Diffraction & Imaging Division update

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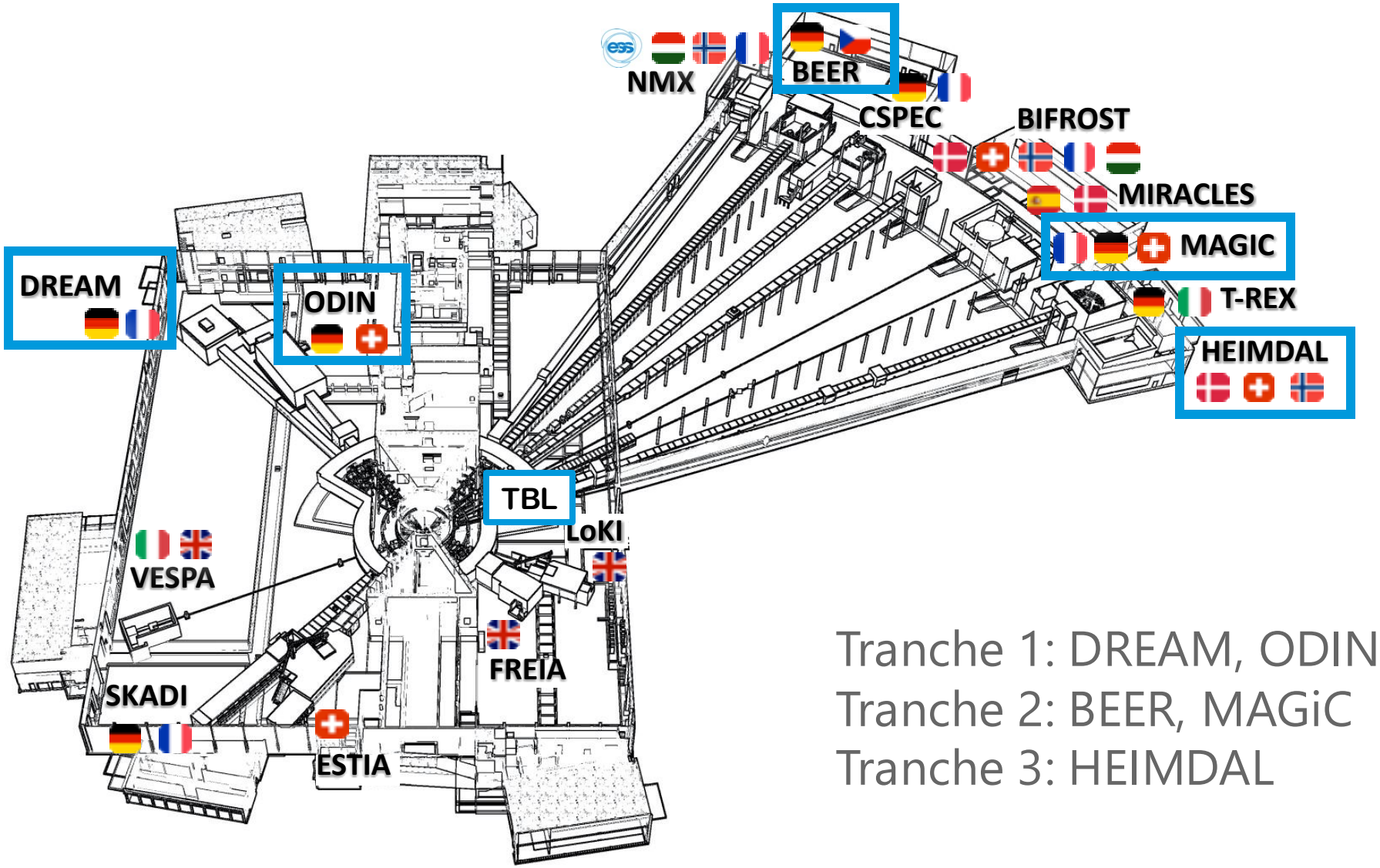
[3] Jülich Center for Neutron Scattering, Forschungszentrum Jülich

Instruments

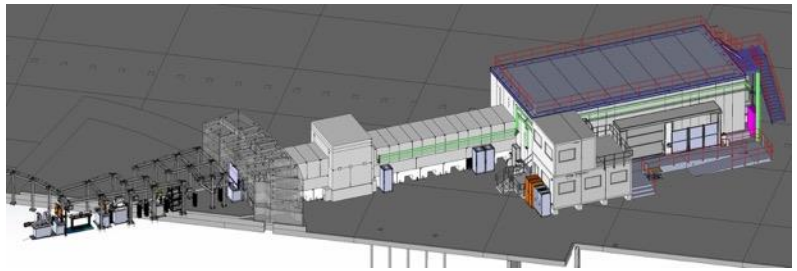


Tranche 1: DREAM, ODIN, TBL
Tranche 2: BEER, MAGiC
Tranche 3: HEIMDAL

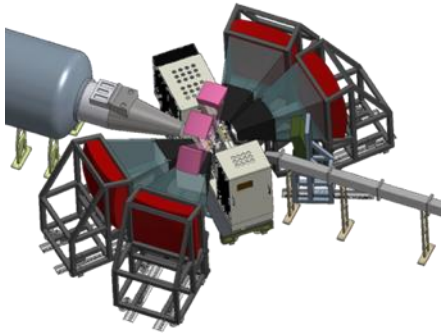
Teams on site

MAGiC
Denis Vasiukov
Moritz Braun (Eng)
1/3 Daniele Erbi (Des)

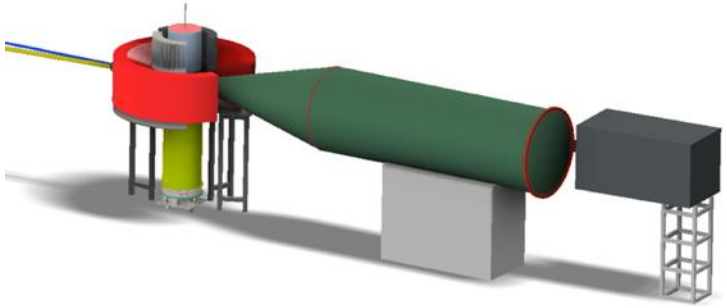
ODIN
Robin Woracek
Stefanos Athanasopoulos(postdoc)
Shuqi Xu (postdoc)



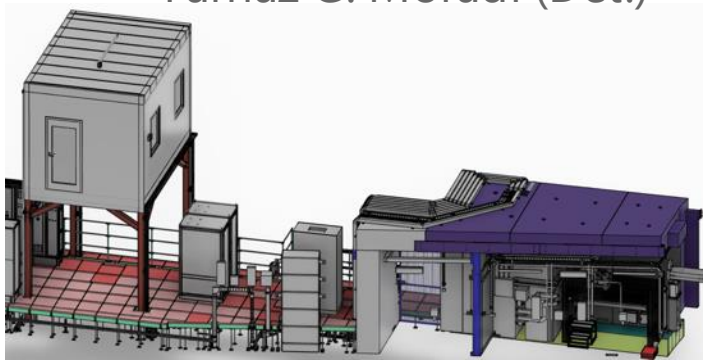
BEER
Premek Beran
Gergely Neméth
Caroline Curfs (SEE)
Grant Wallas (IOE)
Bojan Peric (Eng)



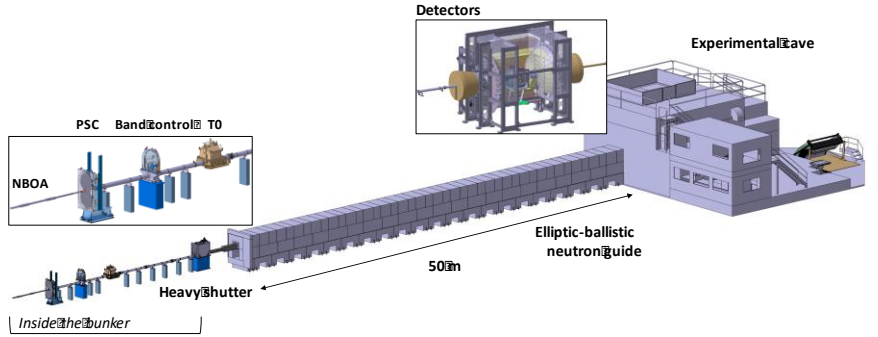
HEIMDAL
Dan Mannix
Siamak Kianzad (Eng)
Bengt Jönsson (Eng)



TBL
Thawatchart Chulapakorn
Zhanwen Ma (TBD)
Jason Morin (IOE)
Christofer Svensson (Eng)
Farnaz G. Moradi (Det.)



