Diffraction & Imaging Division update

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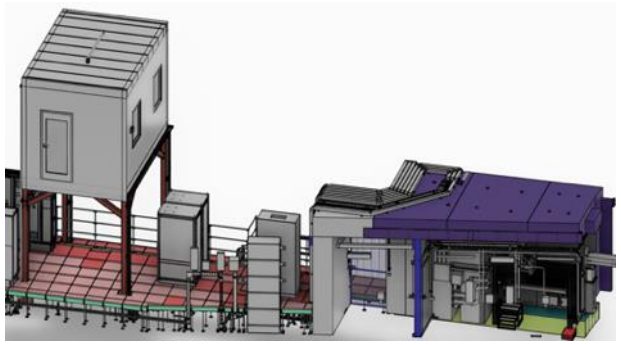
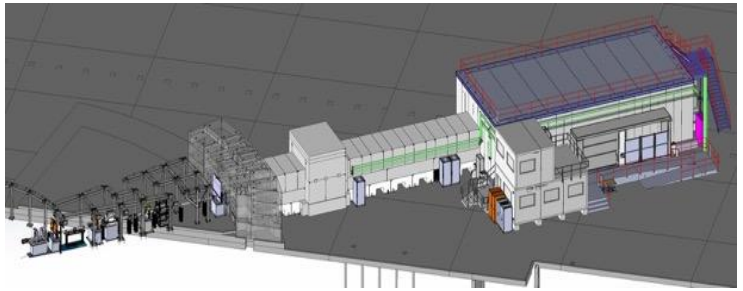
[3] Jülich Center for Neutron Scattering, Forschungszentrum Jülich

TBL (SAR/iSRR* meeting 2025)
Test beamline



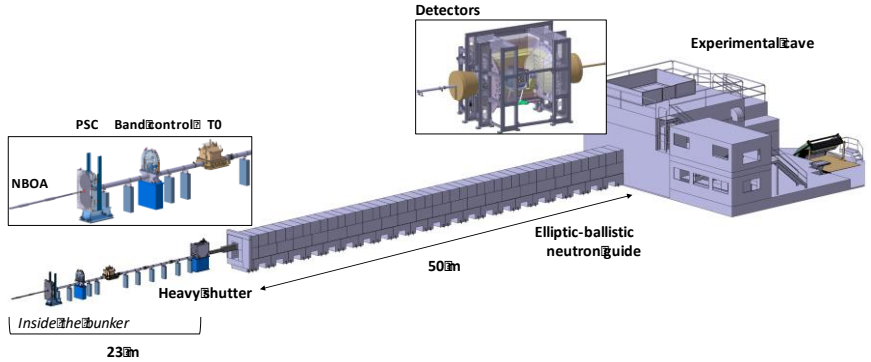
ODIN (SAR/iSRR meeting 2025)
Neutron imaging

DE CH



DREAM (SAR/iSRR meeting 2026)
Powder diffractometer

DE FR

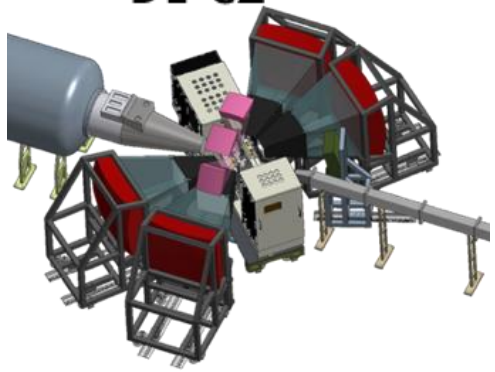


MAGiC (2027)
Polarized diffractometer

DE FR CH

BEER (2027)
Engineering diffractometer

DE CZ



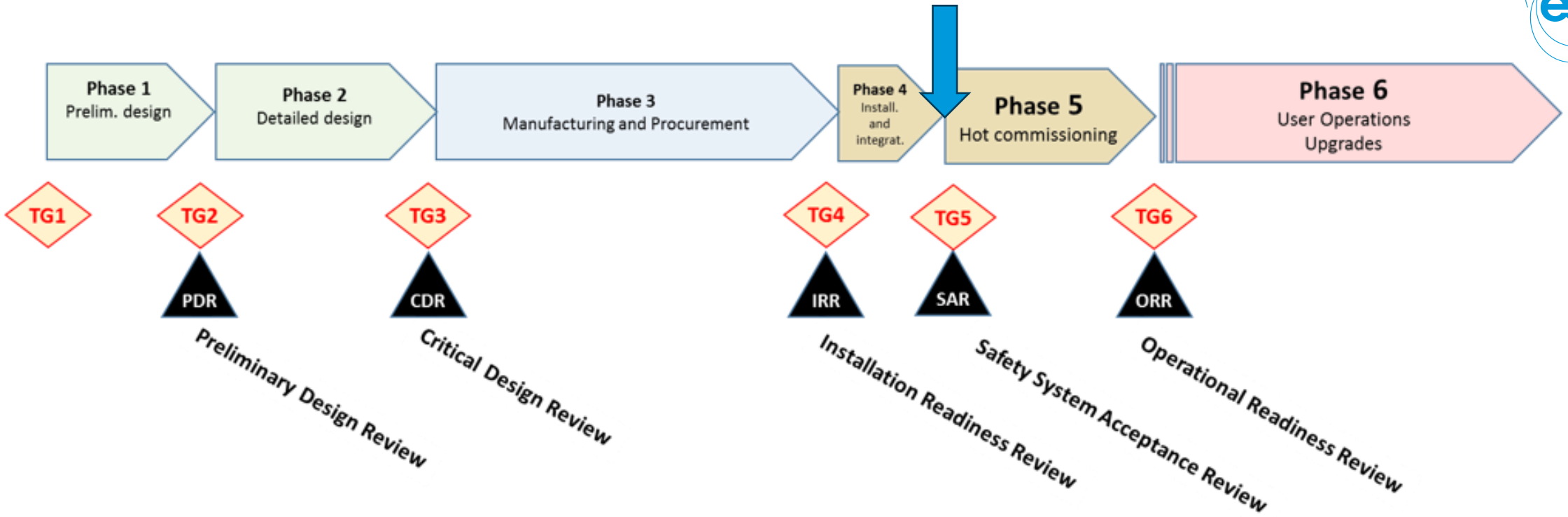
HEIMDAL (2027)
Multiscale diffractometer

DK CH

*SAR = System Acceptance Review
iSRR = instrument Safety Readiness Review

SAR/TG5 and iSRR

Last milestone in TA for partners



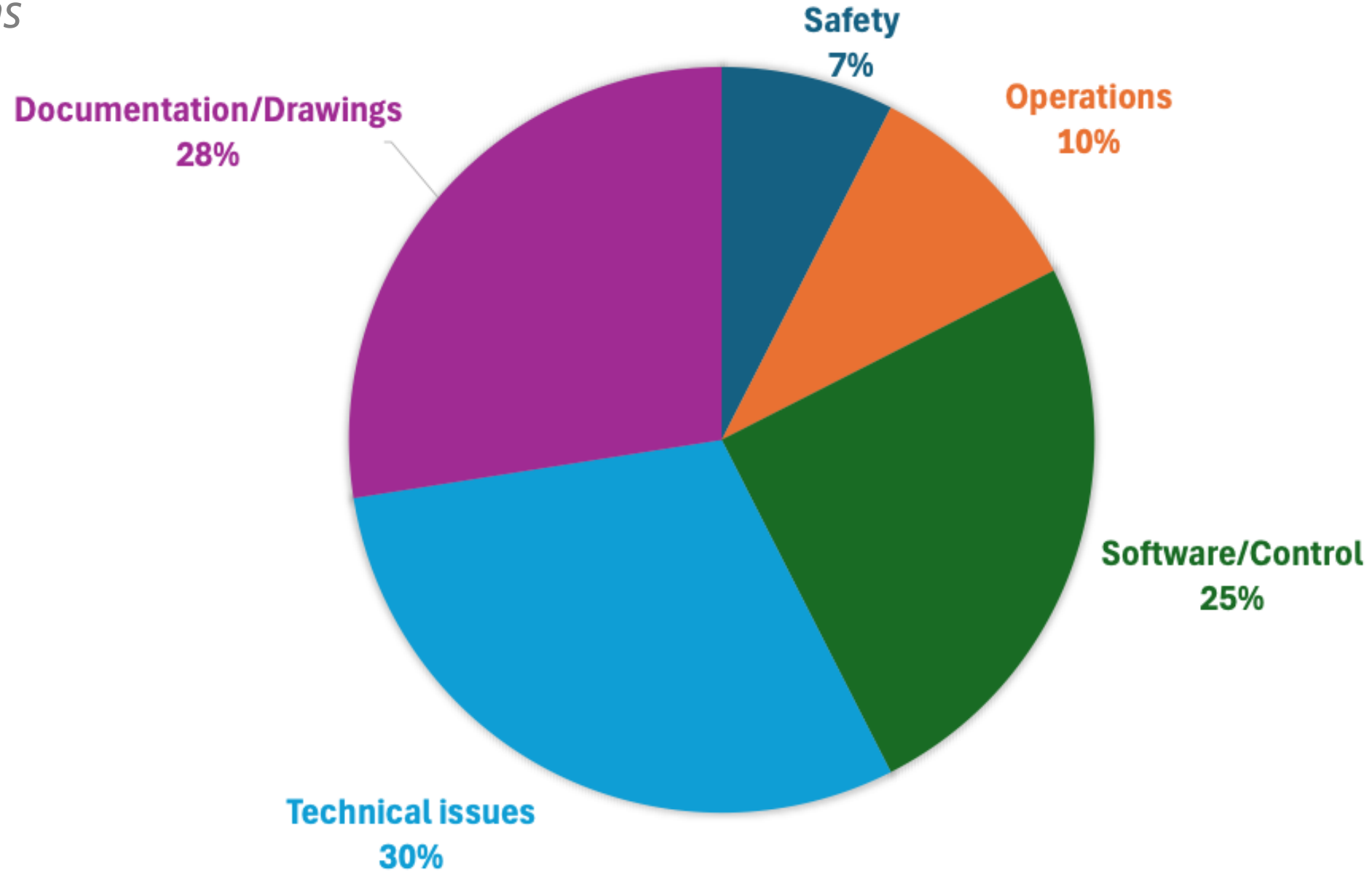
System Acceptance Review (SAR) or TG5: all components installed, integrated commissioning is done, final milestone for in-kind partners

