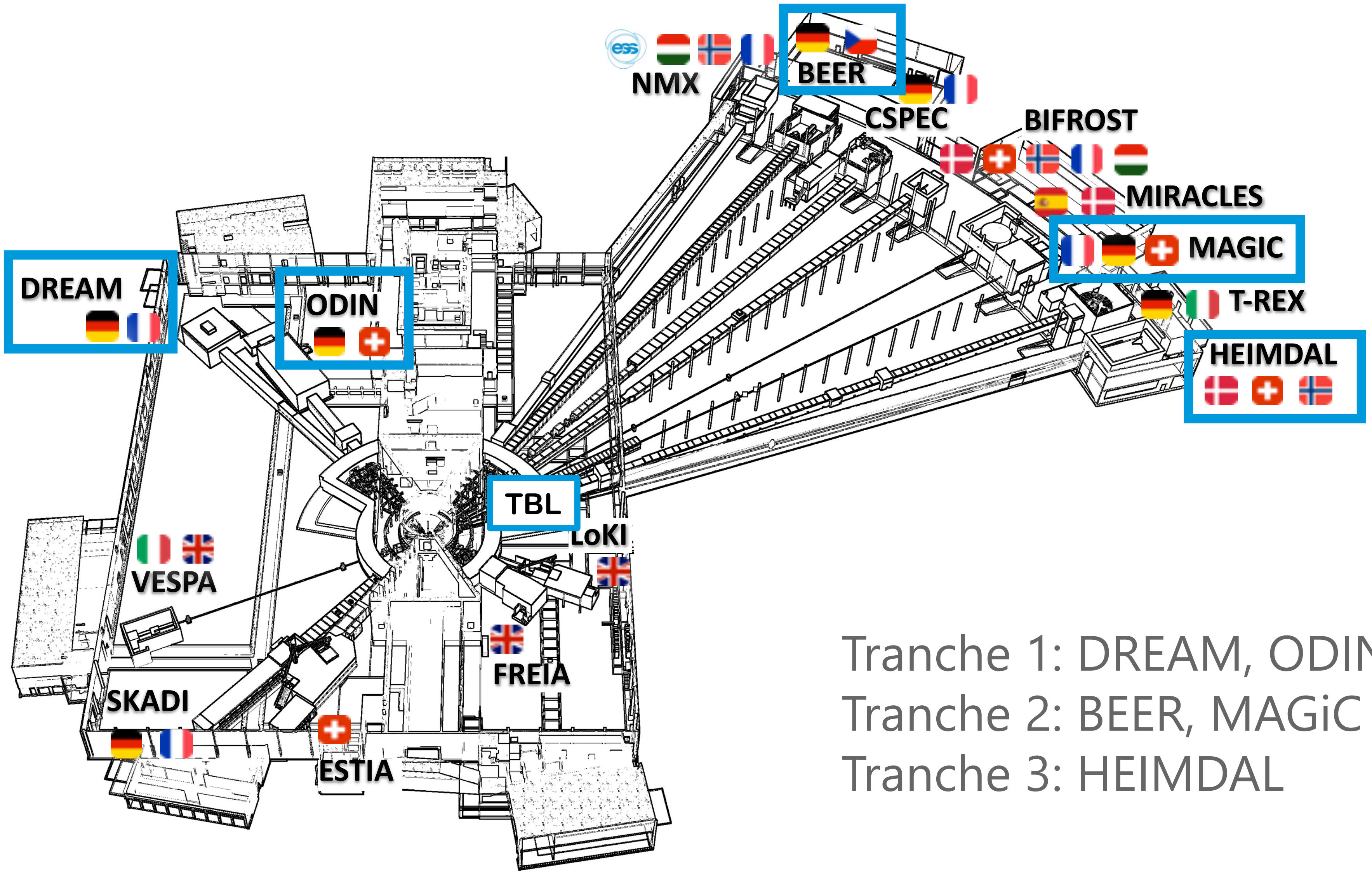
- **Neutron Diffraction Scientist (2021 -):** *Neutron Scattering Systems at* **European Spallation Source**

- **Adjunct Associate Professor (2023 -):** *Department of Materials Science and Engineering at* **Uppsala University**

- **Head of Diffraction & Imaging Division (Feb., 2024 -):** *Science Directorate at* **European Spallation Source**

h-index: 34, i10-index: 61, 80 publications

Instruments



Tranche 1: DREAM, ODIN, TBL
Tranche 2: BEER, MAGiC (tbc)
Tranche 3: HEIMDAL

Division's goals

Gradual transition to Science

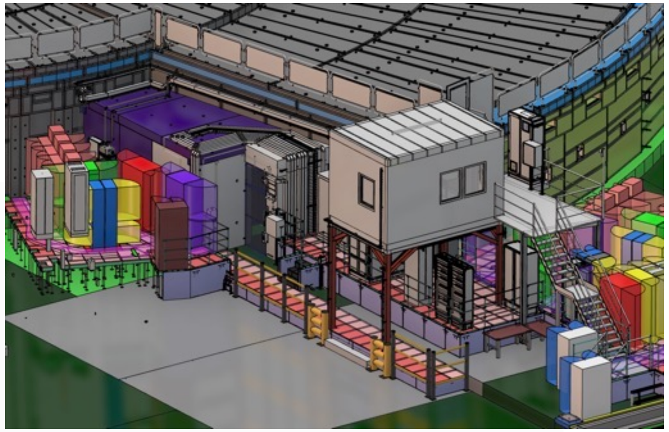
- Work closely with NSS to complete the construction of the instruments
- Work closely with DMSC, Sample Environment, User Office Support to prepare for hot commissioning and first science
- Continue engaging in-kind partners and STAP into preparation for the first science
- Continue hiring instrument staff (MAGiC, DREAM, BEER)
- Ensure smooth integration of first in-kind scientists into the instrument teams (DREAM, BEER)
- Integrate IOEs into the instrument teams
- Support instrument teams in transitioning from a construction project to a science facility

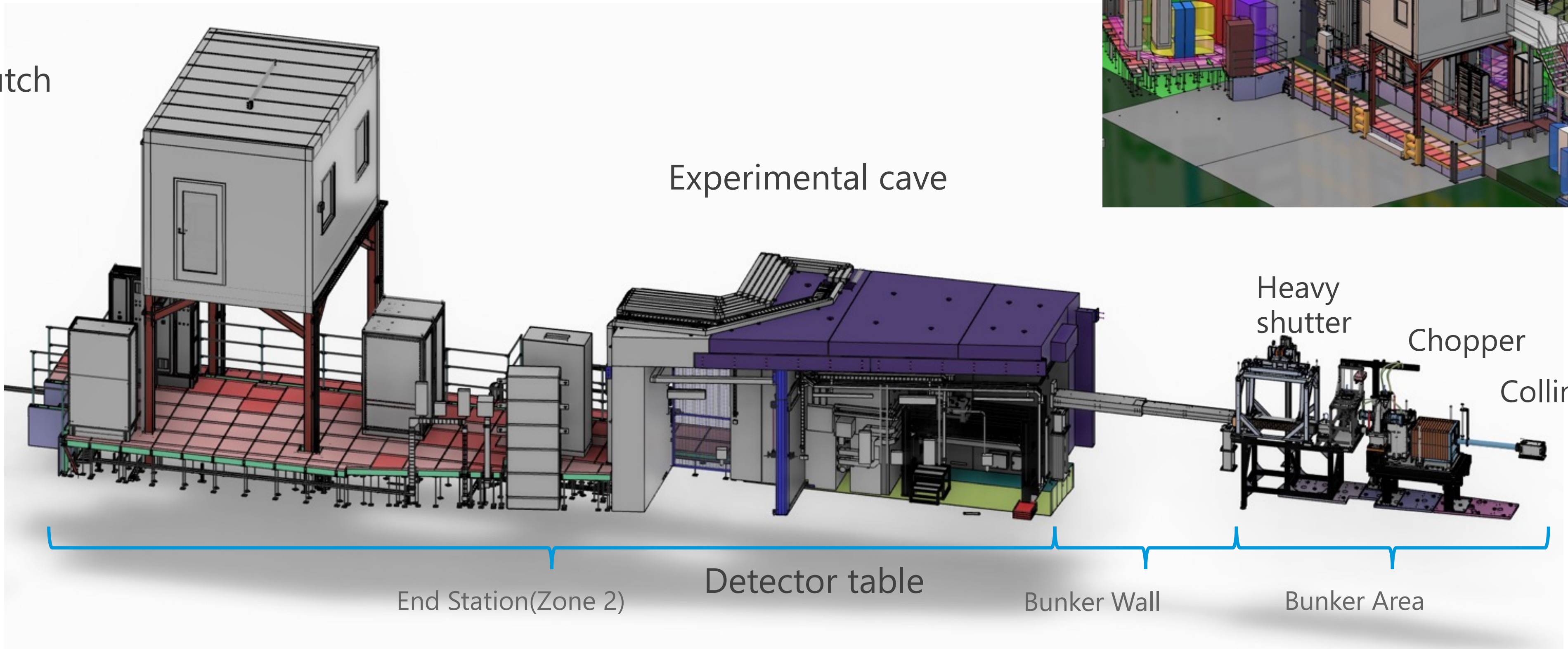
TBL Cold commissioning completed : Q4, 2024