DREAM
Florence Porcher
Paulo Brant Carvalho
Anna Fornell (IOE)
1/3 Sylvain Desert (Eng)



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

ESS BoT milestone

- Measured reasonable thermal and cold neutron spectra on the Test Beam Line (acceptable signal-to-noise ratio)
- Completed a first estimation of the yield of thermal and cold neutrons per proton as measured on the Test Beam Line (no specific threshold value required)

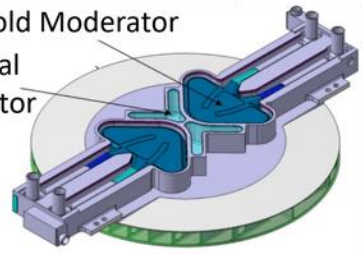
Overview

Principle

'Camera obscura' concept

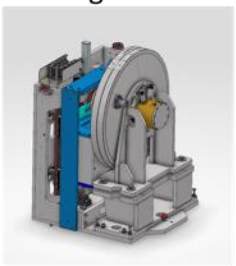
Cold Moderator

Thermal Moderator

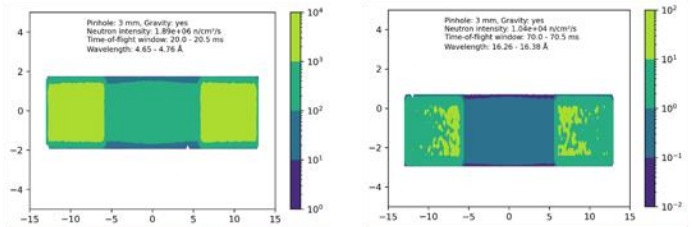


Upgrade from MARK-I (initial) to MARK-II (neutronically optimized) moderator

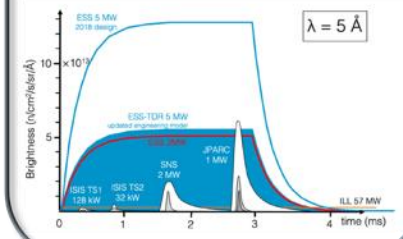
Wavelength Selection



A 2D image of the moderator is obtained the detector by 'pinhole camera concept' and allows to study intensity distributions at different neutron energies.



Measure the pulse shape



Blocks unwanted radiation

Chopper

Bunker Wall

Heavy Shutter

Filters

Thermal neutrons

Pinholes

Moderator

Monolith

Cold neutrons

Light Shutter & Bridge Beam Guide

Collimation system

Cave

Detector

Beam Stop

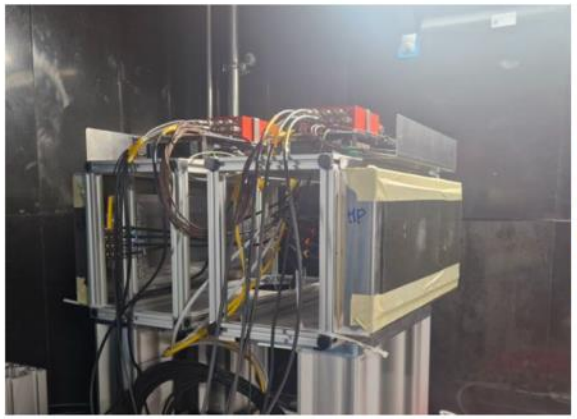
0 m 2.7 m 5.5 m 8.5 m 11.5 m 14.3 m 17 m

Detectors-overview

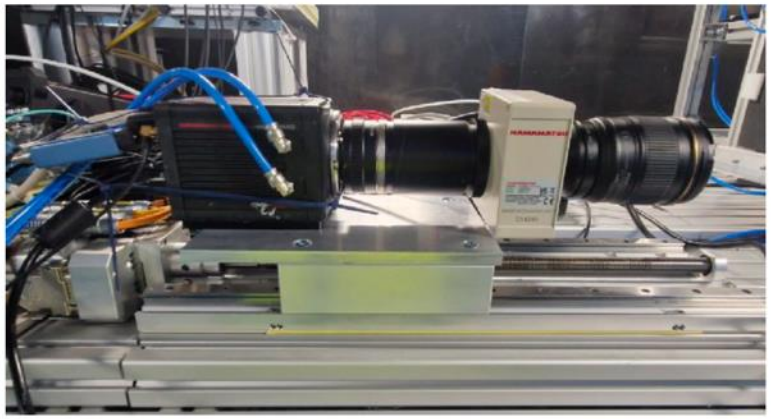
Table 2.: **Summary of TBL detectors**

Detector	He-3	nGEM	CMOS	TimePix3	Multi-Blade
Type	Gas-filled	Micropattern	Scintillator – optical camera (Frame-based)	Scintillator – optical camera (Event-mode)	Multi Wire Proportional Chamber (MWPC)
Neutron Converter	He-3	^{10}B	Scintillators (^{6}LiF, Gadox, etc.)	Scintillator pending (^{6}LiF, Gadox, etc.)	^{10}B
Active Area	312mm × 50.8mm	100mm × 100mm	Up to 280mm × 280mm	Up to 260mm × 260mm	260mm × 140mm
Spatial resolution (mm)	3 mm	0.8mm × 0.8mm	Between 20µm and several hundred µm	Between 5µm and several hundred µm	~ 0.5 mm x ~ 3.5 mm
Time resolution (µs)	10	0.015	10,000 (100 Hz full frame readout)	0.001	< 10
Efficiency @2Å	10 - 63.6	~10%	Scintillator pending		~40%
Count rate capacity	100 kHz	10 MHz	100 Hz	20 MHz	several kHz per mm2

Multi-blade



He-3



CMOS

nGEM

LumaCam

Status

- Installation & integrated tests are completed
- First instrument to have
  System Acceptance Review (SAR) &
  Instrument Safety Readiness Review (iSRR)
- SAR is approved, with the action items
- PSS installation is done
- Fire suppression system is tested
- Deferral scope: automatic door, BM in cave, P2P and diffraction rig
- Instrument and team are ready for BoT goals

iSRR demonstration on-site

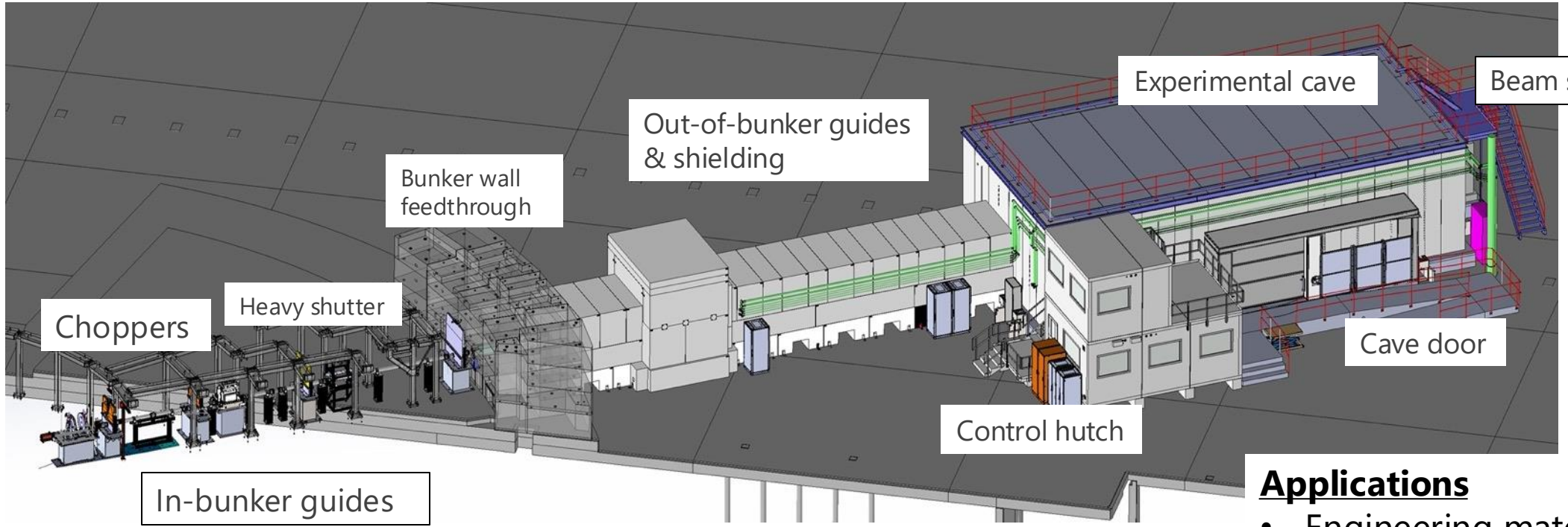
Challenges

- Team is still incomplete (long wait time for visa of 2nd IS)
- Lead engineer will be moving to another project
- Resources will be needed to complete the deferred scope
- No dedicated IDS, DMSC is putting extra resources into TBL

ODIN

Cold commissioning completed : Q4, 2025

Optical and Diffraction Imaging with Neutrons



- Bi-spectral extraction
- Direct line-of-sight (T0 chopper)
- Tailored wavelength resolution
- Variety of imaging techniques, including x-rays (full scope)

- White beam
- High flux wavelength dispersive (basic ToF)
- High-resolution wavelength dispersive (WFM)