instrument Safety Readiness Review (iSRR): PSS, fire suppression, motion safety, team readiness to for hot commissioning

During SAR/TG5 & iSRR reviews

Issues raised during SAR/iSRR meeting (ODIN):

A combination of tasks to pass SAR/iSRR and to be ready for user operations



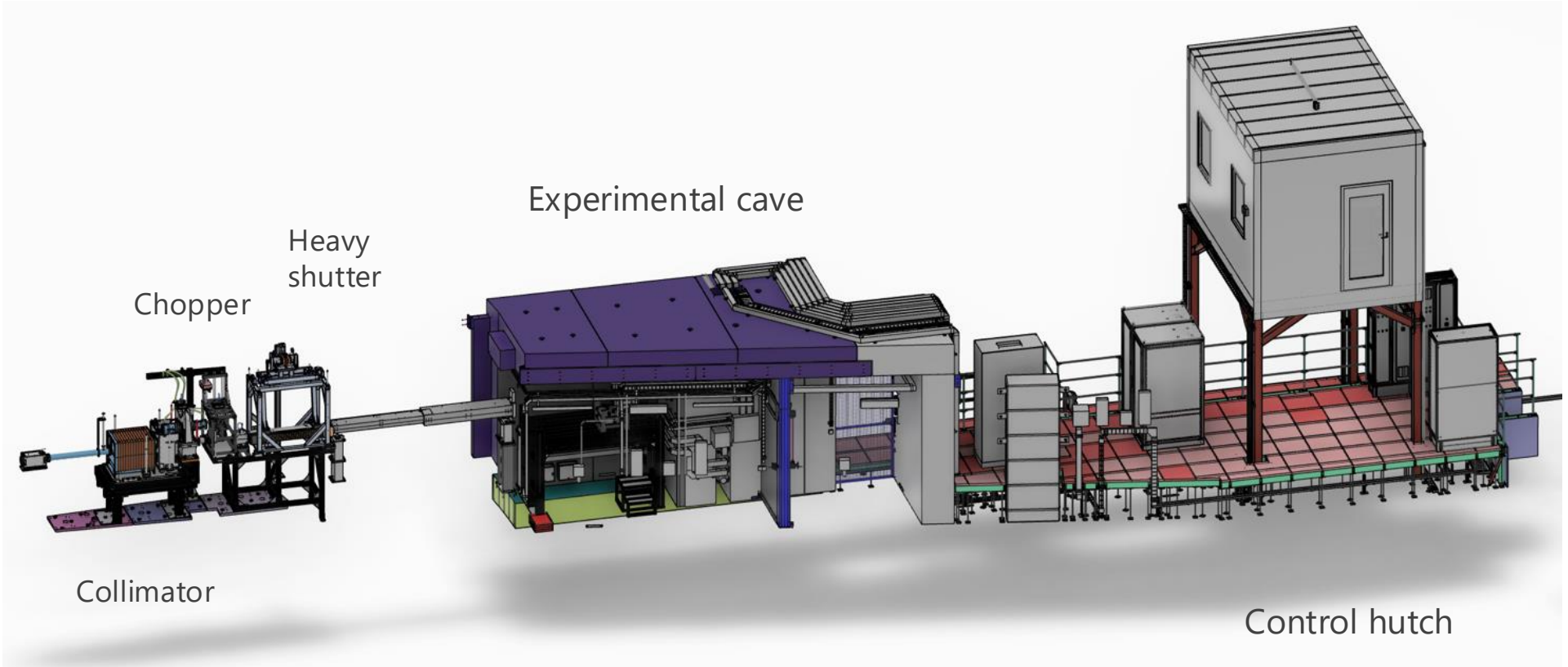
Integrated cold commissioning completed; SAR & iSRR permits are approved

ESS Test Beamline

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

Tasks for TBL for ESS BoT milestone

1. Measured reasonable thermal and cold neutron spectra on the Test Beam Line (acceptable signal-to-noise ratio)
2. 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)



Test Beamline

Early Science Ideas – beyond the source characterization

Idea 1

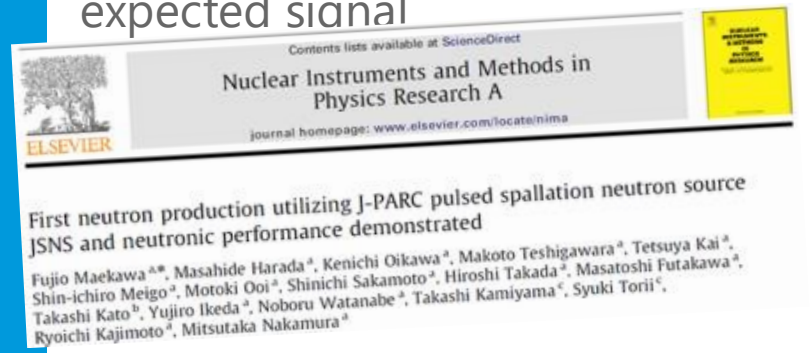
Validation of unique neutronics design features of ESS

- current collaborators: inhouse (e.g. Integrated Commissioning Meetings)

- potential collaborators:

other neutron sources

- requirements for Spallation Physics: Proper simulations of expected signal


Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research A

journal homepage: www.elsevier.com/locate/nima

ELSEVIER

First neutron production utilizing J-PARC pulsed spallation neutron source JSNS and neutronic performance demonstrated

Fujio Maekawa [a,*], Masahide Harada [a], Kenichi Oikawa [a], Makoto Teshigawara [a], Tetsuya Kai [a], Shin-ichiro Meigo [a], Motoki Ooi [a], Shinichi Sakamoto [a], Hiroshi Takada [a], Masatoshi Futakawa [a], Takashi Kato [b], Yujiro Ikeda [a], Noboru Watanabe [a], Takashi Kamiyama [c], Syuki Torii [c], Ryoichi Kajimoto [d], Mitsutaka Nakamura [a]

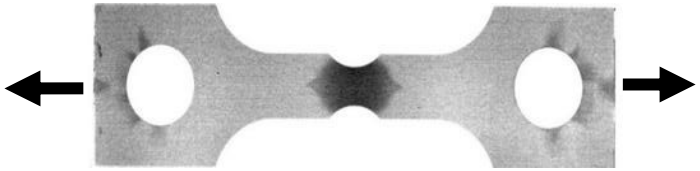
Idea 2

Plastic deformation during mechanical processing (*method development as of now*)

- current collaborators: inhouse (Thawatchart Chulapakorn) + LTH

- potential collaborators: endless *once established*...