ESS Test Beamline

- Characterization of the ESS moderator system
- Proton beam stability/Moderator stability
- Spatial distribution of neutron beam
- Characterize neutron spectrum
- Pulse-shape of cold-thermal neutrons

- Detectors and data processing systems
- Sample (e.g. single crystal) alignment
- Simple imaging and diffraction experiments

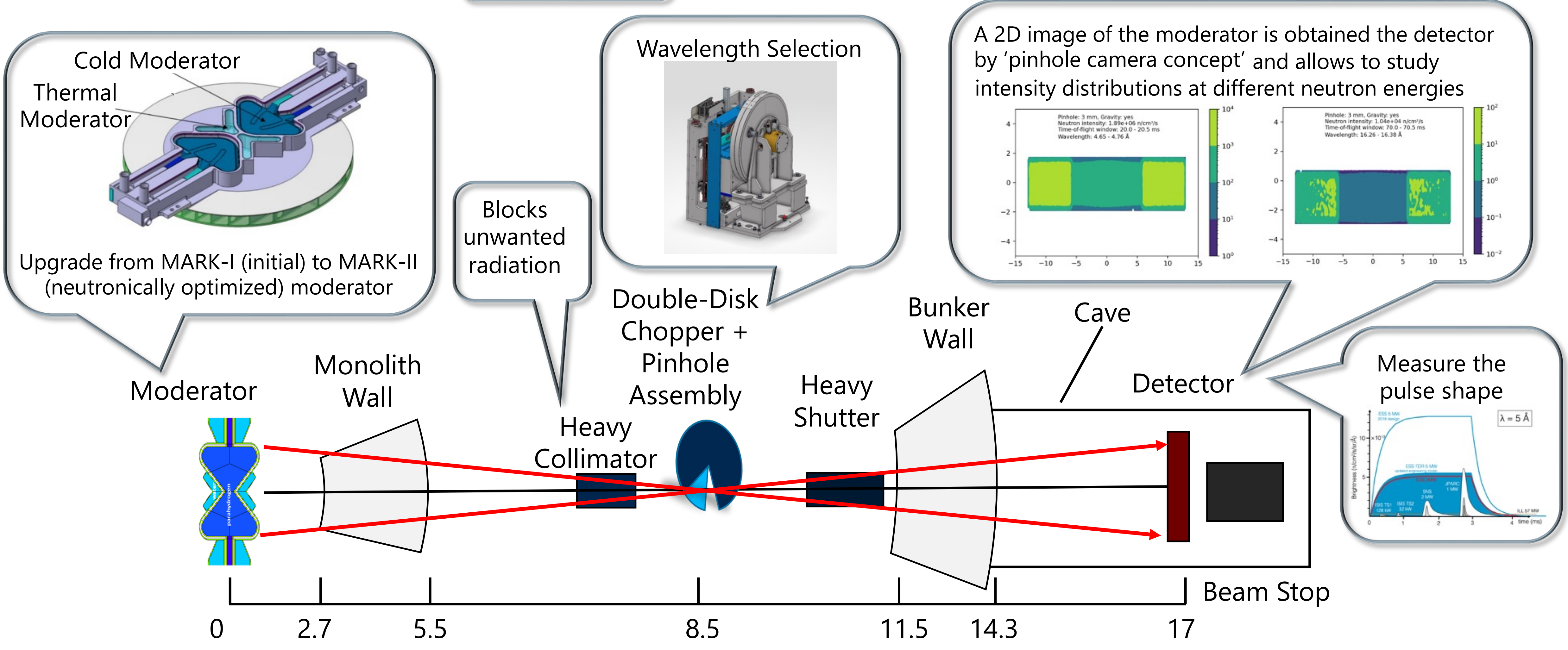




How we want to do it?

Principle

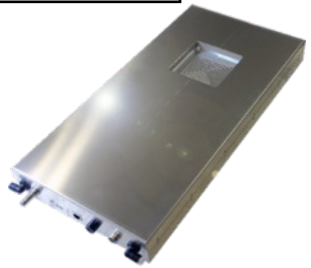
'Camera obscura' concept



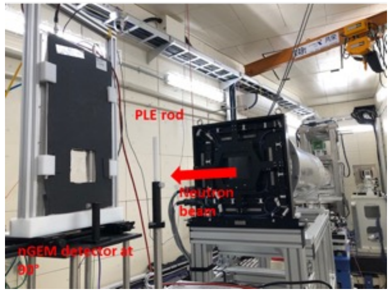
Test beamline (TBL): Detectors

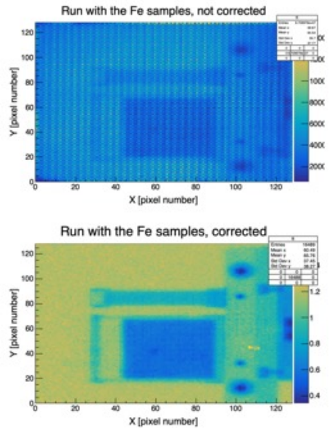
nGEM

Detector	nGEM
Type	Micropattern
Neutron converter	^{10}B
Area (mm^2)	100×100
Time resolution (ns)	15
Spatial resolution (mm)	1
Efficiency @25.3 meV (%)	10
Peak count-rate capacity	4.6 Mcps
Effective peak count-rate	180 kcps



Detector uniformity measured by recording data with a PLE rod (isotropic scattering in 4pi)





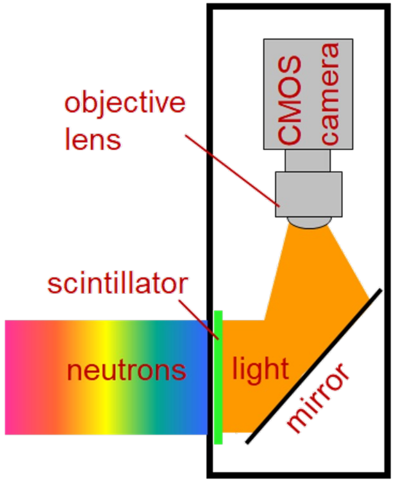
tested at J-PARC and ISIS

^{3}He PSD tubes

1bar/10bar

Scintillator

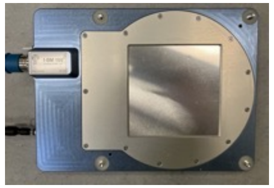
CMOS
+ gated
intensifier



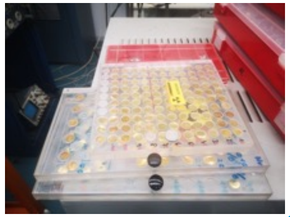
TPX3cam (LumaCAM)

Beam Monitors

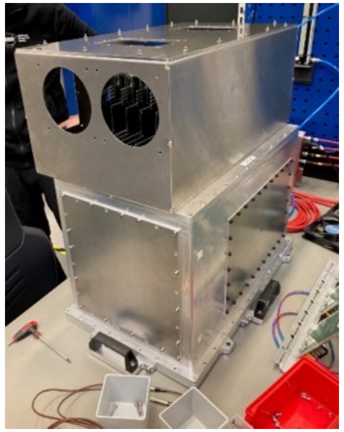
- In bunker (moveable, 5% efficiency)
- In cave (moveable, 5% efficiency)