Applications

- Engineering materials
- Geo- and planetary science
- Paleontology
- Cultural Heritage
- Energy materials
- In-operando fuel cells & batteries
- Soft matter and biology

Contrast Mechanism

Diffraction | Phase | Magnetic | ‚Attenuation‘

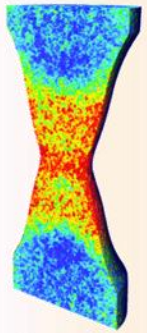
Applications

Metals/ Engineering

Hydrogen

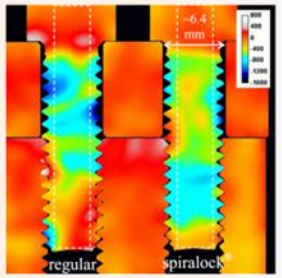
Energy Storage

Cultural Heritage



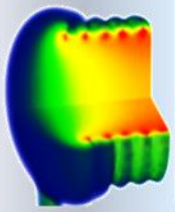
engineering

Strains

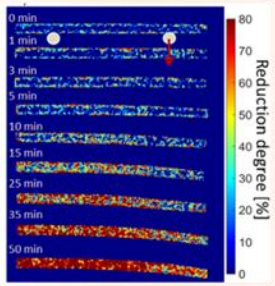


Internal defects

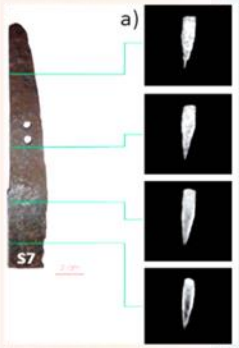
Magnetic fields



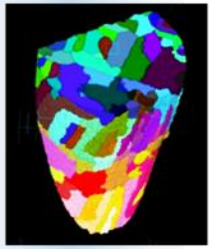
Phase transitions



SOFC’s

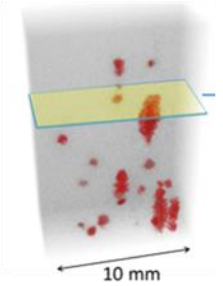


Microstructure in cultural heritage



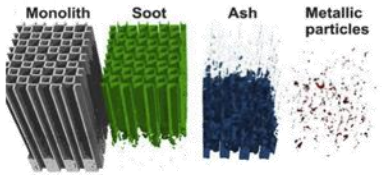
Magnetic domains

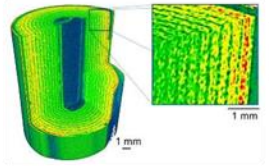
Hydrogen in metals



Device inspection: particle filters

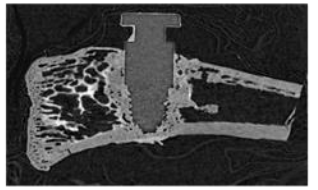
Water uptake in plants





Li transport in batteries

Corrosion



Bone Structures + implants

Å | nm | µm | mm | cm

Contrast mechanism length scales

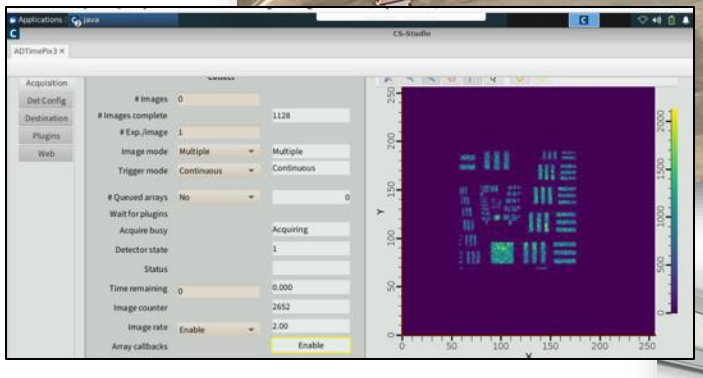
Slide : Robin Woracek

Status

- Installation completed
- Integrated tests ongoing: choppers, ToF camera
- PSS system installed
- Fire-suppression system installed
- Fixed: chopper guide gap, beam stop position
- SAR documentation is almost done
- Many documents/solutions are taken from TBL
- Joint SAR/iSRR review is scheduled for December

Cave and hutch

TPX3 image



Cave interior

Challenges

- Lead scientist is leaving on March 1st, 2026
- More integrated tests: motion, CMOS camera, beam monitor
- No dedicated lead engineer on site
- Many tasks for DMSC, but the timeline is not 100% clear
- Slow progress with x-ray setup (detector procurement delays)

DREAM

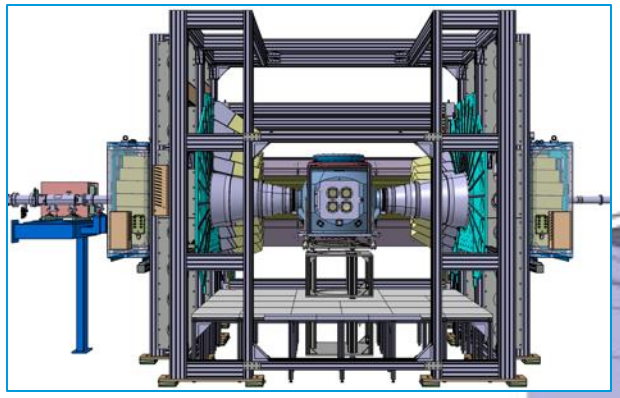
Cold commissioning completed : Q1, 2026

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

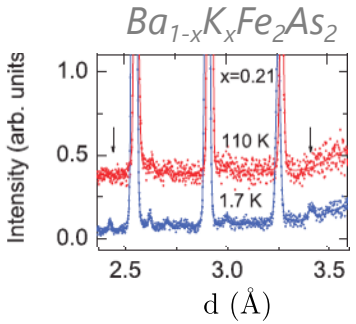


Experimental cave

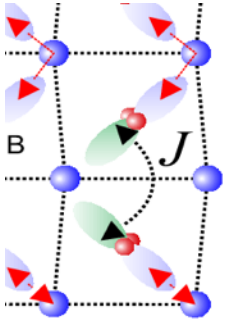


powders
single-crystals
nanoparticles
alloys
liquids

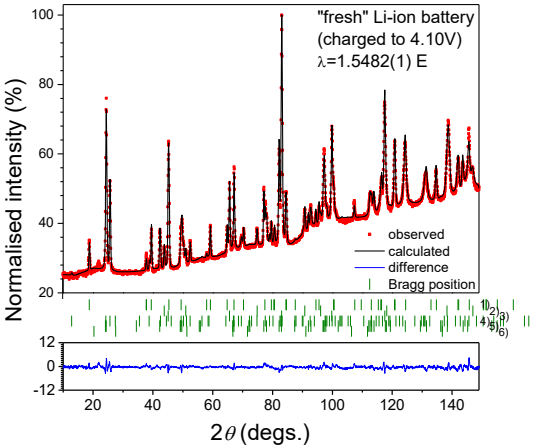
Magnetism



weak moments
phase diagrams of
superconductors
multiferroics



orbital ordering
charge ordering
distortion
magnetic exchange

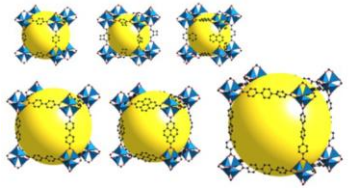


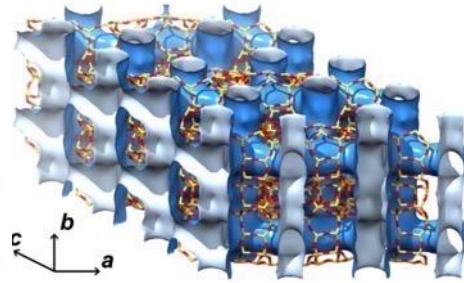
Energy Materials

multiphase
catalysts
in-operando
batteries

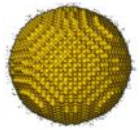
Large Unit Cells

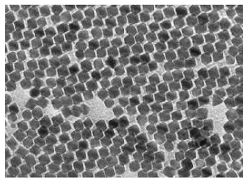
MOFs
thermoelectrics
molecular sieves
H_2 - storage