- requirements from SE/DMSC/Labs/external developmental needs: small stress rig, furnace; incorporate external equipment into NICOS+DAQ



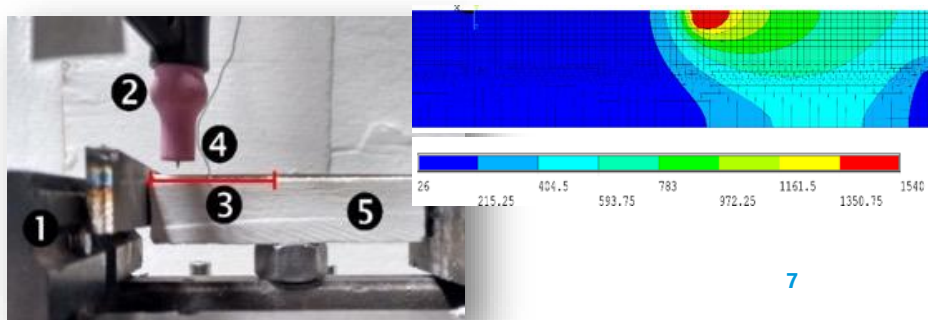
Idea 3

Changes in neutron transmission due to Debye Waller Factor: In-situ welding

- current collaborators: BAM (Berlin), HZB

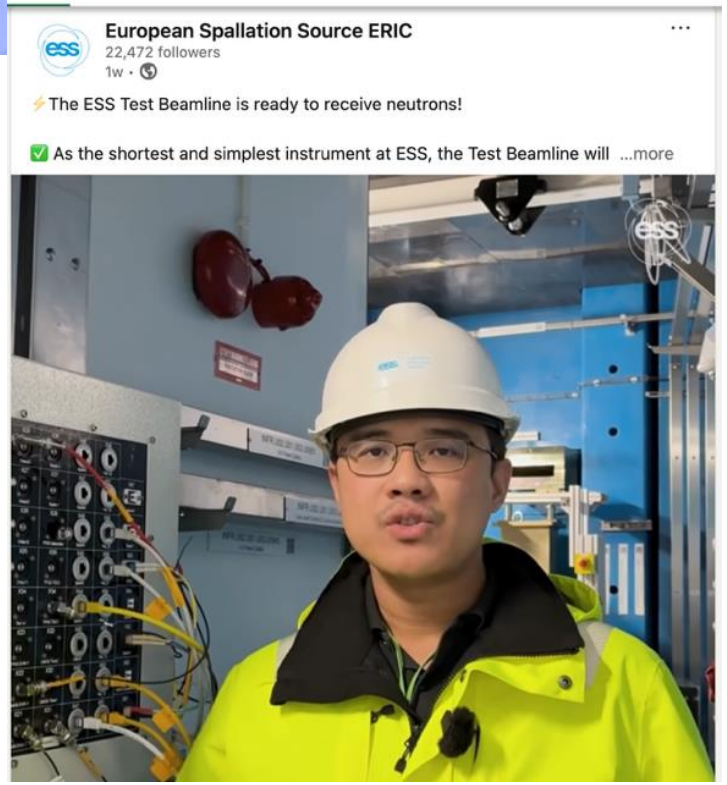
- potential collaborators: Industrial network within Sweden

- requirements from SE/DMSC/external developmental needs: Welding device available and control/DAQ linked



Status

- System Acceptance Review (SAR) is done
- Instrument Safety Readiness Review (iSRR) is done
- Instrument scientist recruitment is almost done
- Ongoing work to fine-tune the instrument for BoT
- Discussion with RP about activated samples/ detectors storage is ongoing
- Work on deferred scope: automatic door, diffraction rig, etc. is ongoing

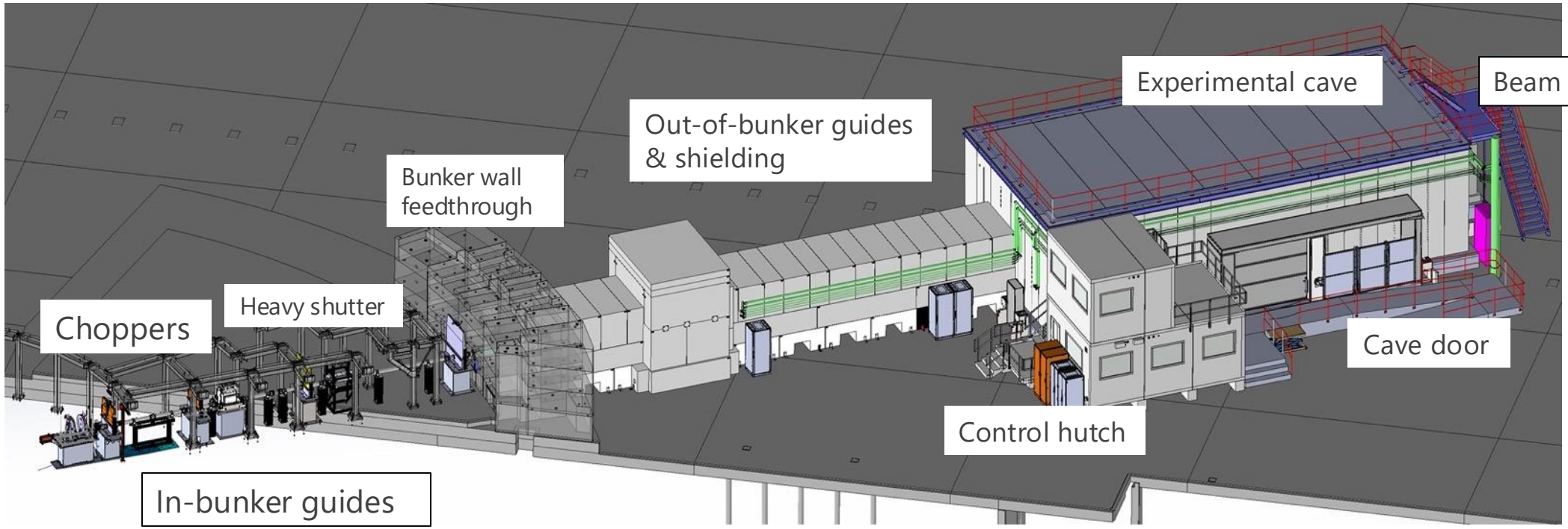


Challenges

- Team is still incomplete
- Reliability and robustness of control and acquisition system
- Scipp and VISA tools need improvement
- Many practical issues have to be raised for entire organization for (RP, NSS, Safety)

ODIN Integrated cold commissioning completed; SAR & iSRR permits are pending

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)

Contrast Mechanism

Diffraction | Phase | Magnetic | ‚Attenuation‘

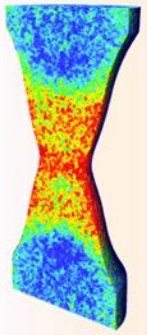
Applications

Metals/ Engineering

Hydrogen

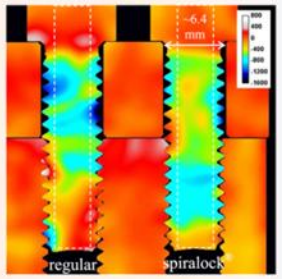
Energy Storage

Cultural Heritage



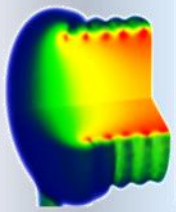
engineering

Strains

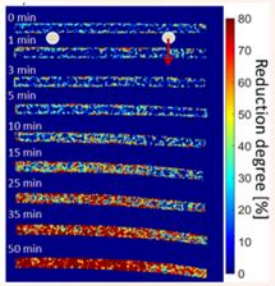


Internal defects

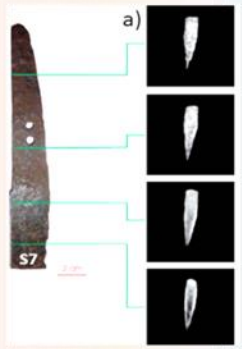
Magnetic fields



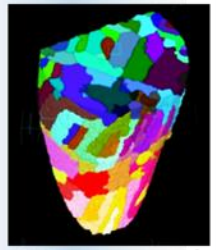
Phase transitions



SOFC’s

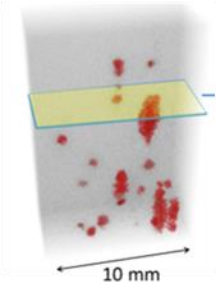


Microstructure in cultural heritage



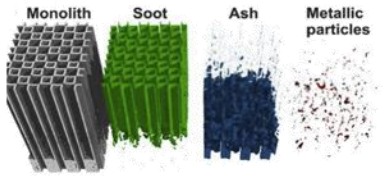
Magnetic domains

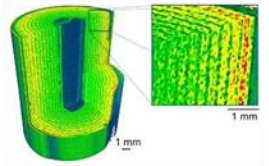
Hydrogen in metals



Device inspection: particle filters

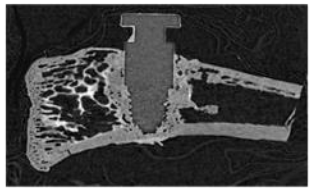
Water uptake in plants





Li transport in batteries

Corrosion



Bone Structures + implants

Å | nm | µm | mm | cm

Contrast mechanism length scales

Slide : Robin Woracek

Status

- New instrument scientist (Stefanos Athanasopoulos)
- System Acceptance Review (SAR/TG5) is done
- instrument Safety System Review (iSRR) is done
- Work ongoing for on remaining actions for SAR/iSRR
- Licensing work on x-ray source authorization is ongoing
- Preliminary x-ray setup design is completed
- Image plate detector for x-ray source is procured
- High-flux detector is procured
- ODIN was part of HERCULES neutron school