Gold foils

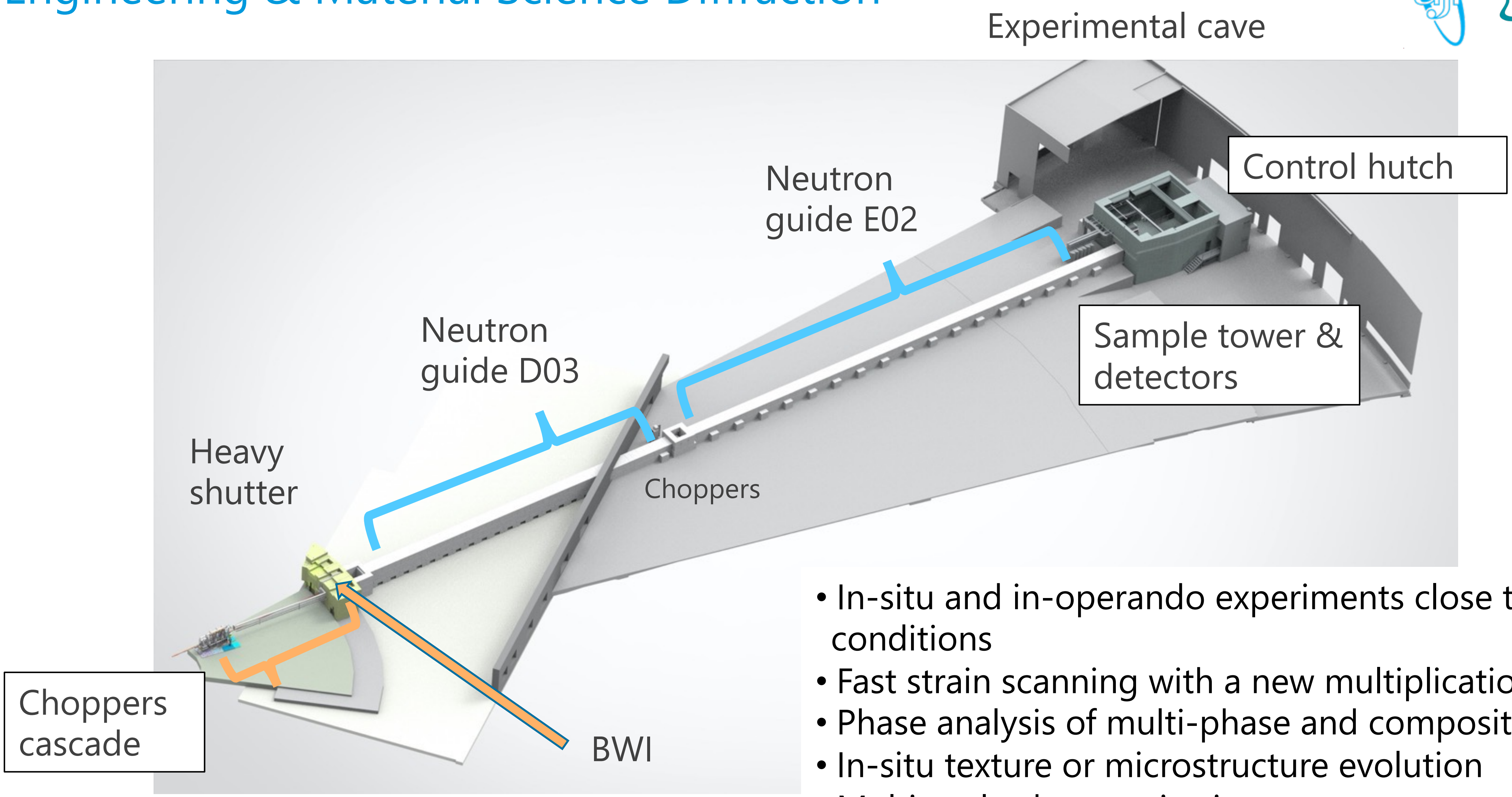


Multiblade



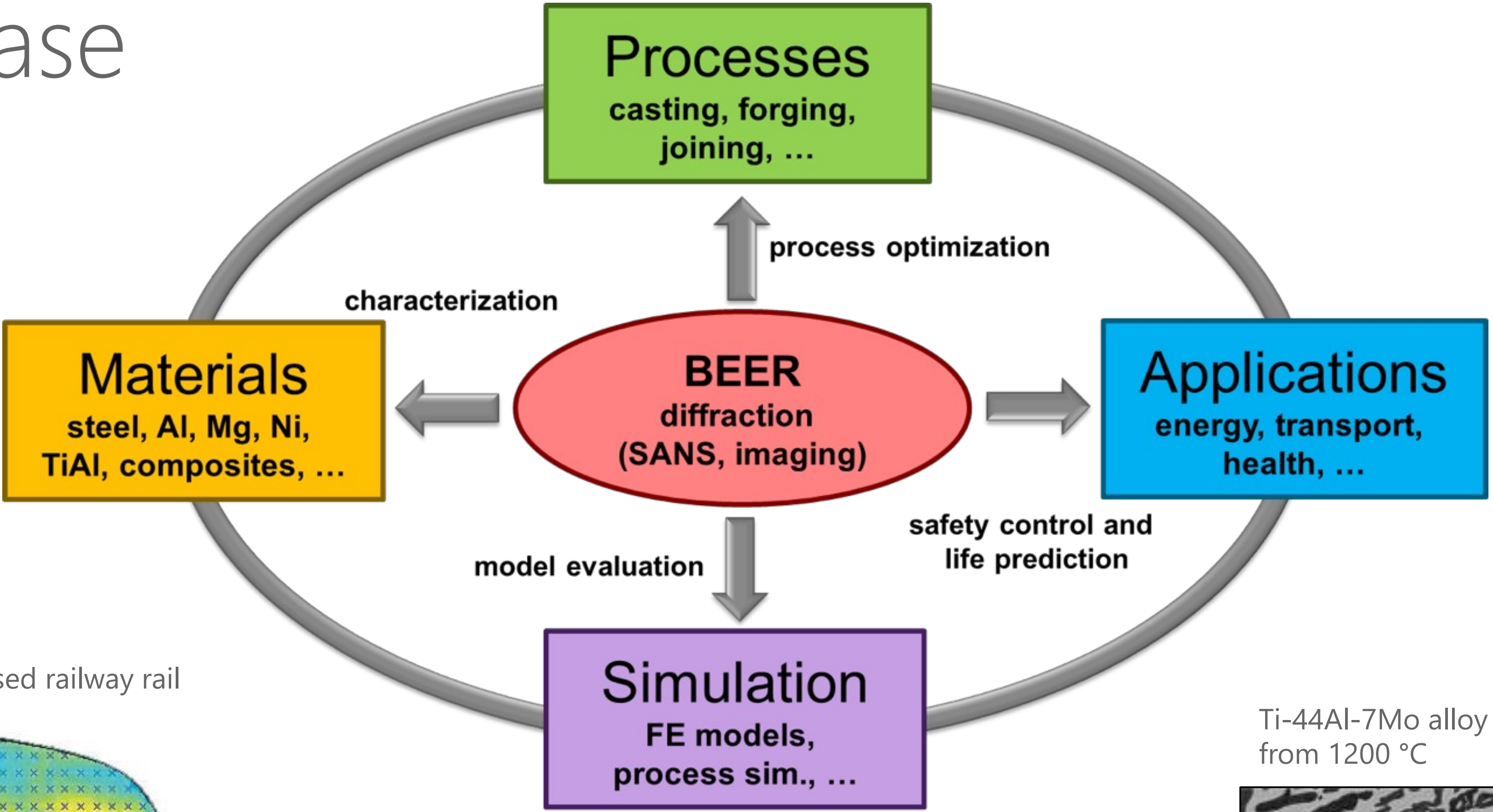
BEER Cold commissioning completed : Q4, 2026