Nanostructures





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

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

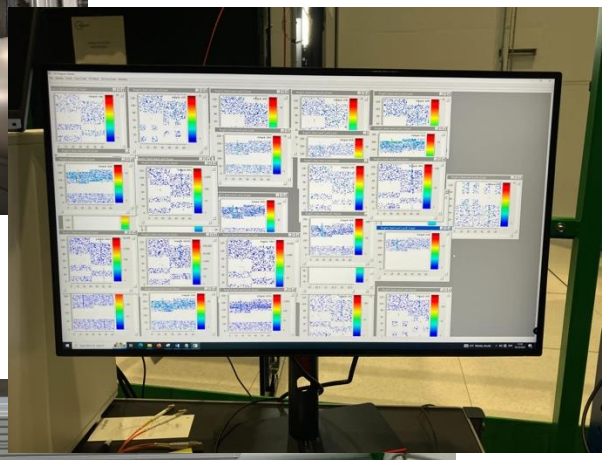
RöntgenÅngströmCluster

Status

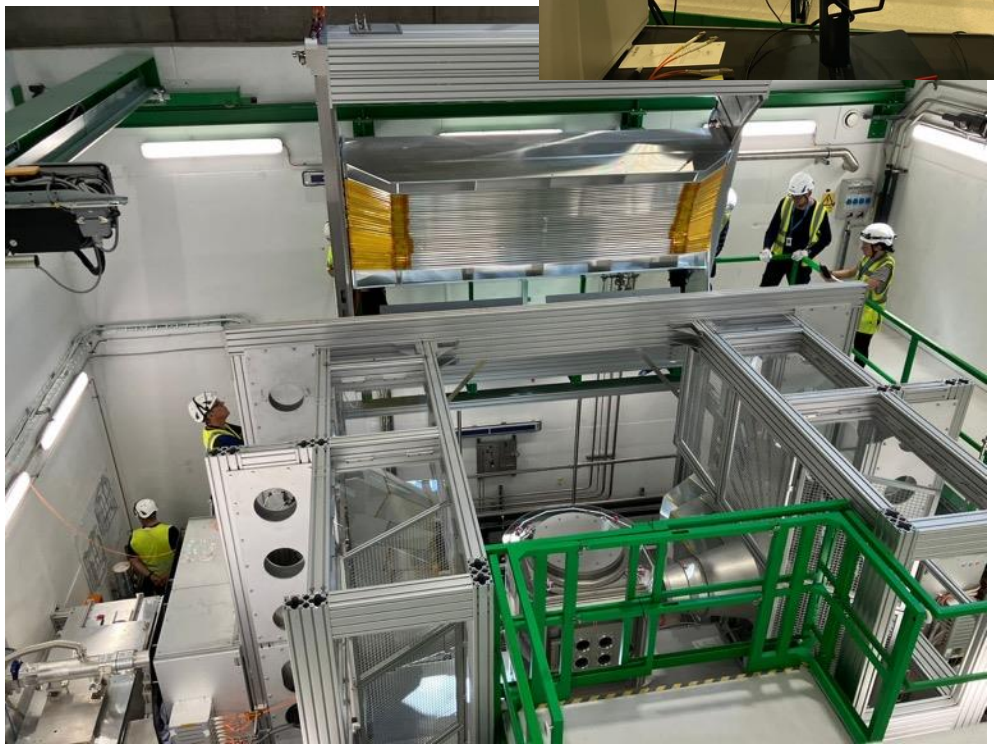
- Mantle detectors were installed
- All components are now installed
- Local SAR of detectors started (LV)
- PSS is installed
- Roof is installed
- Furniture in sample preparation lab is being installed
- T0 chopper SAT is complete
- Steady progress with SAR/TG5 documentation

Sample position

Local SAT Detectors



Mantle detectors installation



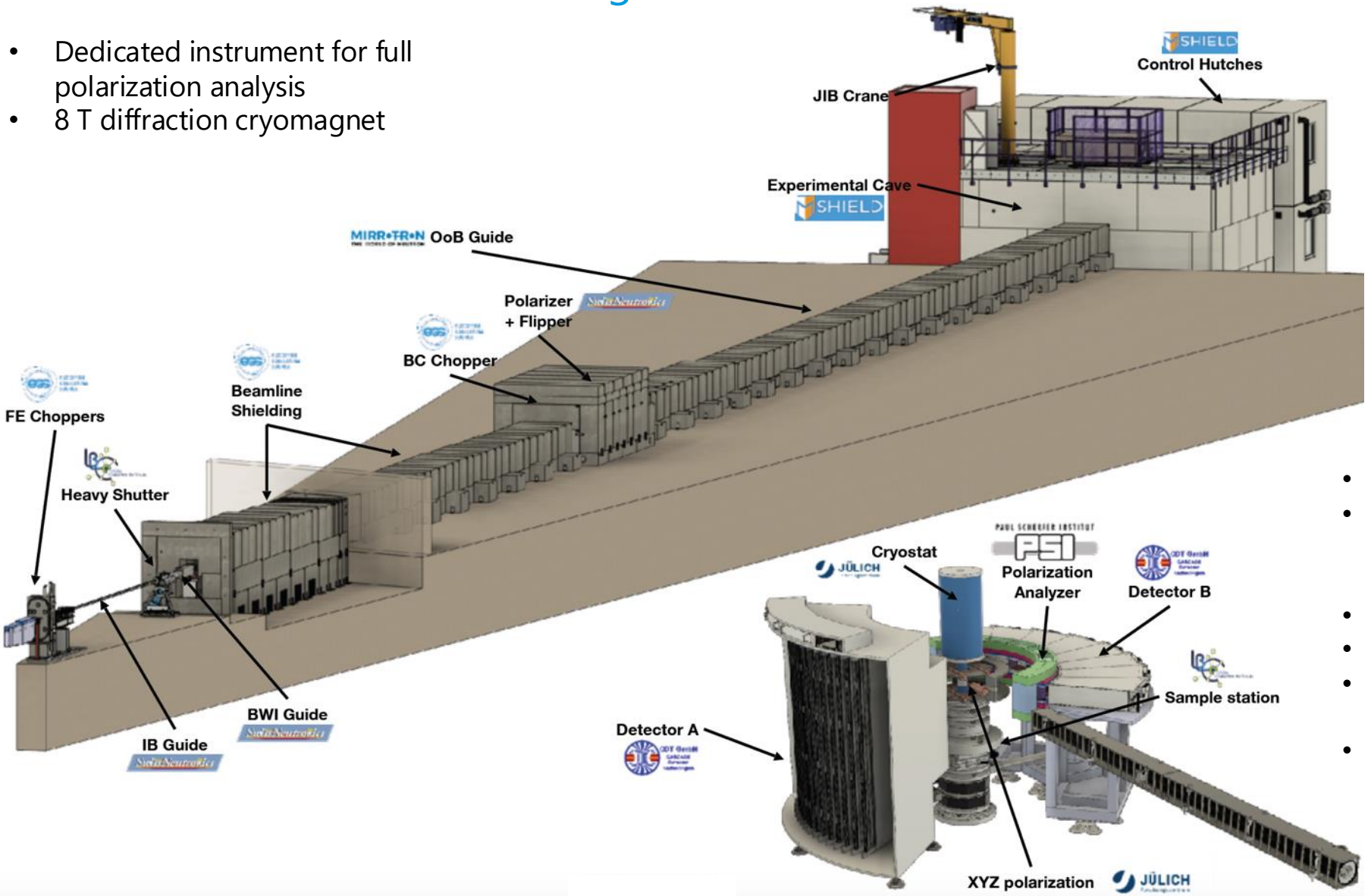
Challenges

- Detector gas supply has to be modified for integrated SAT of detectors (exhaust, flowmeters)
- Detector readout work ongoing
- Beam monitor gas/readout is not ready (DetG is supporting)

MAGiC Cold commissioning completed: Q1, 2027

Polarised Diffractometer for Magnetism

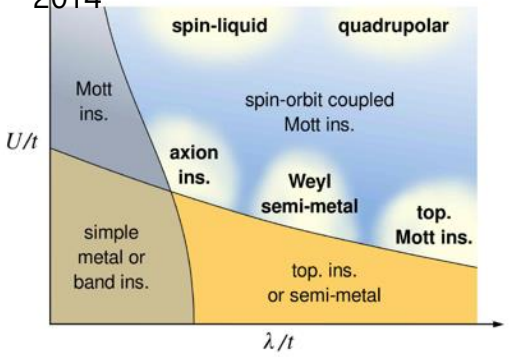
- Dedicated instrument for full polarization analysis
- 8 T diffraction cryomagnet



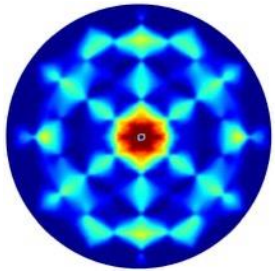
- Local susceptibility and spin densities
- Exotic magnetic structure (long range, non-collinear, anisotropic Hamiltonian)
- Multifunctional materials
- Superconductivity
- Frustrated magnets and quantum spin liquids
- Magnetism in thin films and at interfaces