SAR/iSRR tour

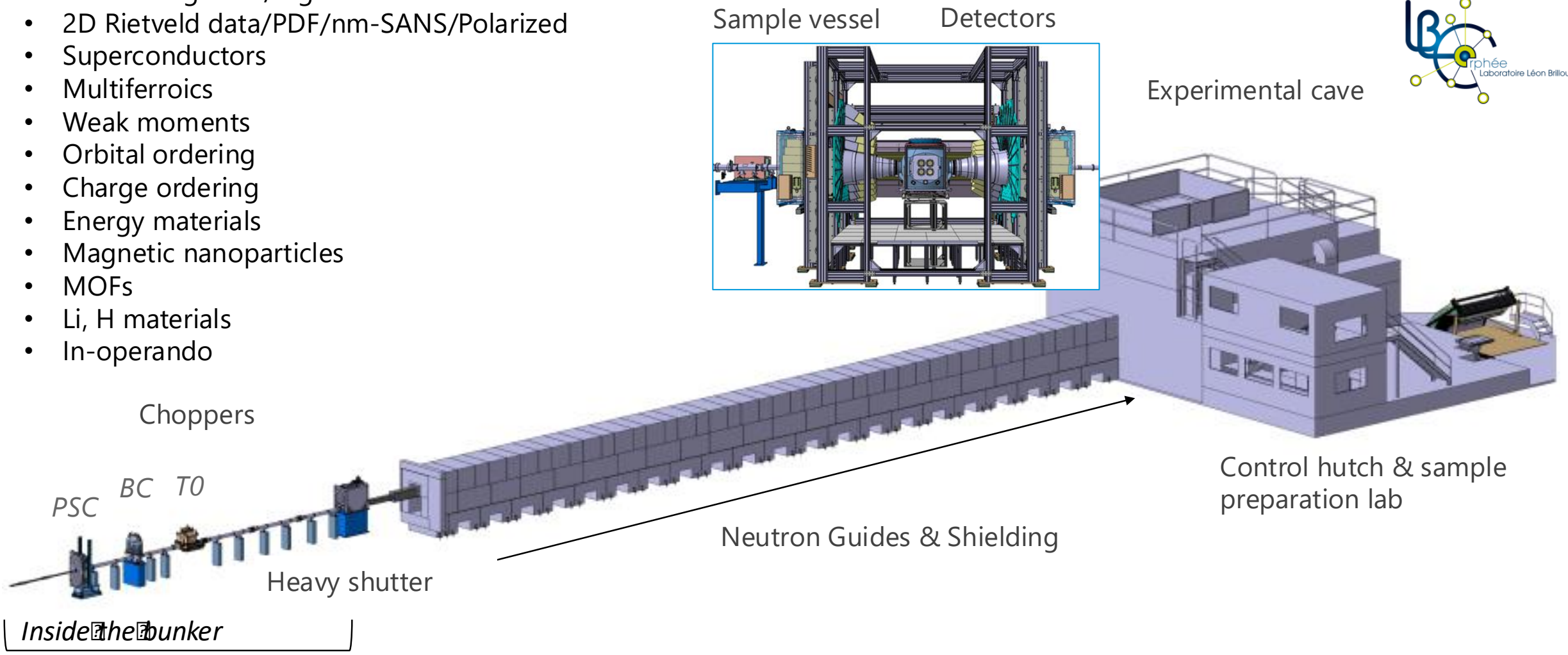
Challenges

- Team is incomplete: another scientist is on LoA (until Sept., 2026)
- Number of outstating DMSC tasks for first science
- Data workflow for ToF imaging data has to be optimized

DREAM Integrated cold commissioning completed; SAR & iSRR permits are pending

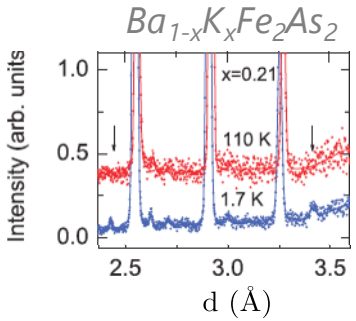
Diffraction Resolved by Energy and Angle Measurements

- 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

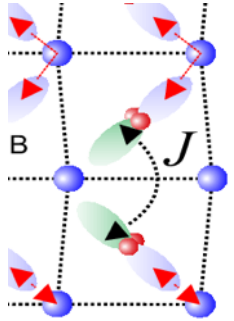


powders
single-crystals
nanoparticles
alloys
liquids

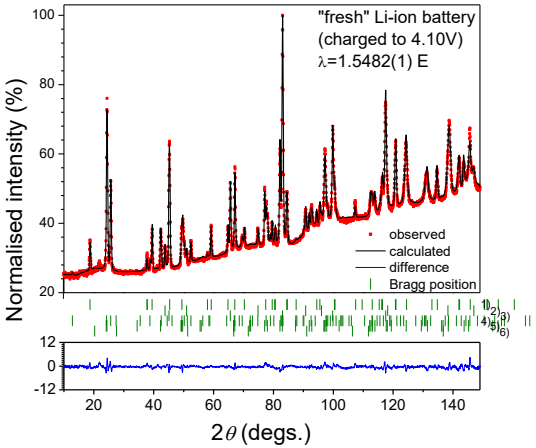
Magnetism



weak moments
phase diagrams of
superconductors
multiferroics



orbital ordering
charge ordering
distortion
magnetic exchange

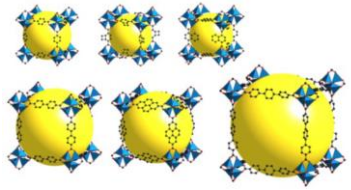


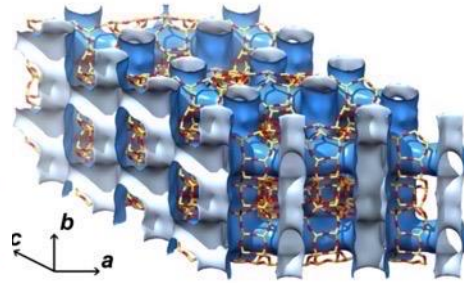
Energy Materials

multiphase
catalysts
in-operando
batteries

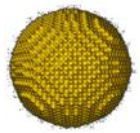
Large Unit Cells

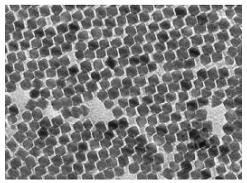
MOFs
thermoelectrics
molecular sieves
H_2 - storage





Nanostructures





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

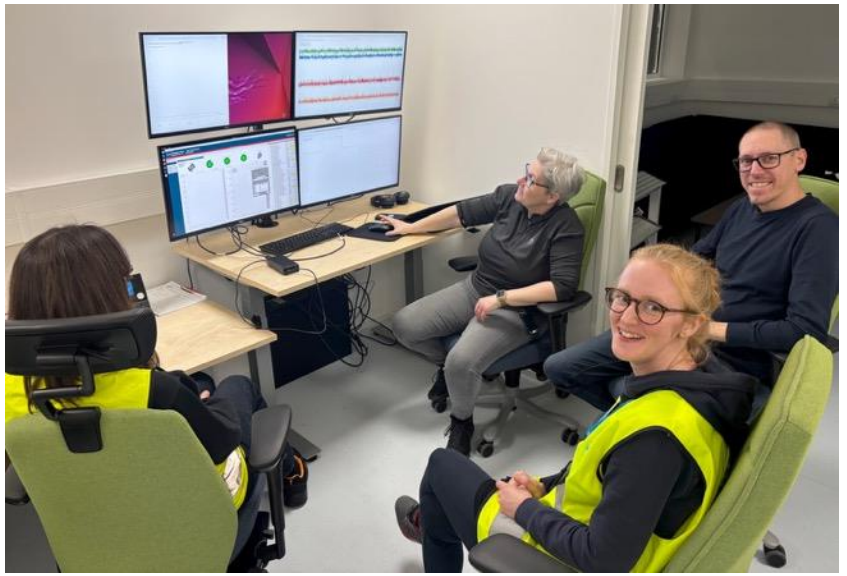
Third-party funding:
Polarized (cold) neutrons +
nm-SANS detector

RöntgenÅngströmCluster

Status

- All integrated tests are completed
- System Acceptance Review (SAR/TG5) is done
- instrument Safety Readiness Review (iSRR) is done
- Work on SAR/iSRR remaining tasks
- Part of HERCULES neutron school
- Detector rescoping activities started