Engineering & Material Science Diffraction

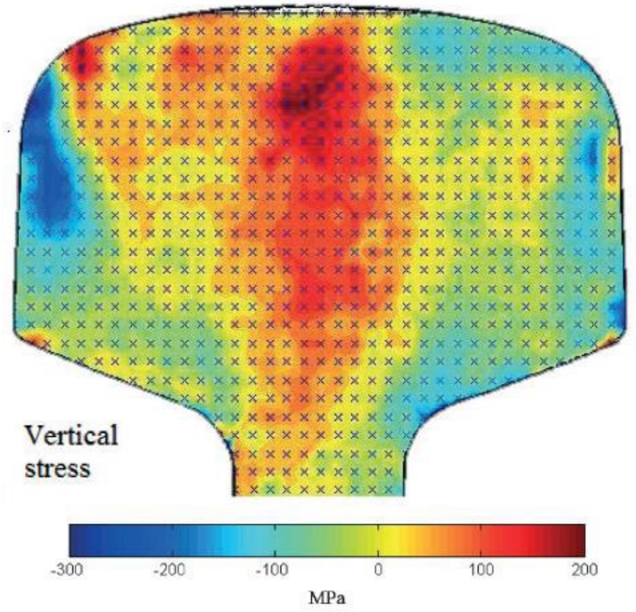


- In-situ and in-operando experiments close to the real conditions
- Fast strain scanning with a new multiplication technique
- Phase analysis of multi-phase and composite materials
- In-situ texture or microstructure evolution
- Multi-scale characterisation
- Long term experiments

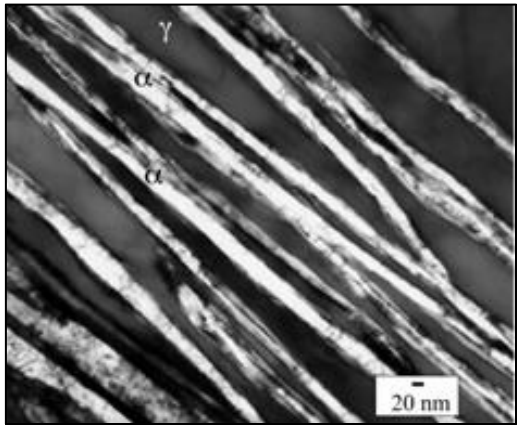
Science case



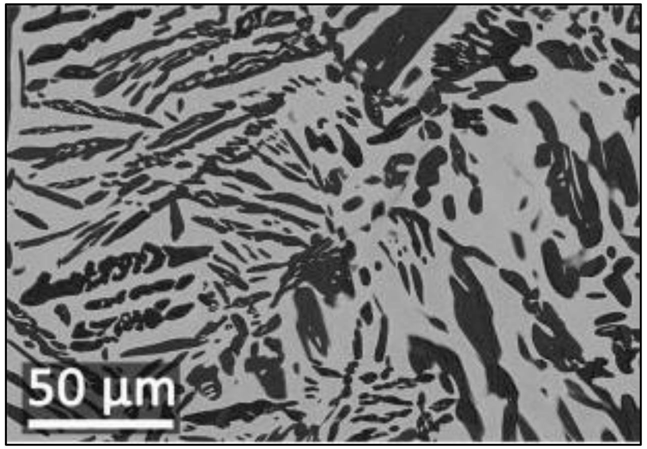
16 mm thick slice cut from a used railway rail



Superbainite nanolamellar structure



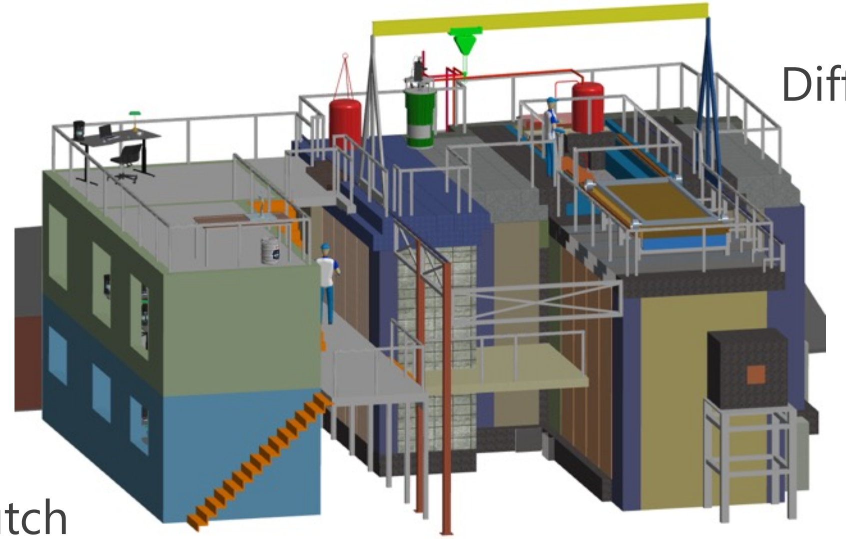
Ti-44Al-7Mo alloy (at%) quenched from 1200 °C