Novel metals and insulators

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

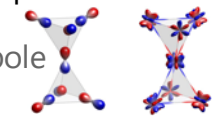


Frustrated magnetism spin-liquid



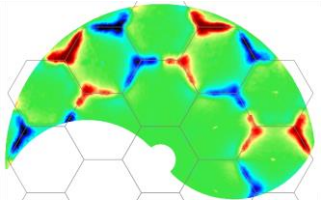
Spin-Ice model

dipole
monopole



quadrupole
Sibille, Nature Physics 2020

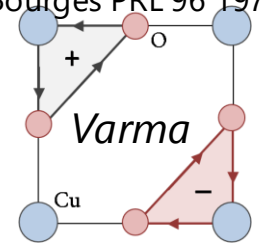
Fennell, Science 2009



Chirality
PRX 12 021029 2022

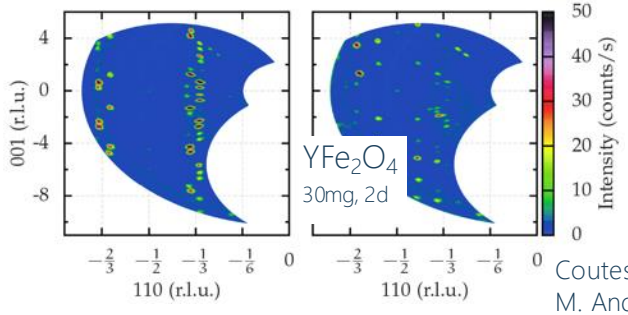
Superconductivity

Loop current order
P. Bourges PRL 96 197001 (2006



Spin and charge order

@ DNS



Coutesy of M. Angst

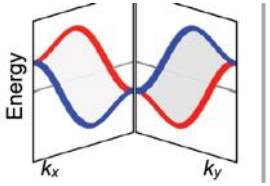
MAGIC proposal

high resolution

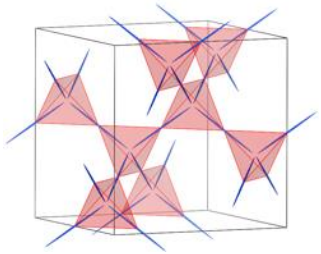
$\Delta Q \sim 10^{-2} \ldots 10^{-3} \text{Å}^{-1}$

altermagnetism

new phases / spintronics
PRX 12 040501 2022

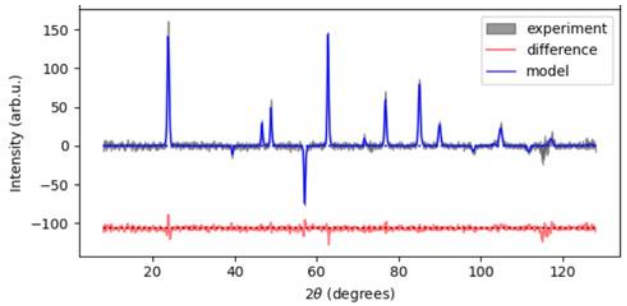


spin anisotropies



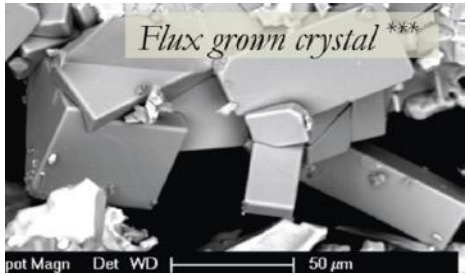
Iurii Kibalin & Arsen Gukasov
PRB 2019

from powders



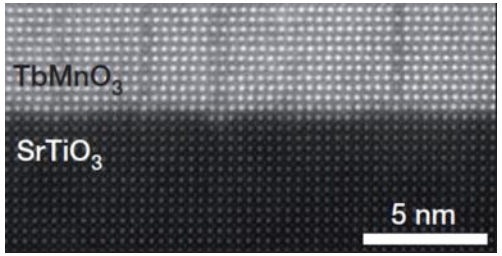
small moments S=1/2

small crystals

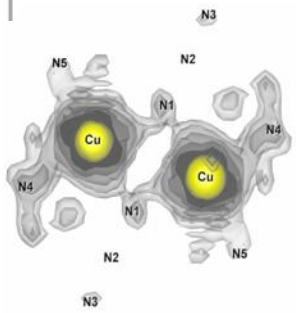


M. Valldor

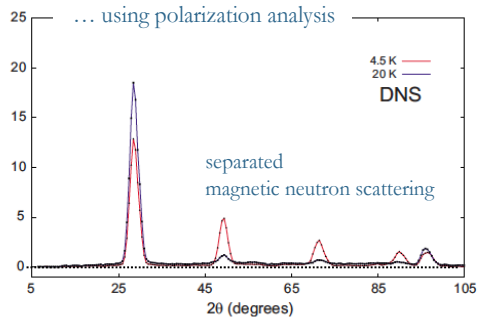
small (hetero) structures

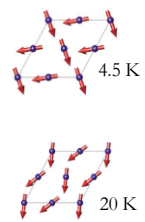


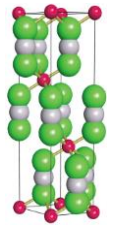
S. Farokhipoor et al
Nature Materials 515 , 379 (2015)



Molecular magnets
spin densities







MnNCN

background suppression (nucl, magn, inc)
hydrogeneous materials
Li, Na- batteries

Status

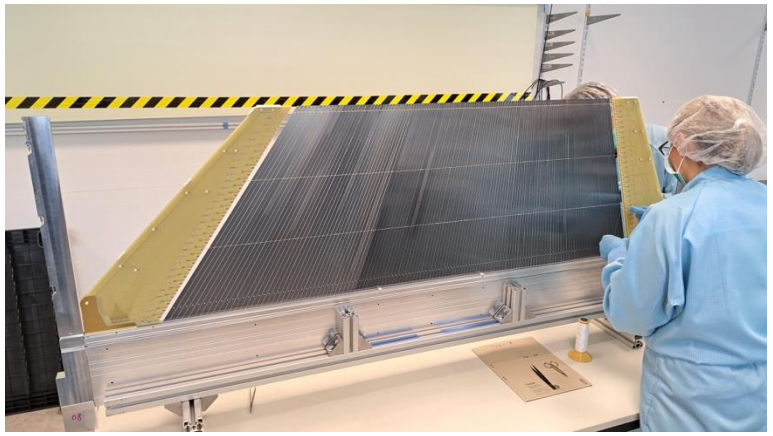
- Instrument Data Scientist – Iurii Kibalin started on September 1st
- IOE recruitment is ongoing
- Tender for the BWI opened by LLB on September 15th
- Beamstop+evac. flight path passed Sub-TG3
- The tests of the XYZ magnetic assembly began at FZJ
- Neutron tests with the spin analyzer prototype at PSI
- Detector A manufacturing has started
- Design of sample environment elevated platform is ready
- In-Bunker Vacuum Housing has been manufactured

Challenges

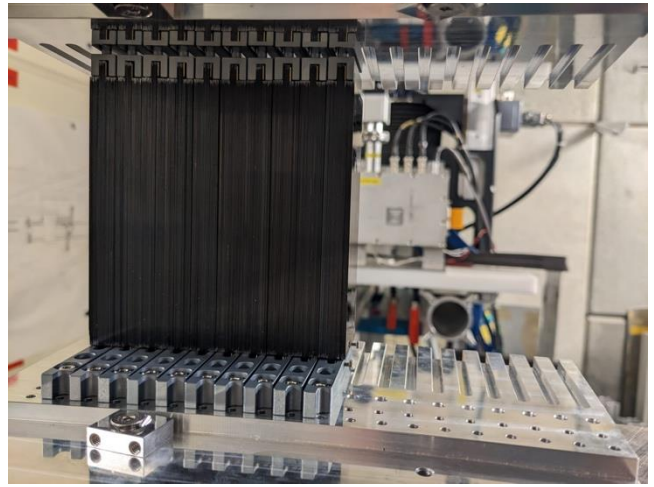
- Installation of bunker-wall insert before the BoT
- Out-of-Bunker neutron guide vacuum housing procurement (moved to ESS)