Choppers integrated tests



iSRR/SAR tour

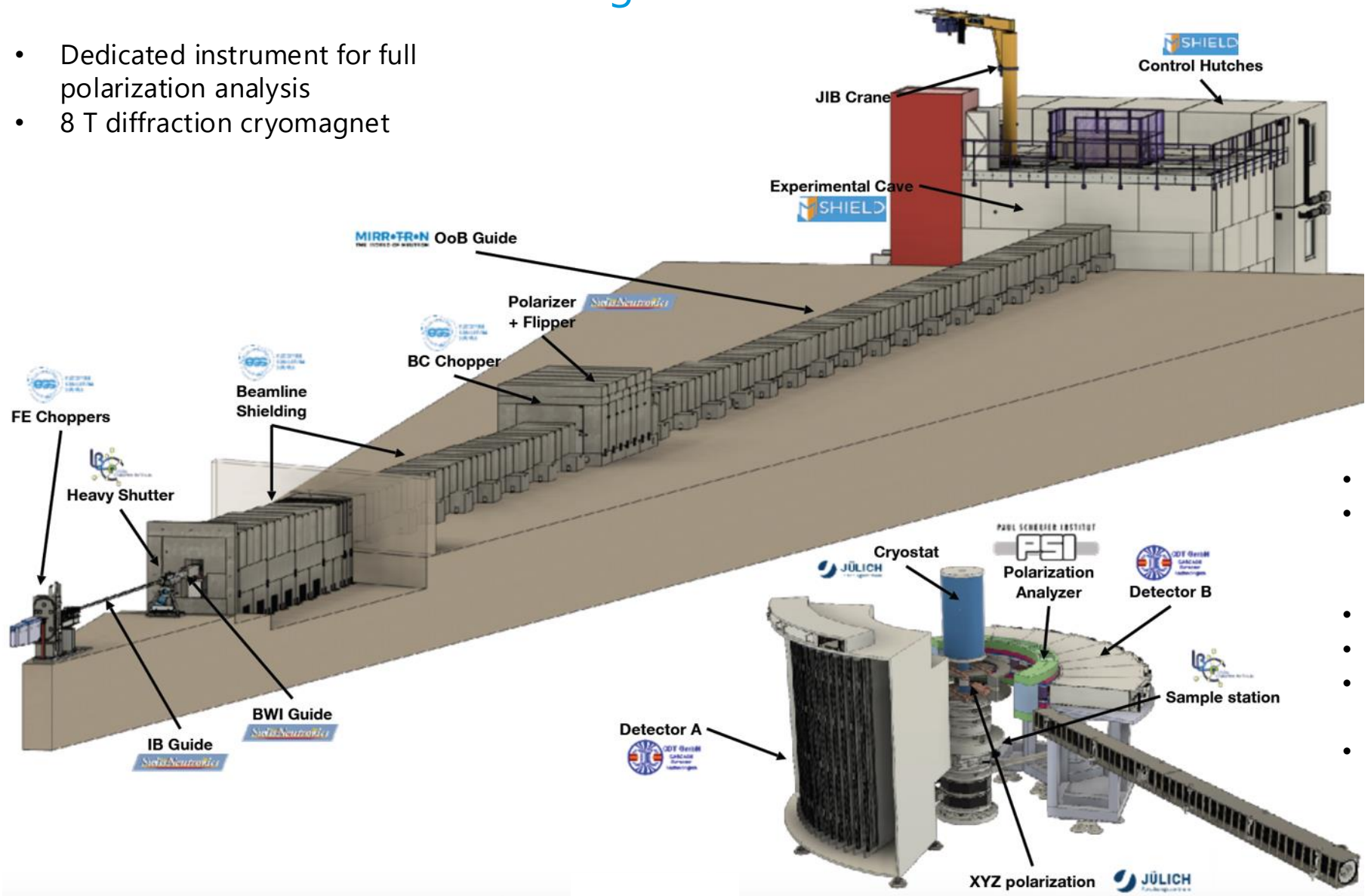
Challenges

- Faulty detector modules have to be shipped back to manufacturer
- Engineering support after TG5 (common for all)
- Delays in cryofurnace sample changer procurement

MAGiC Cold commissioning completed: Q2, 2027

Polarised Diffractometer for Magnetism

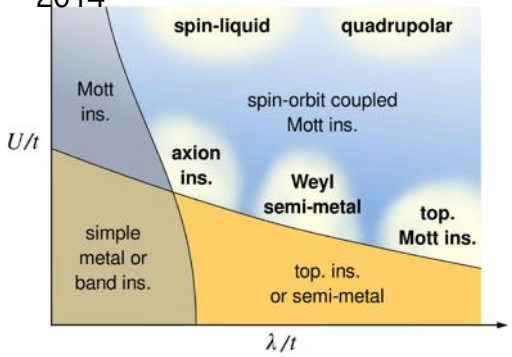
- Dedicated instrument for full polarization analysis
- 8 T diffraction cryomagnet



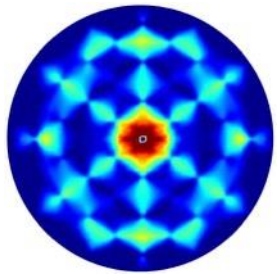
- Local susceptibility and spin densities
- Exotic magnetic structure (long range, non-collinear, anisotropic Hamiltonian)
- Multifunctional materials
- Superconductivity
- Frustrated magnets and quantum spin liquids
- Magnetism in thin films and at interfaces

Novel metals and insulators

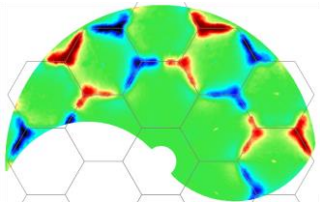
W. Witczak-Krempa et al
Ann Revi Cond Matt Phys 5 57 2014



Frustrated magnetism spin-liquid

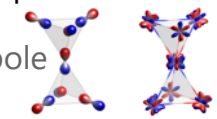


Spin-Ice model



Chirality
PRX 12 021029 2022

dipole
monopole

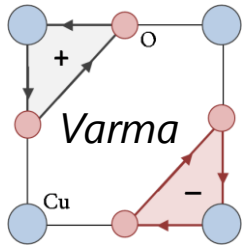


quadrupole
Sibille, Nature Physics 2020

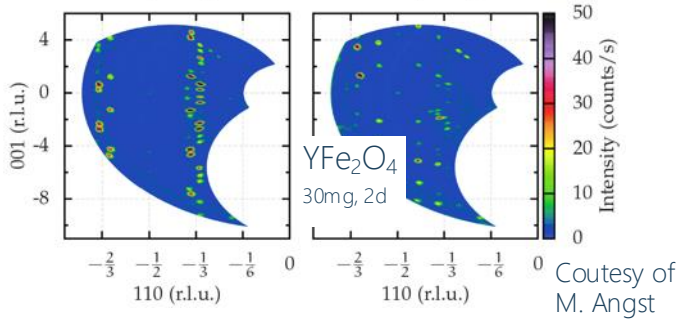
Fennell, Science 2009

Superconductivity

Loop current order
P. Bourges PRL 96 197001 (2006



Spin and charge order



Coutesy of M. Angst

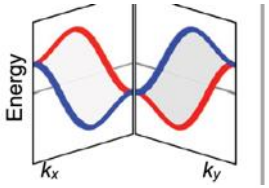
MAGIC proposal

high resolution

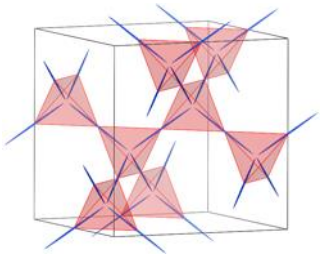
$\Delta Q \sim 10^{-2} \ldots 10^{-3}$ Å^{-1}

altermagnetism

new phases / spintronics
PRX 12 040501 2022

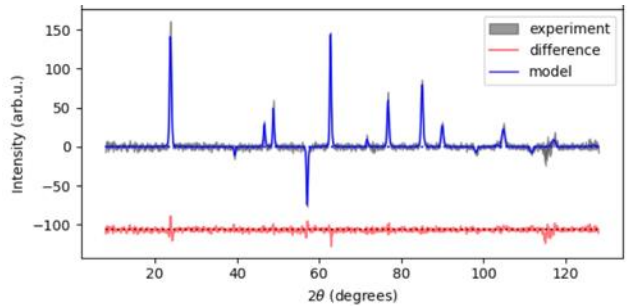


spin anisotropies



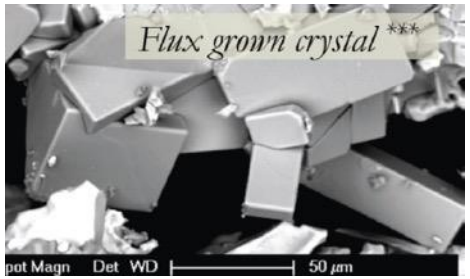
Iurii Kibalin & Arsen Gukasov
PRB 2019

from powders



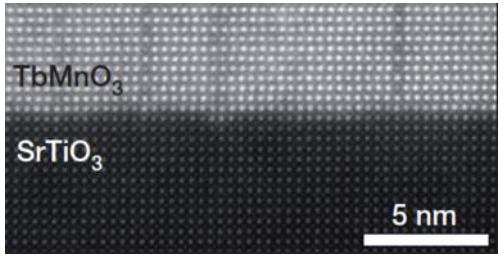
small moments S=1/2

small crystals

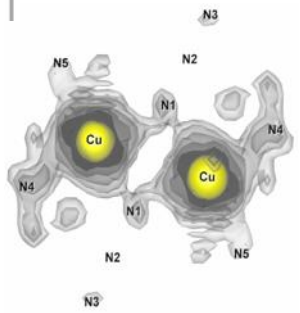


M. Valldor

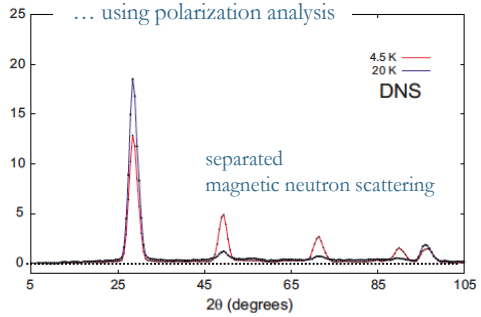
small (hetero) structures

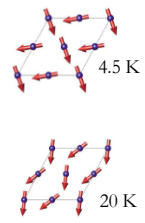


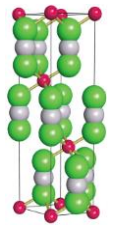
S. Farokhipoor et al
Nature Materials 515 , 379 (2015)