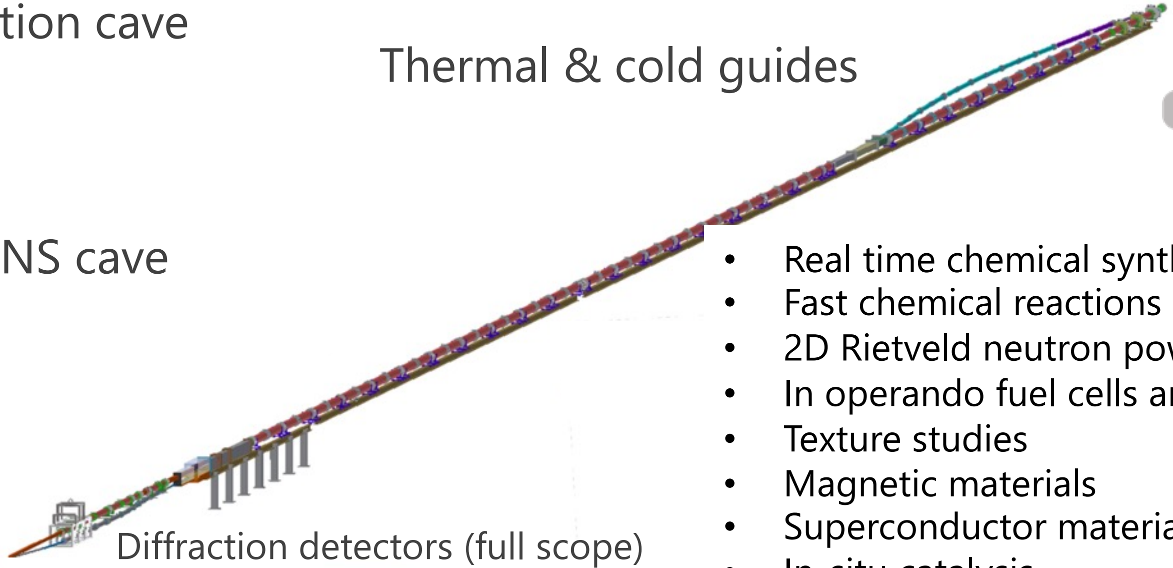


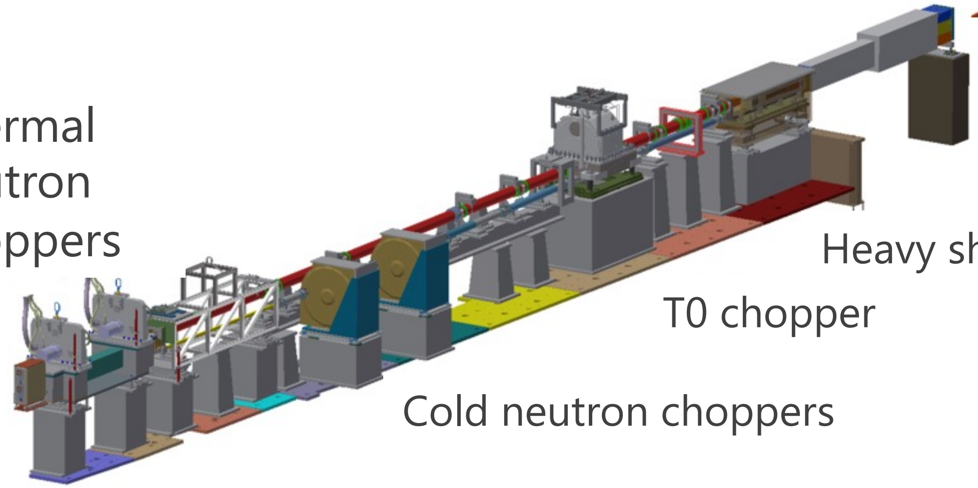
HEIMDAL

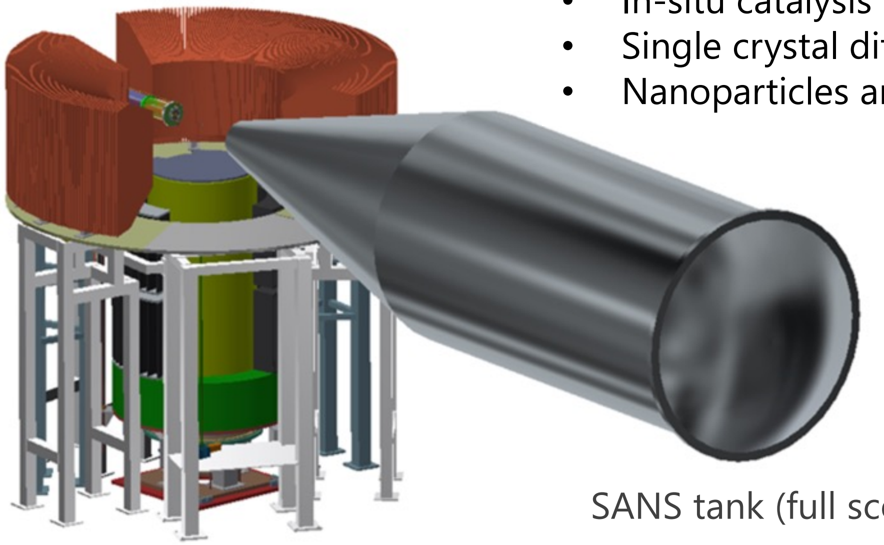
Cold commissioning completed : Q1, 2027

Hybrid Diffractometer: Combined Diffraction and SANS and Imaging









- Real time chemical synthesis
- Fast chemical reactions and kinetics
- 2D Rietveld neutron powder diffraction
- In operando fuel cells and batteries
- Texture studies
- Magnetic materials
- Superconductor materials
- In-situ catalysis
- Single crystal diffraction of small samples
- Nanoparticles and core-shell structures

Science case

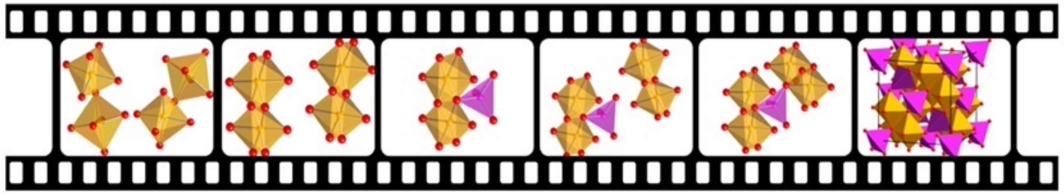
By combining diffraction and SANS HEIMDAL probes an extended q-range of
10^{-3} Å^{-1} < q < 15 Å^{-1}

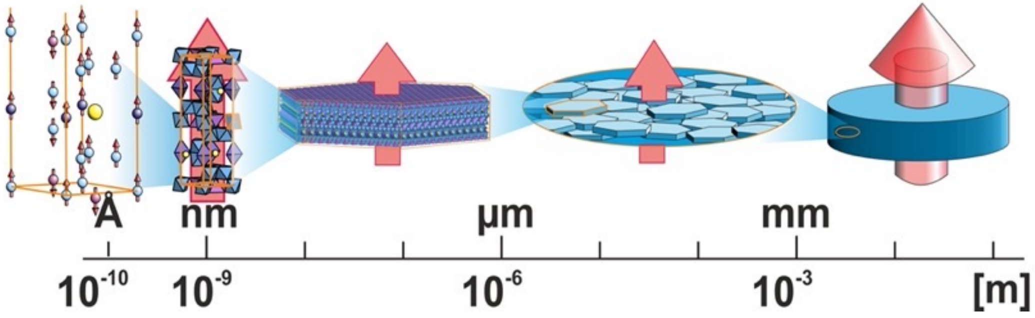
This enables studies of chemical and physical processes as they happen rather than attempts to combine data from several instruments recording almost identical processes.

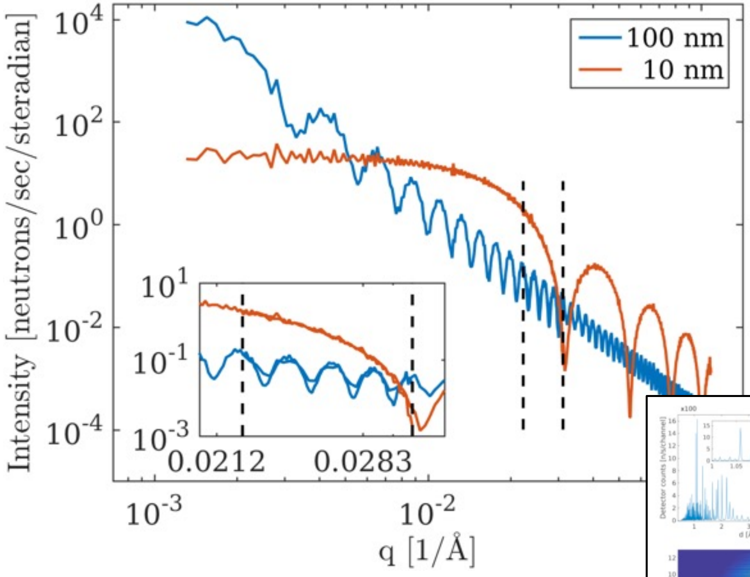
It can also be useful when examining both types of data are required to determine the next step in the experiment.

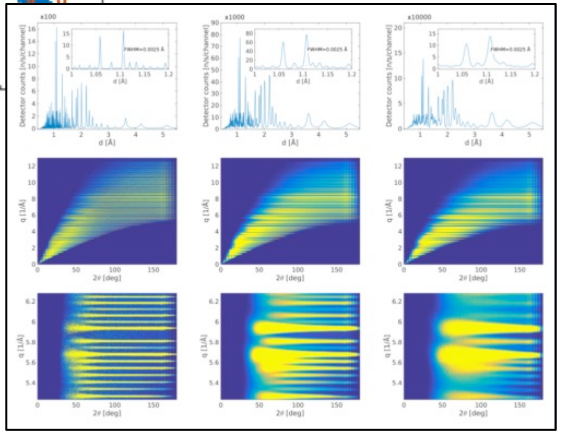
Energy Materials; Hydrogen storage materials, batteries, fuel cells, thermoelectric,…