Manufactured in-Bunker Vacuum Housing

Detector A manufacturing



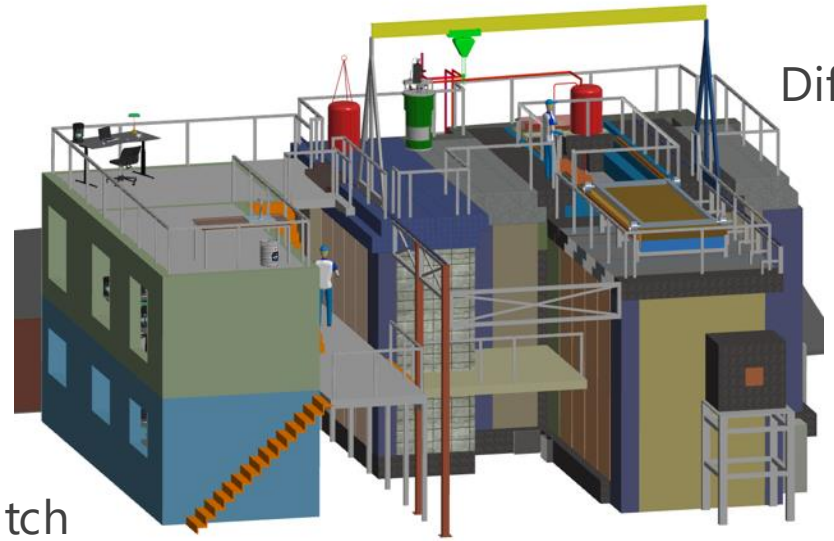
Analyzer prototype



HEIMDAL

Cold commissioning completed : Q2, 2027

Hybrid Diffractometer: Combined Diffraction and SANS and Imaging

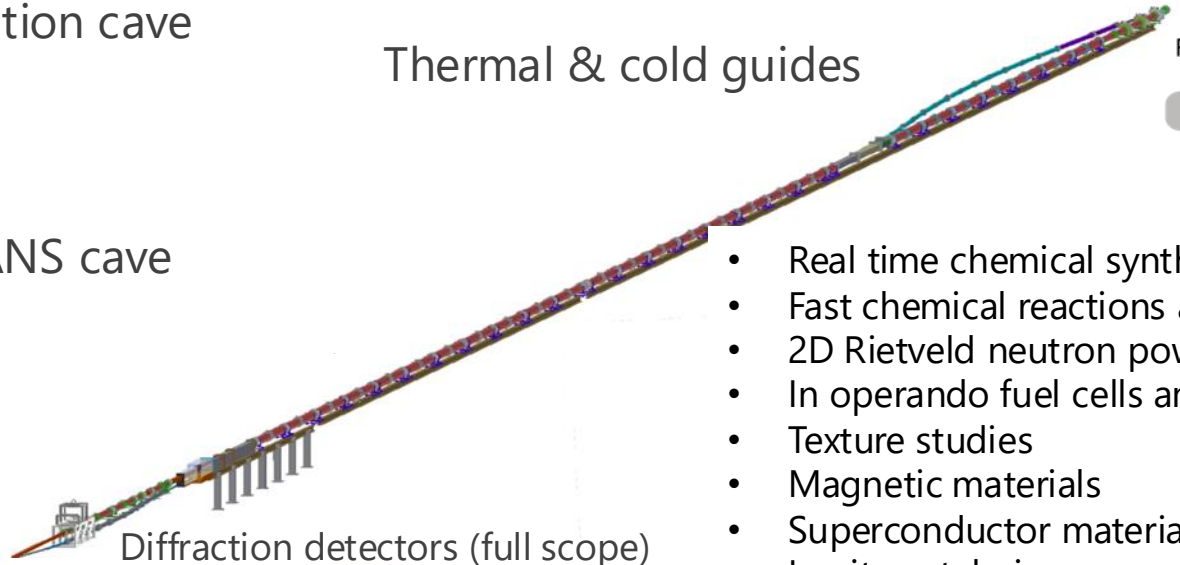


Diffraction cave

SANS cave

Hutch

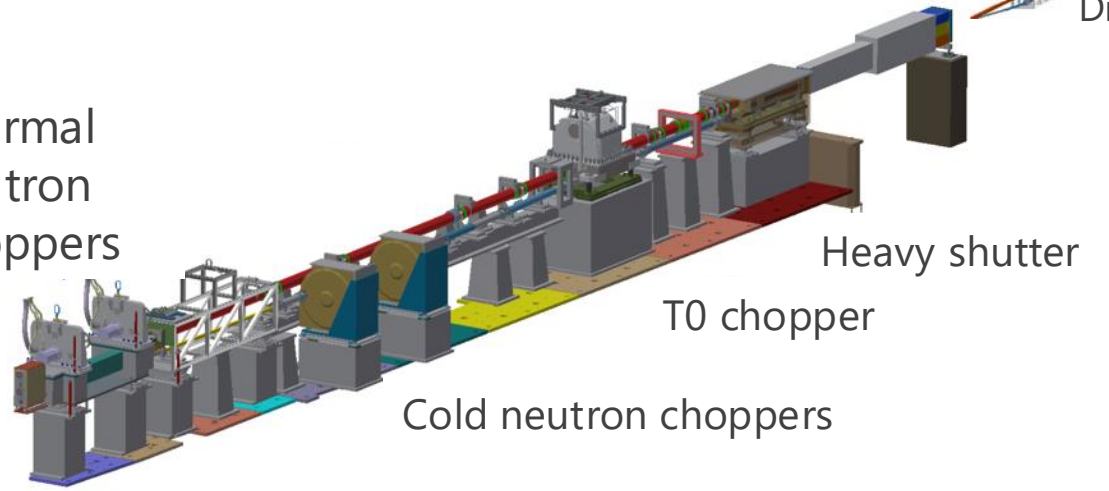
Thermal & cold guides



Diffraction detectors (full scope)

- 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

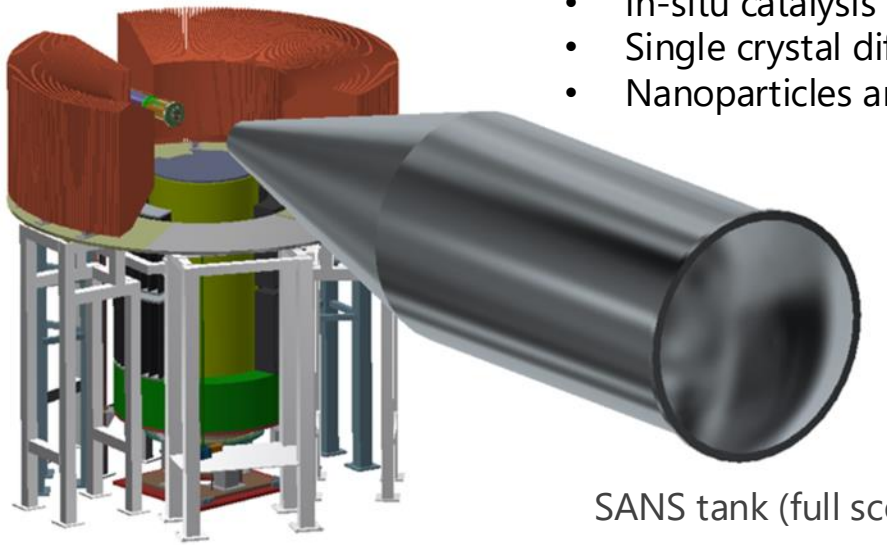
Thermal neutron choppers



Heavy shutter

T0 chopper

Cold neutron choppers



SANS tank (full scope)

Science case

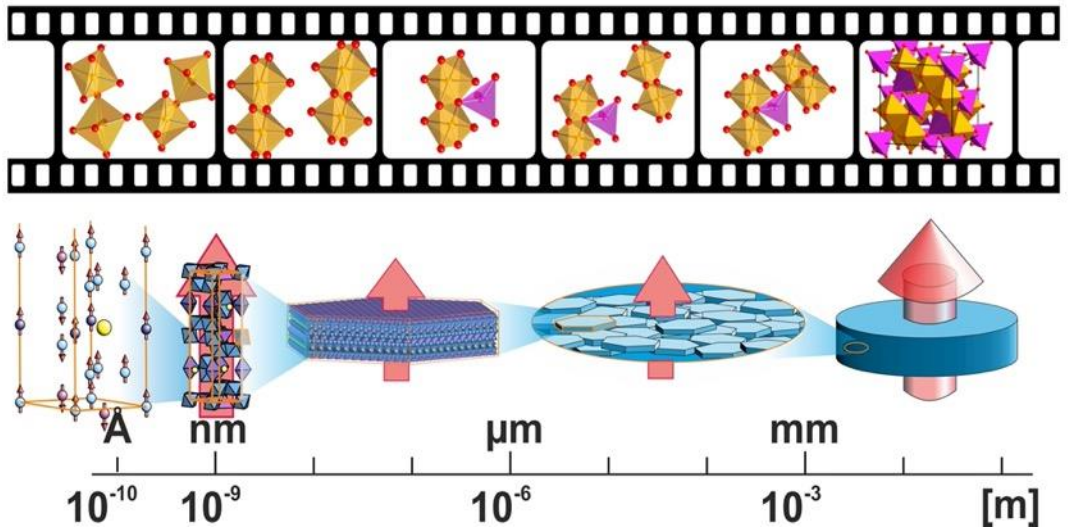
By combining diffraction and SANS HEIMDAL probes an extended q-range of
10^{-3} Å^{-1} < q < 15 Å^{-1}

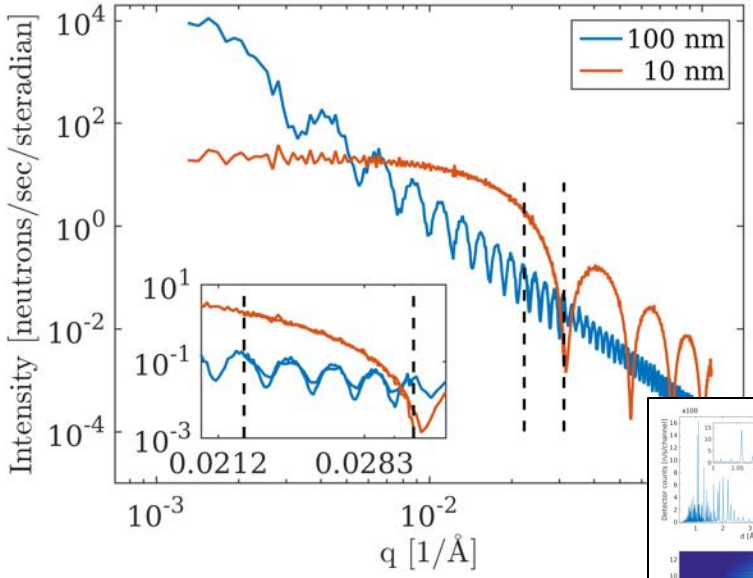
This enables studies of chemical and physical processes as they happen rather than attempts to combine data from several instruments recording almost identical processes.