Molecular magnets
spin densities







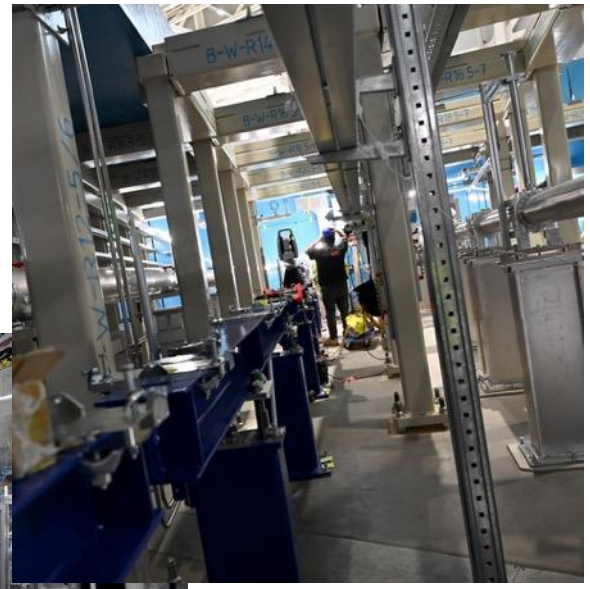
MnNCN

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

Status

- IOE is hired (Moritz Braun)
- Replacement of Moritz will start on May 4th
- In-bunker neutron guides have been installed
- Supplier for the out-of-bunker vacuum housing found
- FE chopper is installed
- Design of CEP and CUP is completed, installation in June
- Design of elevated platform is completed, installation June
- Tender for the sample stage was open at the end of March (last big procurement)

In-bunker installation



Challenges

- Tight installation schedule in autumn for the equipment inside the cave
- Front-End chopper system position needs to be corrected, after installation

HEIMDAL

Cold commissioning completed : Q3, 2027

Hybrid Diffractometer: Combined Diffraction and SANS and Imaging

Hutch

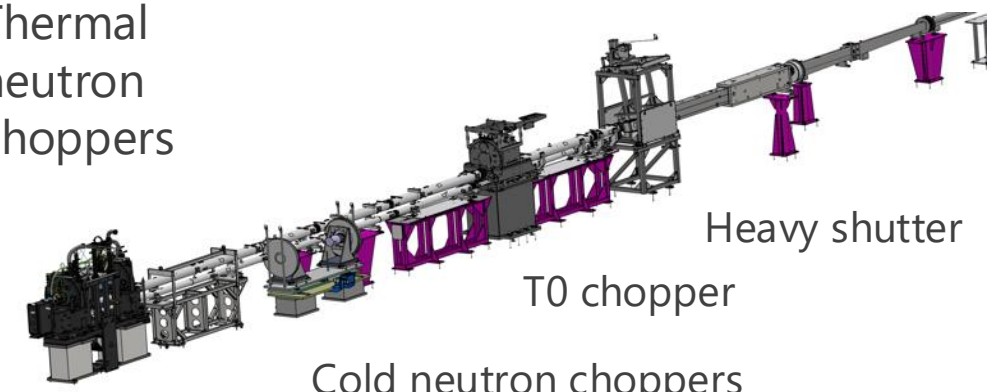
Diffraction cave

SANS cave

Thermal & cold guides

- 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

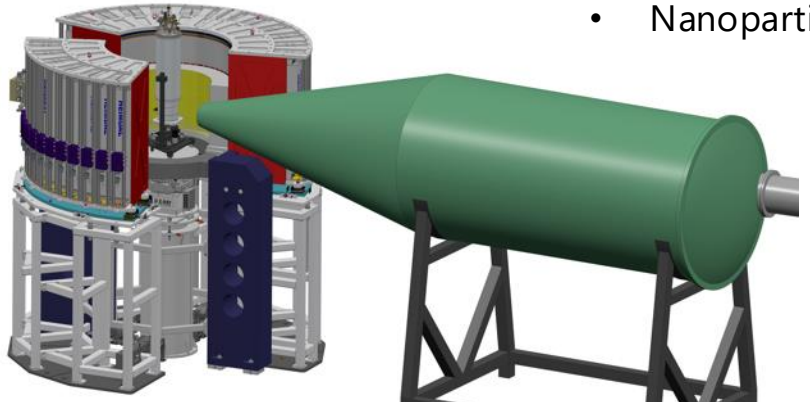


Heavy shutter

T0 chopper

Cold neutron choppers

Diffraction detectors (full scope)



SANS tank (full scope)

Science case

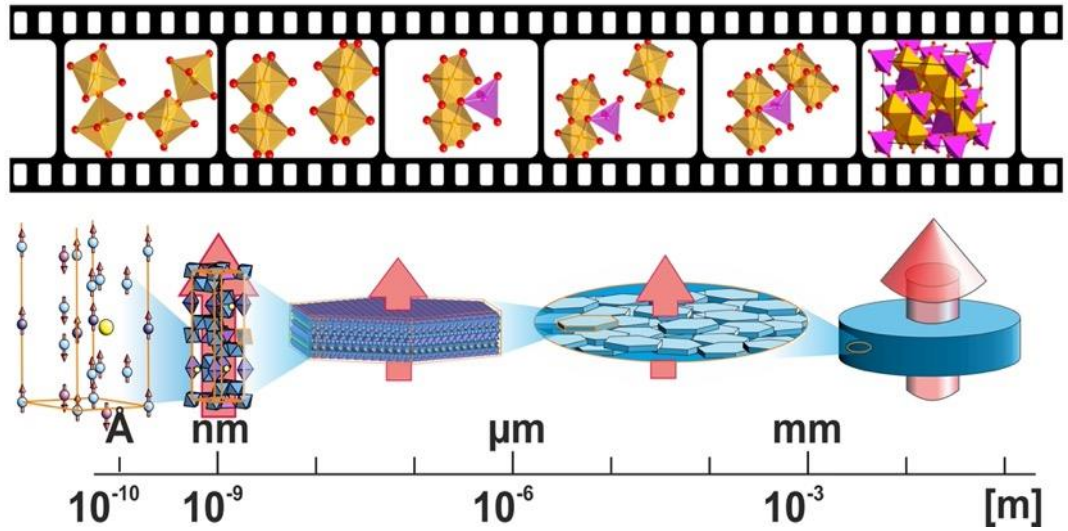
By combining diffraction and SANS HEIMDAL probes an extended q-range of
10^{-3} Å^{-1} < q < 15 Å^{-1}

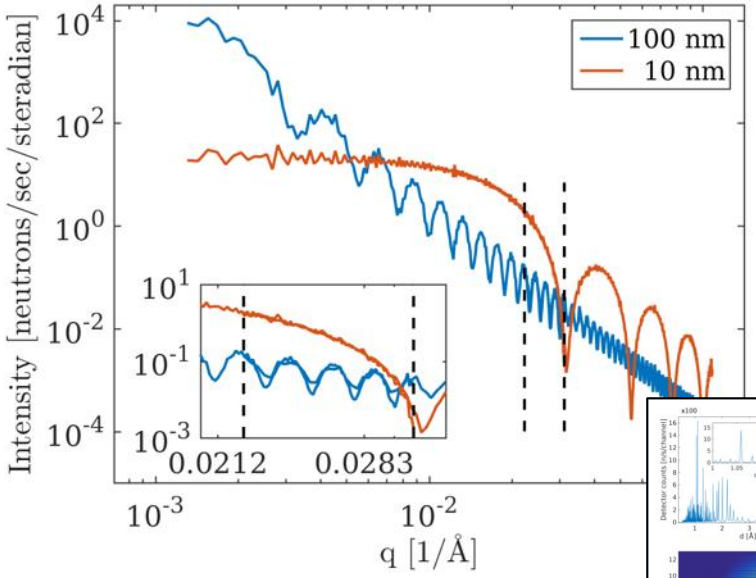
This enables studies of chemical and physical processes as they happen rather than attempts to combine data from several instruments recording almost identical processes.