Hierarchical systems; Catalysts Cement, bone, biominerals, magnetic materials,…





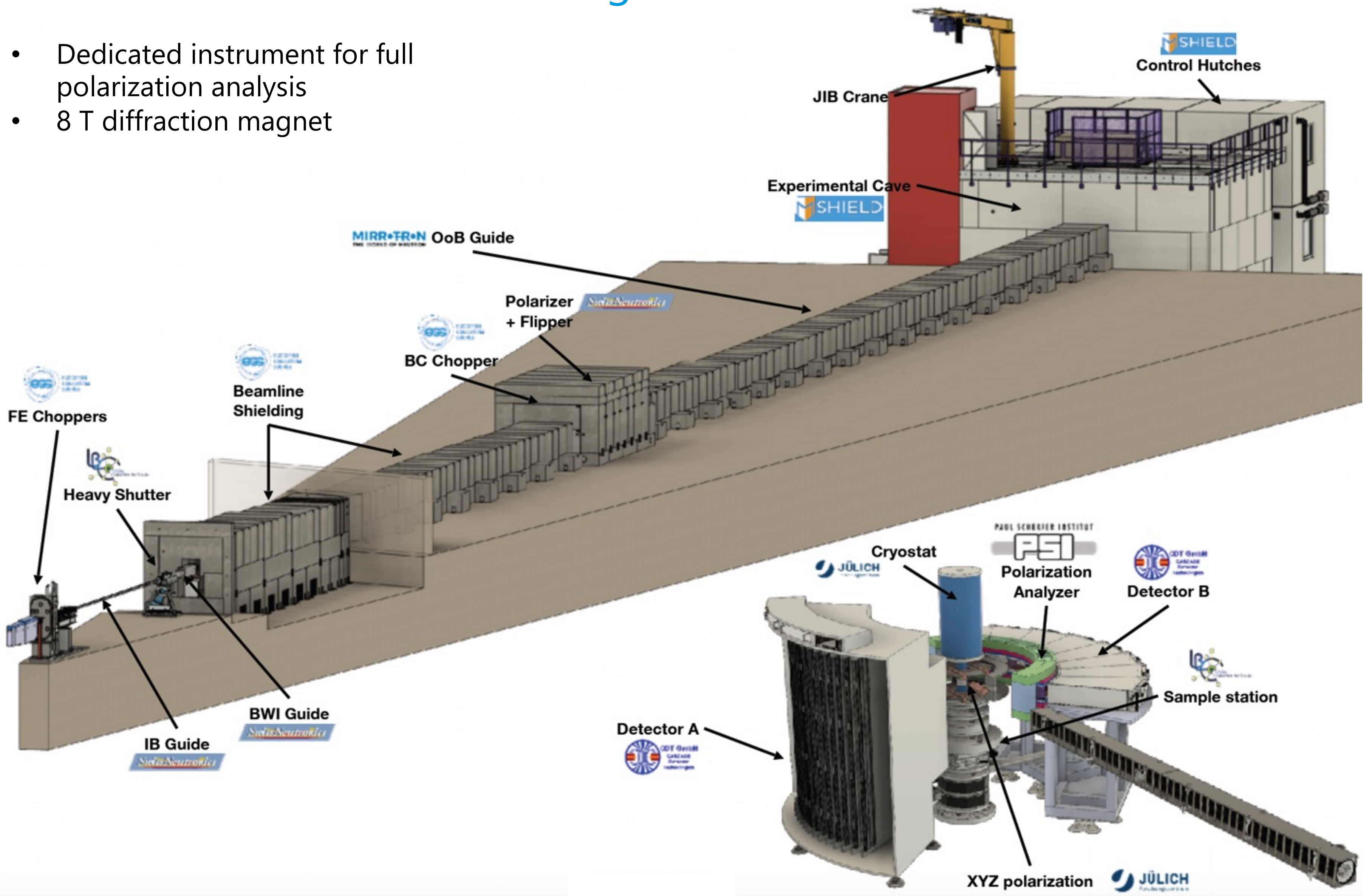




MAGiC Cold commissioning completed : Q4, 2025 (TBC)

Polarised Diffractometer for Magnetism

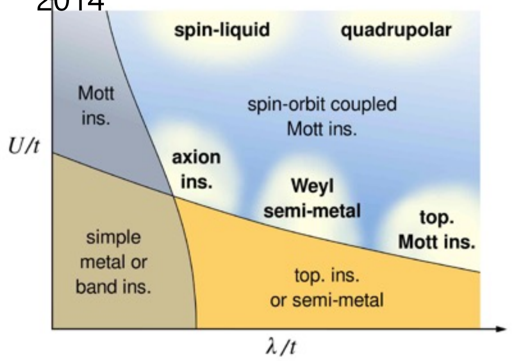
- Dedicated instrument for full polarization analysis
- 8 T diffraction magnet



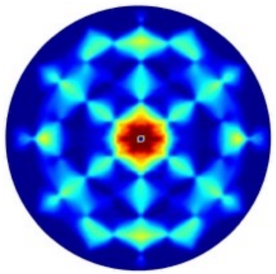
High polarised intensity
Larger Q-range
Flexible resolution

Novel metals and insulators

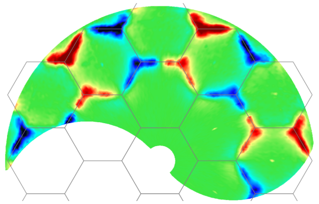
W. Witczak-Krempa et al
Ann Revi Cond Matt Phys **5** 57
2014



Frustrated magnetism spin-liquid



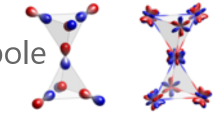
Spin-Ice model



Chirality

PRX 12 021029 202
2

dipole
monopole

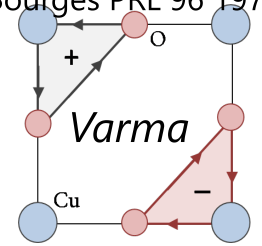


quadrupole
Sibille, Nature Physics 2020

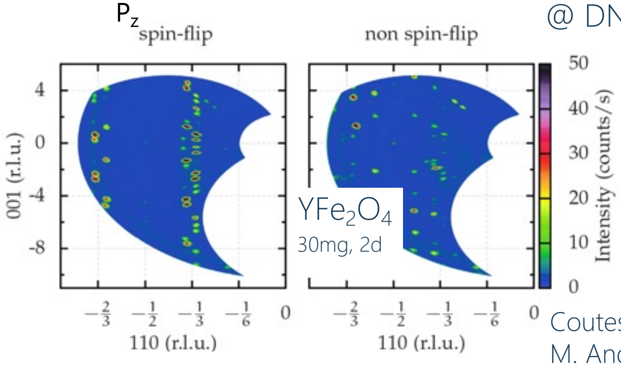
Fennell, Science 2009

Superconductivity

Loop current order
P. Bourges PRL 96 197001 (2006



@ DNS



Coutesy of
M. Angst

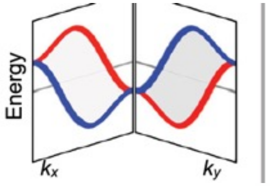
MAGIC proposal

high resolution

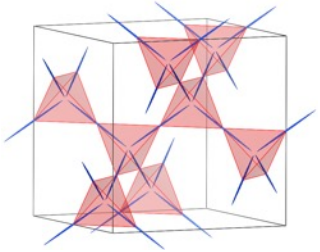
$\Delta Q \sim 10^{-2} ... 10^{-3} \text{Å}^{-1}$

altermagnetism

new phases / spintronics
PRX 12 040501 2022

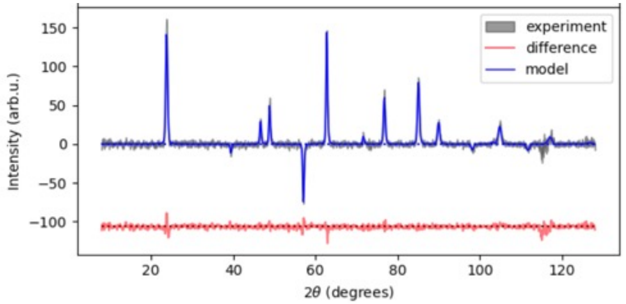


spin anisotropies



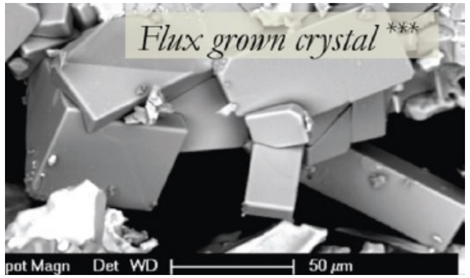
Iurii Kibalin & Arsen Gukasov
PRB 2019

Charge and spin order



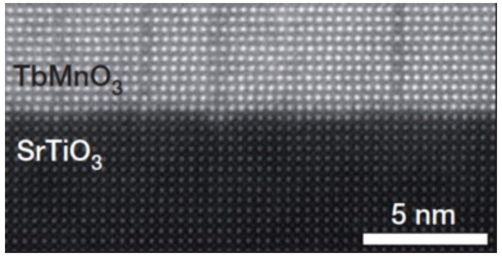
small moments S=1/2

small crystals

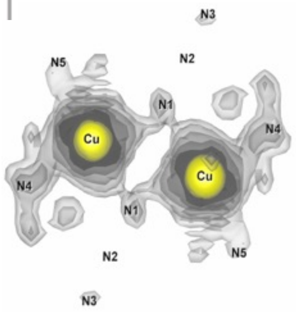


M. Valldor

small (hetero) structures

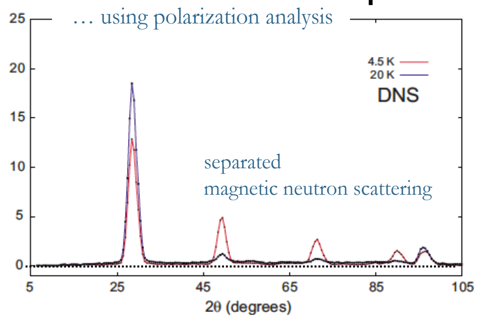


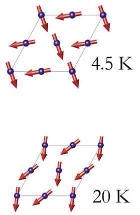
S. Farokhipoor et al
Nature Materials **515** , 379 (2015)