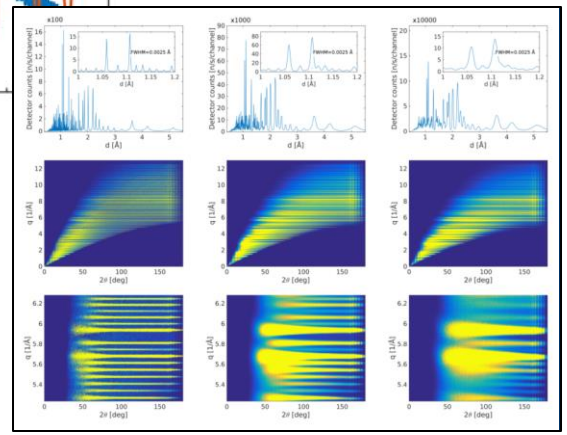
It can also be useful when examining both types of data are required to determine the next step in the experiment.

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

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







Status

- New team at partner university
- IOE recruitment is ongoing
- Bi-spectral switch successfully tested with neutrons at PSI
- Cave structure Sub-TG3 approved
- First cave installation starts in early December
- Hutch preliminary design is completed
- PSS Preliminary design is completed
- Collimator lift & support design started
- End guide detailed design started
- Thermal chopper manufactured
- BBG housing manufactured/optics delivered
- Current priority for re-scoping in the Diffraction & Imaging Division

Chopper cascade & Dan Mannix

Thermal neutrons chopper

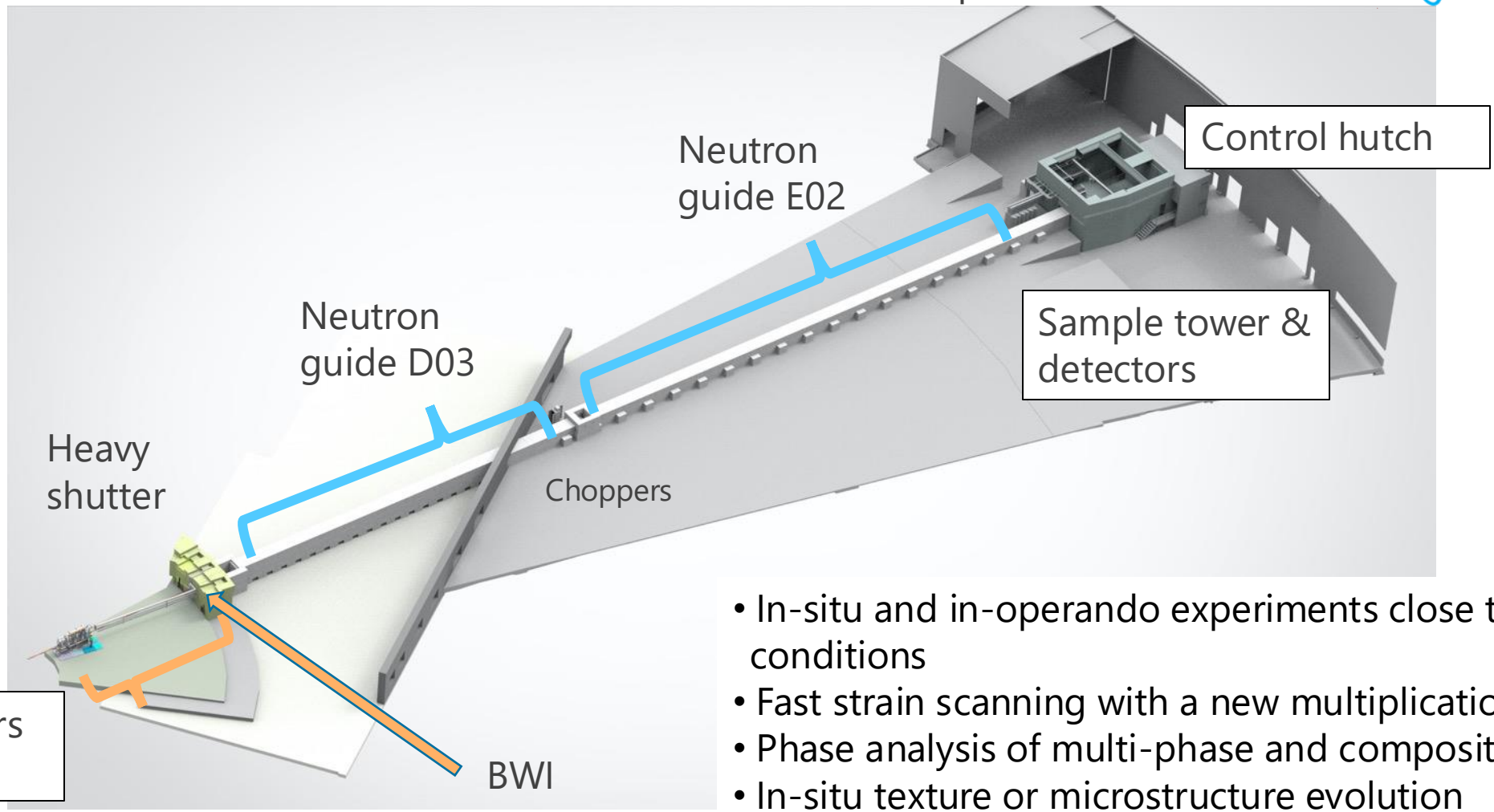
Issues

- No dedicated Instrument Data Scientist
- Minimalistic day one scope: 0.8 sr diffraction detector, coverage, no SANS, no cold guide
- Partner lacks resources to finish the detector support design

BEER

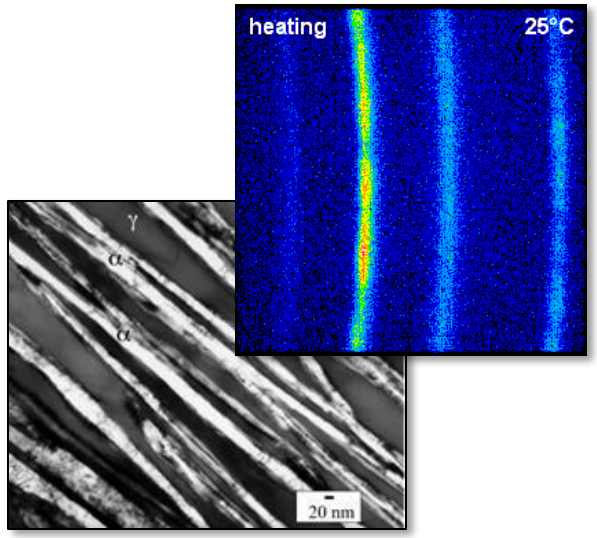
Cold commissioning completed : Q1, 2027

Engineering & Material Science Diffraction

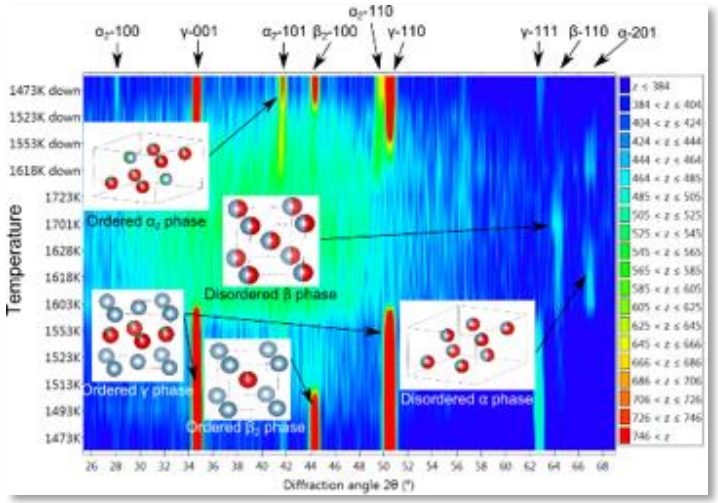


- In-situ and in-operando experiments close to the real conditions
- Fast strain scanning with a new multiplication technique
- Phase analysis of multi-phase and composite materials
- In-situ texture or microstructure evolution
- Multi-scale characterisation
- Long term experiments