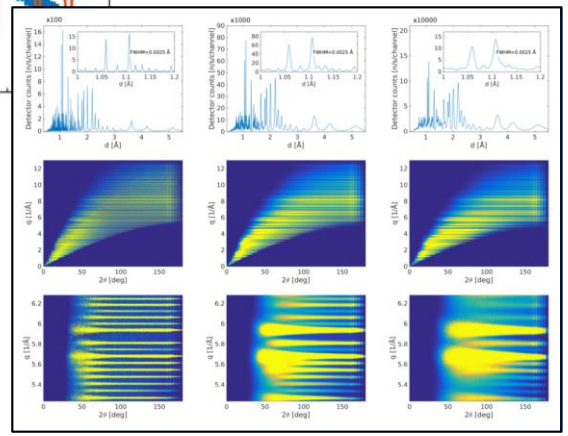
It can also be useful when examining both types of data are required to determine the next step in the experiment.

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

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



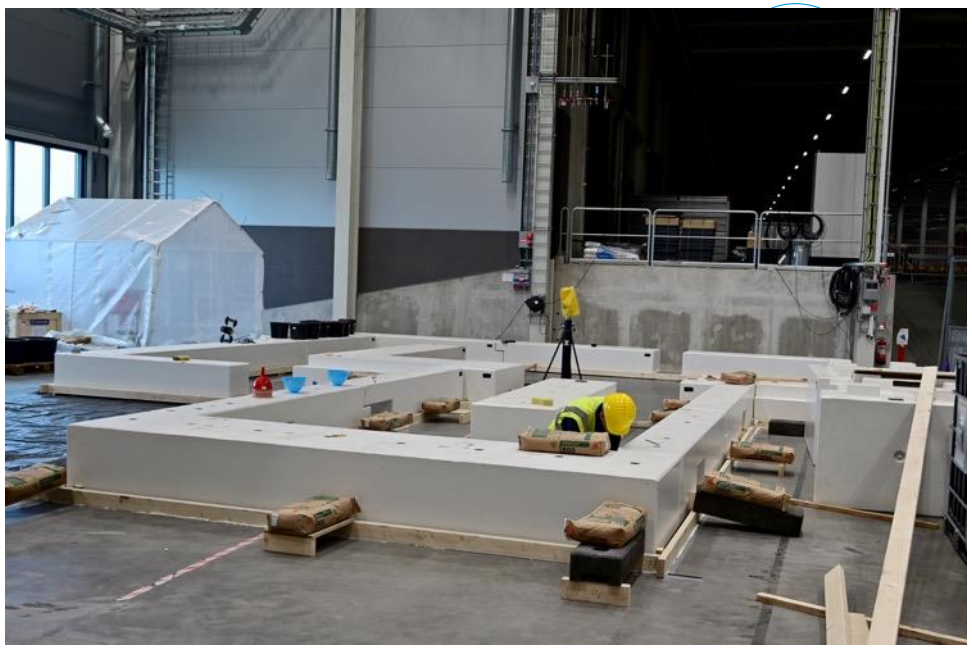




Status

- New IOE has started (Mathieu Leme)
- Instrument data scientist position is open
- Work on TG3 documentation is ongoing
- SubTG3 of the cave is approved
- SubTG3 of the sample stage is approved
- FAT of the cave wall blocks is completed
- FAT out-of-bunker guides is completed
- Jib crane is procured
- T0 chopper manufacturing is ongoing
- Current priority for rescoping in Diffraction & Imaging division

Cave slab installed



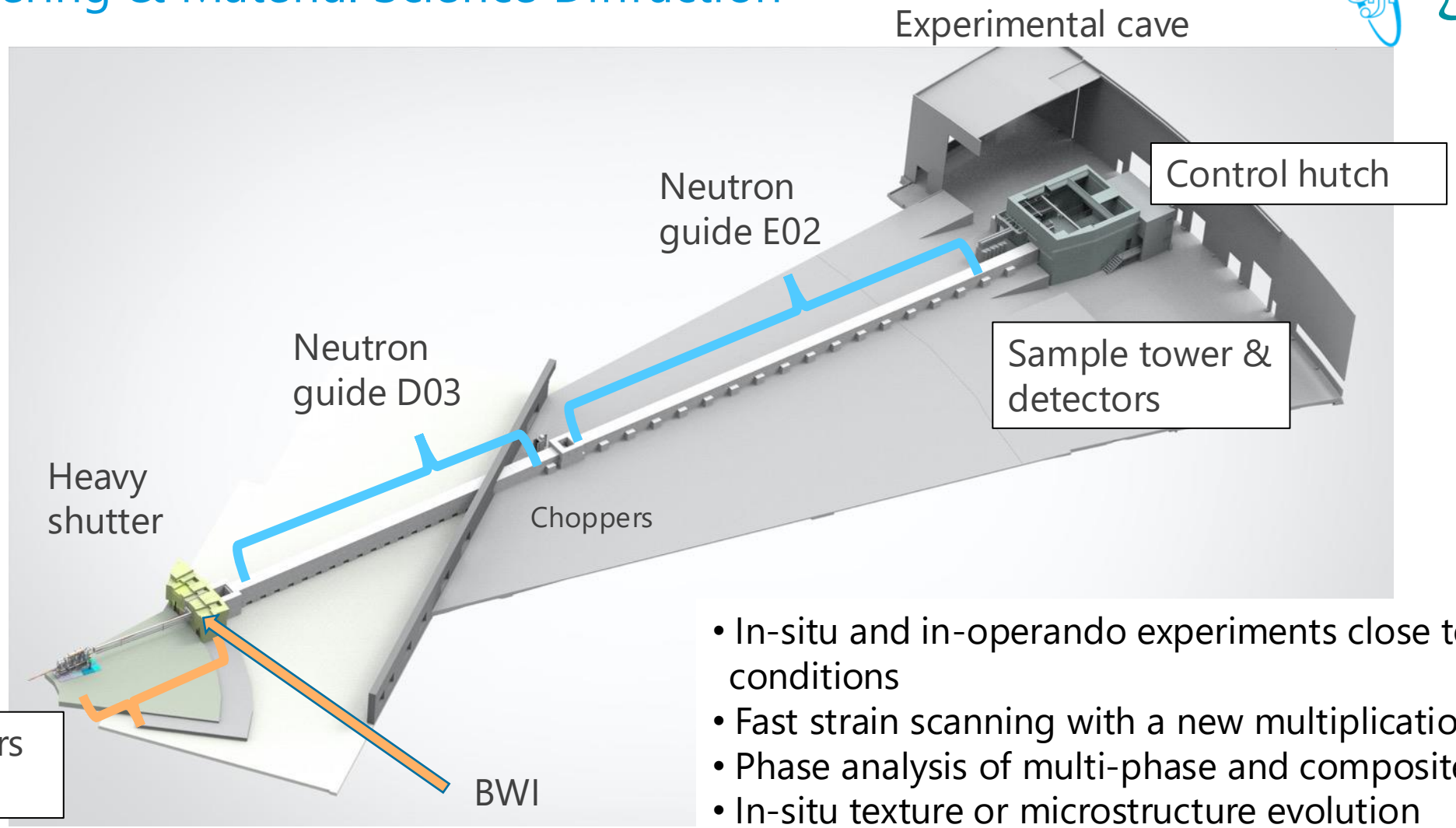
Challenges

- High risk of data reduction software not being ready (mitigation: new IDS, reuse DREAM workflow)
- Collimator Lift & Support final design is being delayed, due to number of interfaces and dependences
- Minimalistic day one scope: 0.8 sr diffraction detector, coverage, no SANS, no end part of cold guide