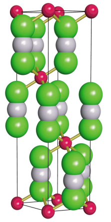


Molecular magnets spin densities

powders







MnNCN

background suppression (nucl, magn, inc)

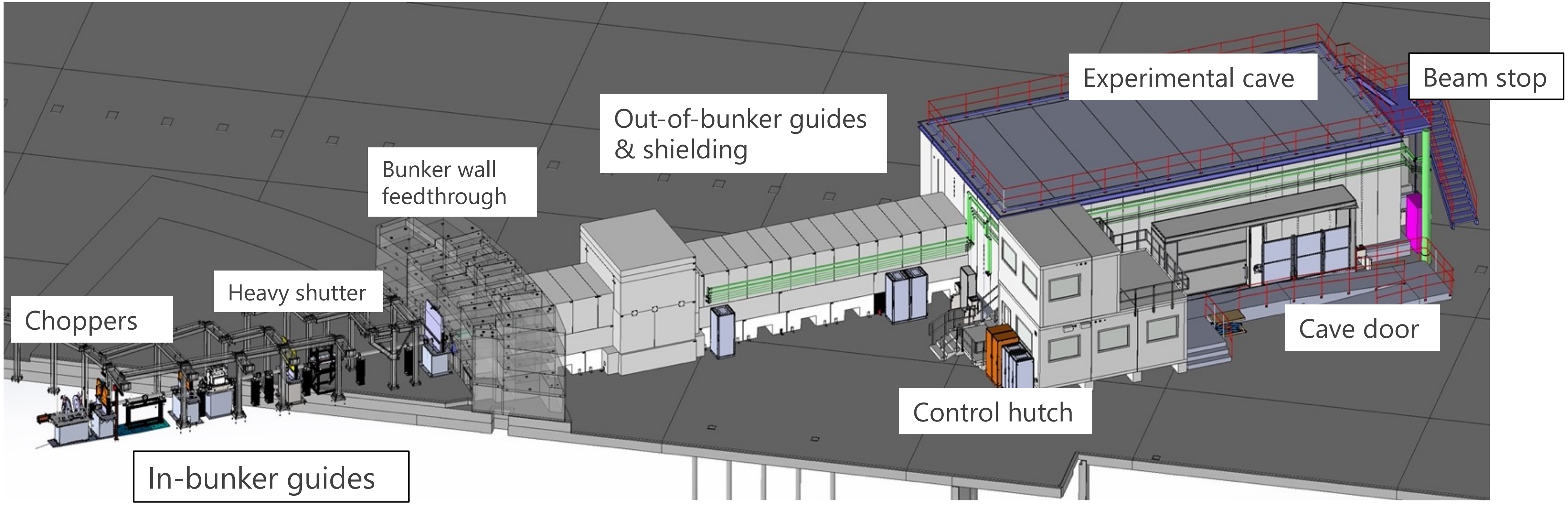
hydrogeneous materials

Na- batteries

ODIN

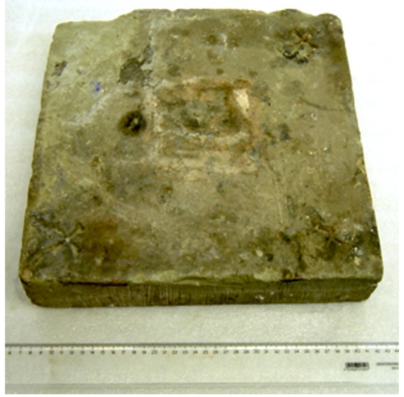
Cold commissioning completed : Q1, 2025

Optical and Diffraction Imaging with Neutrons

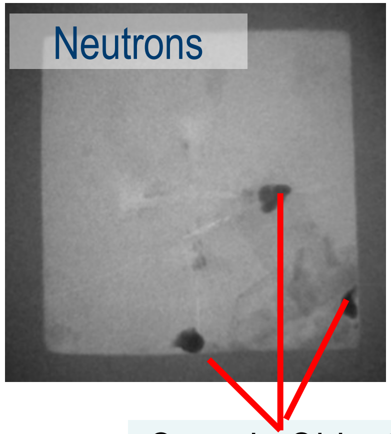


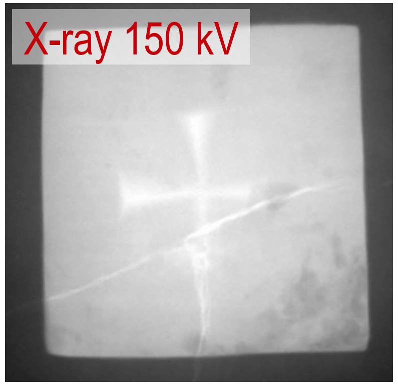
- Spatial resolutions down to the µm-range
- Engineering materials
- Geo-science
- Paleontology
- Energy materials
- Fuel cells
- Magnetism
- Soft matter and biology
- In-operando studies
- Variety of imaging techniques (full scope)

High societal impact early science



Altar stone (33.5cm x 33.5cm x 7cm) from a church (église des Augustins) in Friborg (CH) with a recessed plate with a cross.





Mannes et al. (2014) Archaeometry¸

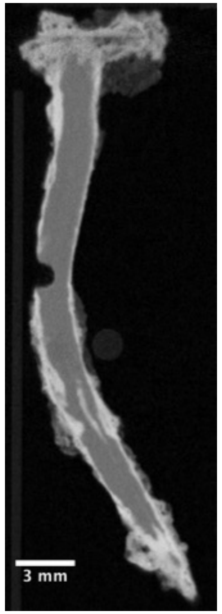
In 2023 Lund’s cathedral will celebrate its 900th anniversary from its foundation

Some discussion already started with the responsible persons (including ESS’ user office) for collaboration and for samples

Similar experiments already performed at existing facilities → low risk/high reward

Neutron Imaging is a well established diagnostic technique for such use cases

High societal impact early science



Vasa ship, Stockholm (1628)

Famous ship that sank in her maiden voyage

Recovered in 1961

Constant preservation efforts

NI could help visualizing the corrosion of the bolts or the swelling in the wood

High societal impact early science

Impossible to predict now what will the trending topic be in 2-3 years from now.

Conversely, if I have a killer application already now, I can perform the same experiment, with more reliability, at an existing source

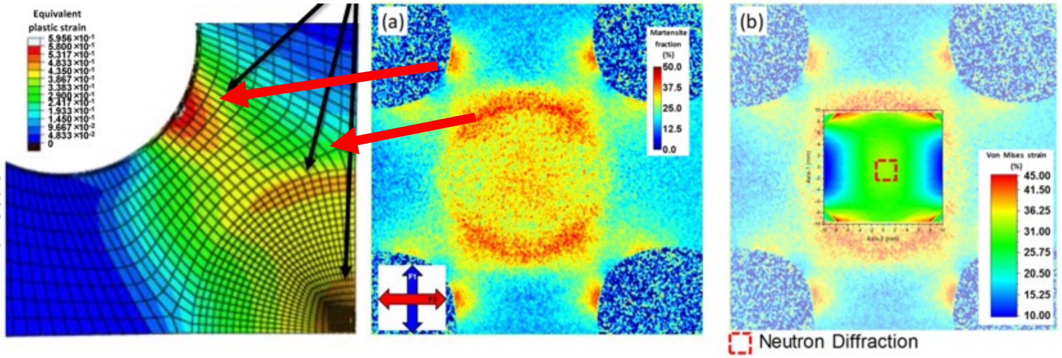
We need to keep being active in the field