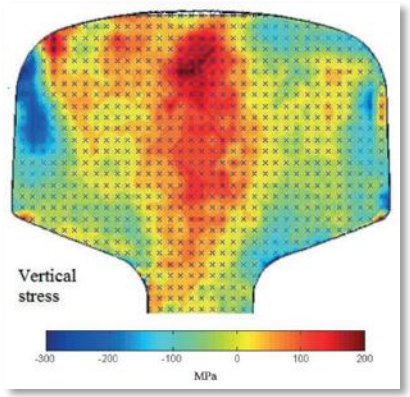
Science case



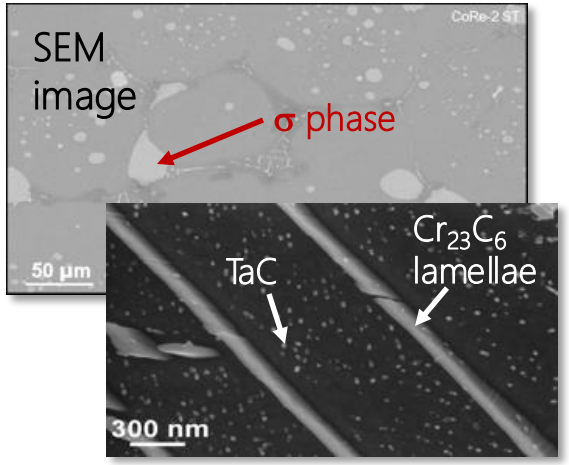
In-situ texture or microstructure evolution:
Re-crystallisation in CoRe alloys
Microstructure of γ-Ti allys



In-situ phase analysis of multi-phase materials:
Phase diagram of alloyed (Mo, C) β-TiAl alloy



Fast strain scanning:
16 mm thick slice cut from a used railway rail



Multi-scale characterisation:
Precipitate characterisation of HT CoRe-based superalloys

Slide : Premek Beran

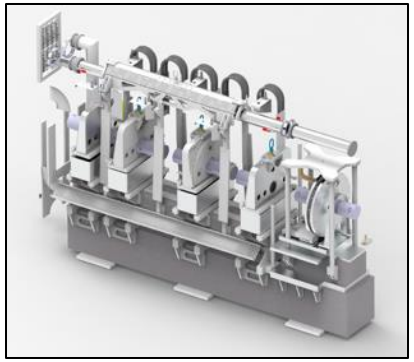
Status

- New IS started Gergely Neméth
- New SEE Eng. started Caroline Curfs
- Celine Durniak (IDS) started with data reduction protocols
- Cave & hutch are in final stages of installation
- Neutron guide/shielding installed
- Heavy shutter installed
- CUP & CEP design frozen
- Bi-spectral switch was successfully tested with neutrons (IMAT@ISIS)
- Choppers ready for installation, chopper cascade is in design

Neutron guides & shielding

Hutch

Chopper cascade



Challenges

- In-bunker installation: what & when?
- Chopper cascade design finalization is slow
- Deformation rig integration is slow
- Complicated interfaces ECDC/ICS/DMSC, MCA/CEP/ECDS
- Lack of good communication with PSS team

Fast chopper disks

First Science Activities

VR workshops

Support first science at DREAM & ODIN and experiments in > 2030

A DREAM come true – Sustainable and functional materials from local resources (Upsalla University)

1. Time-resolved structural evolution in metallic alloys during solidification and nonisothermal conditions
2. Nanoparticle formation in cellulose-based systems in humidity-controlled conditions
3. Separation, Purification and Reduction

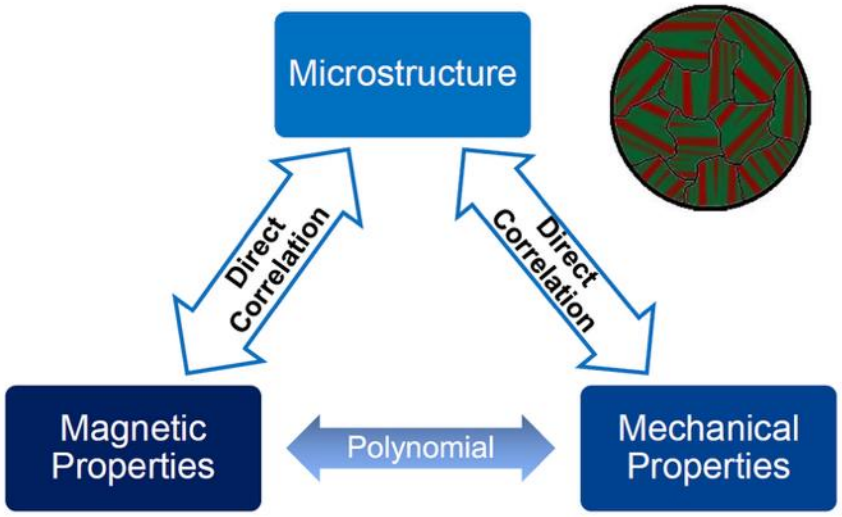
Hyperspectral, multidimensional Imaging with Neutrons to explore material processes and processing for a sustainable society (Lund University)

1. Crystalline Insights with hyperspectral Imaging
2. Decoding Materials and processes in 3D with ToF Tomography.
3. Pioneering ToF Imaging for new challenges and materials

ESS early science postdocs (Q2, 2026)

Two postdoc positions were awarded for imaging and diffraction

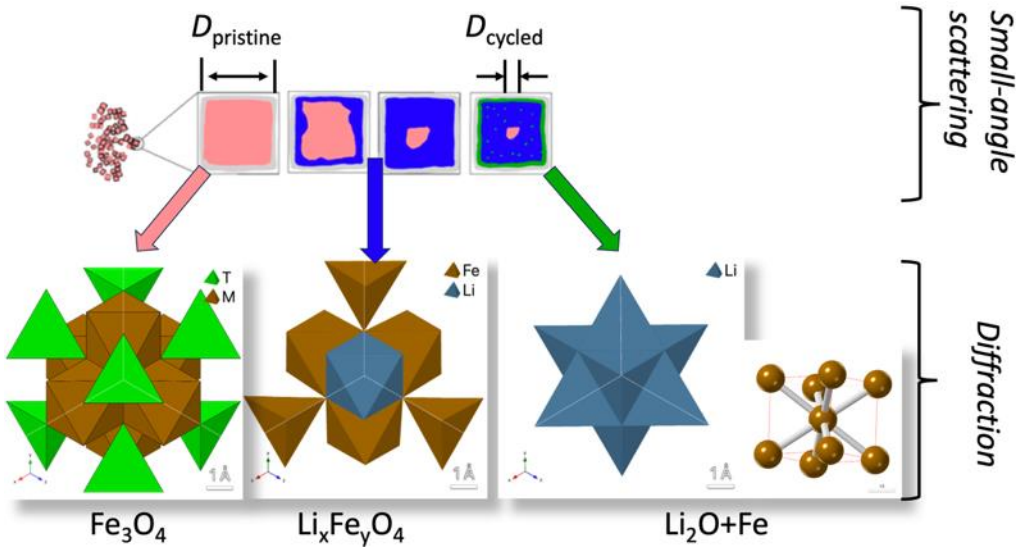
ODIN: Microstructural Characterization of Ferritic Alloys by Neutron Time-Of-flight and Grating Interferometry for Improved Materials



Collaborations: Lund University, Technical University of Munich, TBL team

Supervisor: R. Woracek (TBC)

DREAM: Correlation of Structural and Morphological Changes to Novel Electrode Materials for Li/Na-ion Batteries



Collaborations: Uppsala University, University of Duisburg-Essen

Supervisor: M. Feygenson

Ideas for new instruments under discussion in the Diffraction & Imaging division

1. **Single-crystal diffractometer with high-pressure capabilities** (ESS, PSI, ESS Bilbao, ISIS, Edinburgh University)
2. **PDF dedicated diffractometer with Q_{MAX} ~50 $Å^{-1}$** (PSI, ESS, TUM, ISIS, Duisburg-Essen University, Uppsala University)
3. **MAGNI—Microscopy, Advanced and Grating Neutron Imaging-** neutron imaging instrument optimized for high neutron flux (PSI, DTU, ESS)
4. **IDUN - Guide bundle instrument** for imaging, engineering diffraction and SANS (DTI, ESS)

Concluding remarks

- Overall, good progress with instruments, but there are still challenges
- Division is growing, three more hires since last STAP
- TBL is the first instrument to go through SAR/iSRR
- Challenge of providing engineering support to the teams after TG5
- T2 & T3 instruments suffer from a lack of attention from technical support groups (T1 instruments, SAR/iSRR are the focus)
- Homework from the Imaging & Engineering Diffraction STAP: roleplay of bringing external SEE (quality, safety, delivery, acceptance and etc)
- Good progress towards first science for all teams
- Industry outreach: ZeroSteel (EU-H) & MetalBeams meetings