BEER

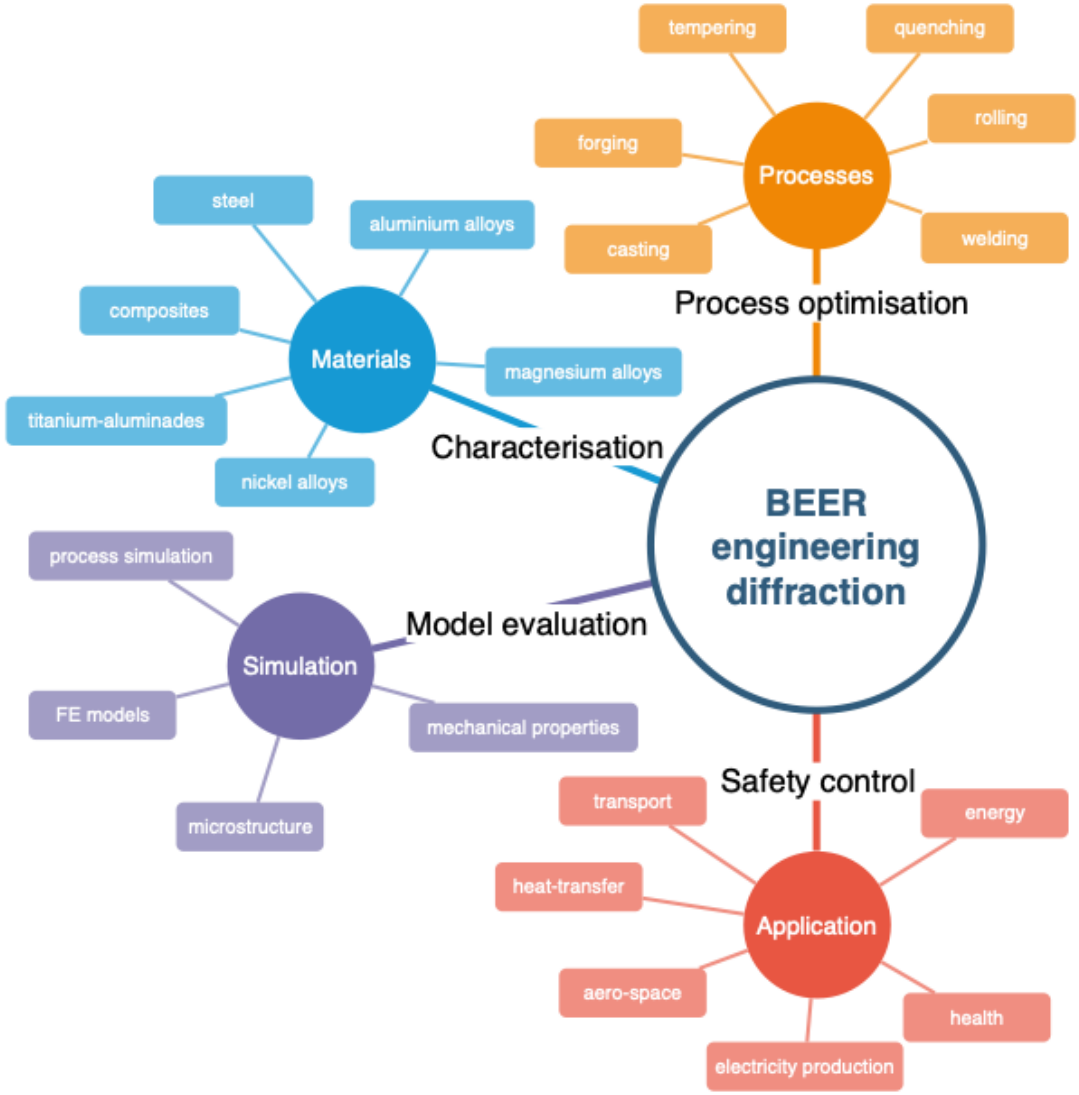
Cold commissioning completed : Q2, 2027

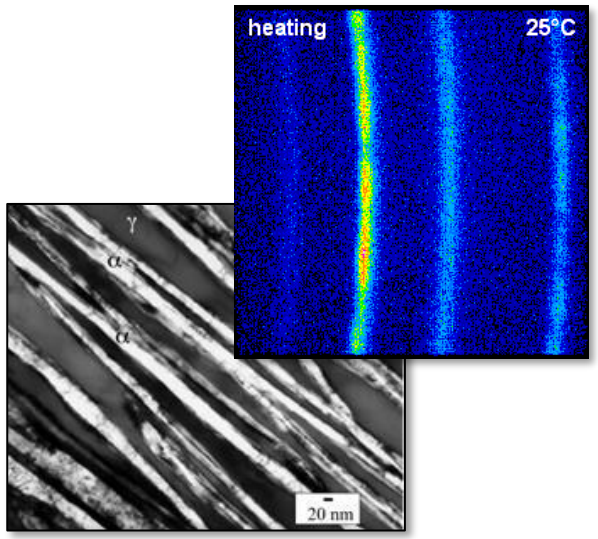
Engineering & Material Science Diffraction



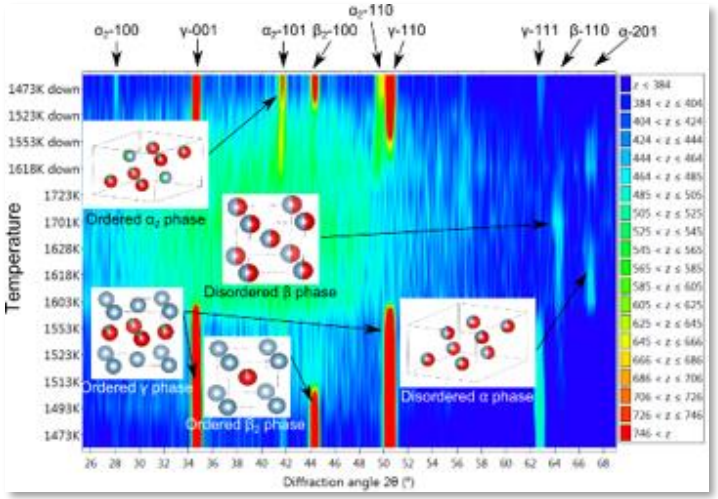
- In-situ and in-operando experiments close to the real conditions
- Fast strain scanning with a new multiplication technique
- Phase analysis of multi-phase and composite materials
- In-situ texture or microstructure evolution
- Multi-scale characterisation
- Long term experiments

Science case

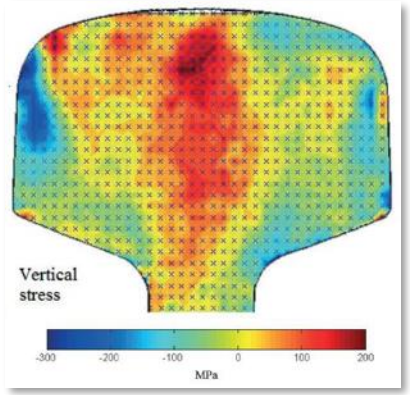




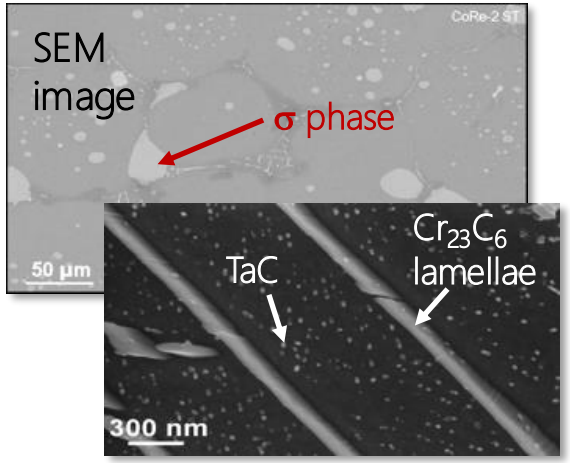
In-situ texture or microstructure evolution:
Re-crystallisation in CoRe alloys
Microstructure of γ-Ti allys



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

- Cave and hutch SATs are completed
- CEP finalization of the installations is ongoing
- Cave and hutch energized
- False-floor and all cabinets installed
- PSS and ICS installations are ongoing
- Neutron guides from the chopper cascade to the cave are fully installed
- Procurement of a dilatometer is ongoing

Cave outside & inside

Challenges

- Radial collimator manipulators FAT is delayed (new MCA requirements)
- Detector 1 FAT is delayed (manufacturing issues)
- Assembly of chopper cascade (Array 1) is delayed (complicated interfaces with many stakeholders)
- Detector support design delayed (lack of resources)

Concluding remarks

- Overall good progress with the instrument projects, but some issues remain
- First three instruments (TBL, ODIN, DREAM) went through TG5/iSRR meeting
- No major roadblocks: those instruments will be ready for hot commissioning
- Readiness for hot commissioning is not the same as readiness for user operations
- There are technical and operational tasks remaining for the instrument teams, even after TG5/SAR
- Post TG5 instruments challenge: engineering resources from partners reassigned, NSS moved resources to the next instruments, but some of the tasks require engineering support
- Robustness of the data visualization & reduction tools have to be improved
- More stability and endurance tests unveil new issues even after passing TG5
- Successful recruitments for MAGiC, ODIN, HEIMDAL

New instrument proposals for DID

HUGIN & MUNIN: Single crystal diffraction
(ESS, PSI, ESS Bilbao, ISIS, Edinburgh University)

BRAGI : Total scattering diffractometer
(PSI, ESS, TUM, ISIS, Duisburg-Essen University, Uppsala University)

MAGNI : Microscopy, Advanced and Grating Neutron Imaging
(PSI, DTU, ESS)

SLEIPNIR: A high-capacity instrument cluster for ESS
(DTU, ESS)

IDUN - Industrial & utilitarian neutron instruments
(DTI, ESS)