Focus on the strengths of ODIN → medium resolution

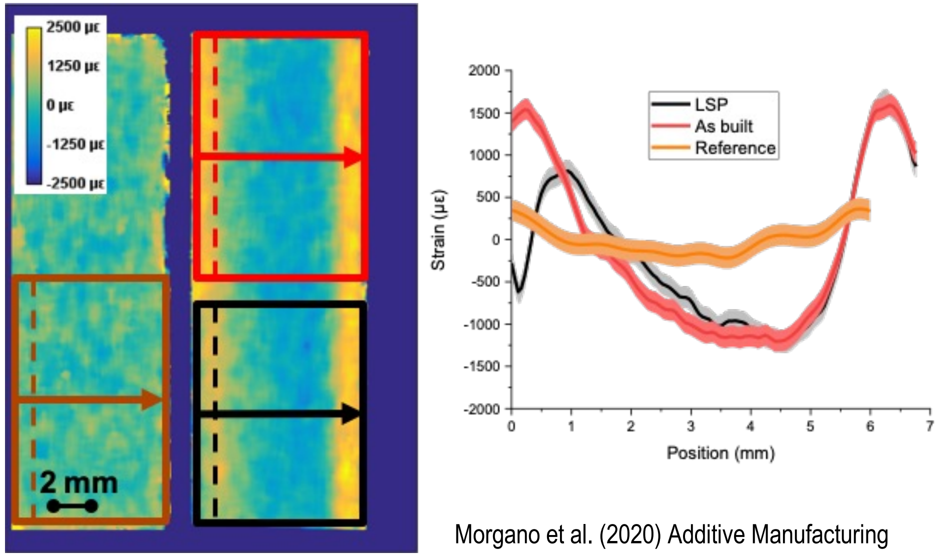
Additive manufacturing of metal is a hot topic now, so it can be expected to still be interesting by BoT

Medium resolution: phase fraction mapping of steel

Polatidis et al. (2020) Materials



Hot topic: residual strain mapping in AM steel



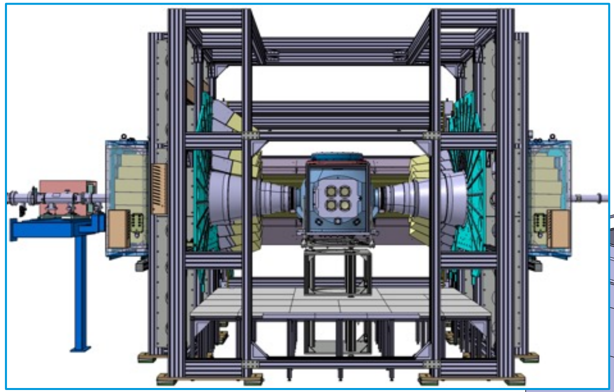
Morgano et al. (2020) Additive Manufacturing

DREAM Cold commissioning completed : Q1, 2025

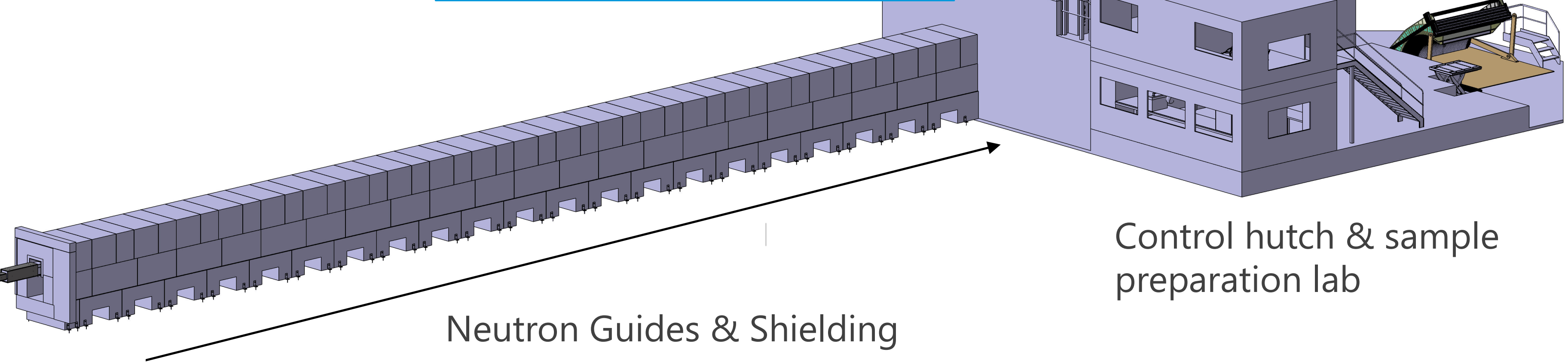
Diffraction Resolved by Energy and Angle Measurements

- Powder diffraction
- Flexible high flux/high resolution
- 2D Rietveld data/PDF/nm-SANS/Polarized
- Superconductors
- Multiferroics
- Weak moments
- Orbital ordering
- Charge ordering
- Energy materials
- Magnetic nanoparticles
- MOFs
- Li, H materials
- In-operando

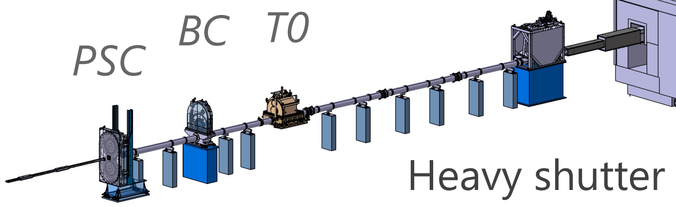
Sample vessel Detectors



Experimental caves



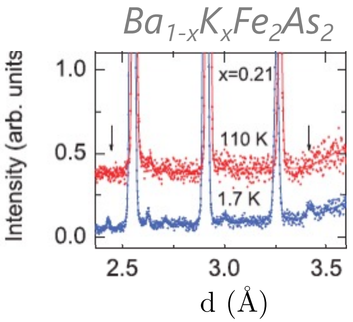
Choppers



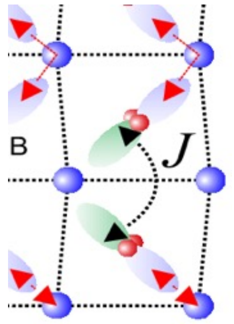
Inside the bunker

powders
single-crystals
nanoparticles
alloys
liquids

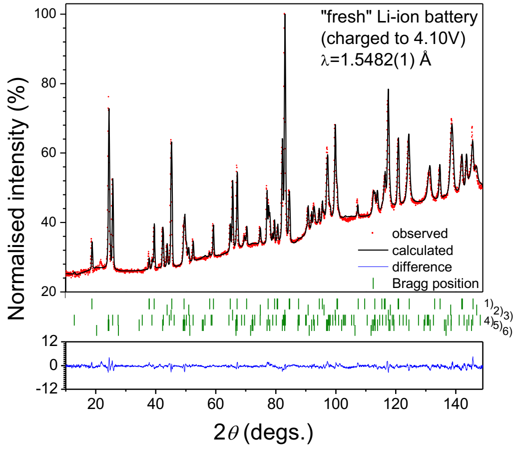
Magnetism



weak moments
phase diagrams of superconductors
multiferroics



orbital ordering
charge ordering
distortion
magnetic exchange

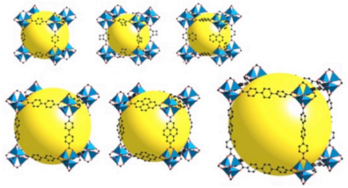


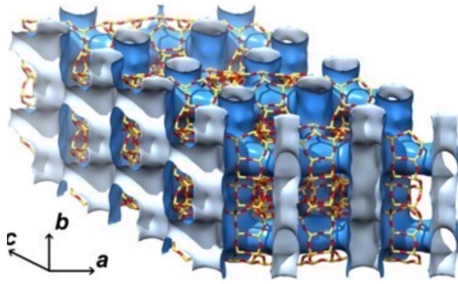
Energy Materials

multiphase
catalysts
in-operandi
batteries

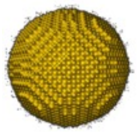
Large Unit Cells

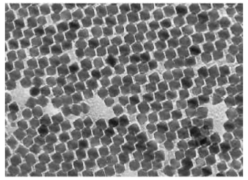
MOFs
thermoelectrics
molecular sieves
H_2 - storage





Nanostructures





many novel samples come in np
magnetic nanoparticles
core-shell structures
self-assembly
synthesis

Third-party funding:
Polarized (cold) neutrons +
nm-SANS detector

RöntgenÅngströmCluster