Opportunities in Neutron Diffraction and Time-of-Flight Imaging at ESS

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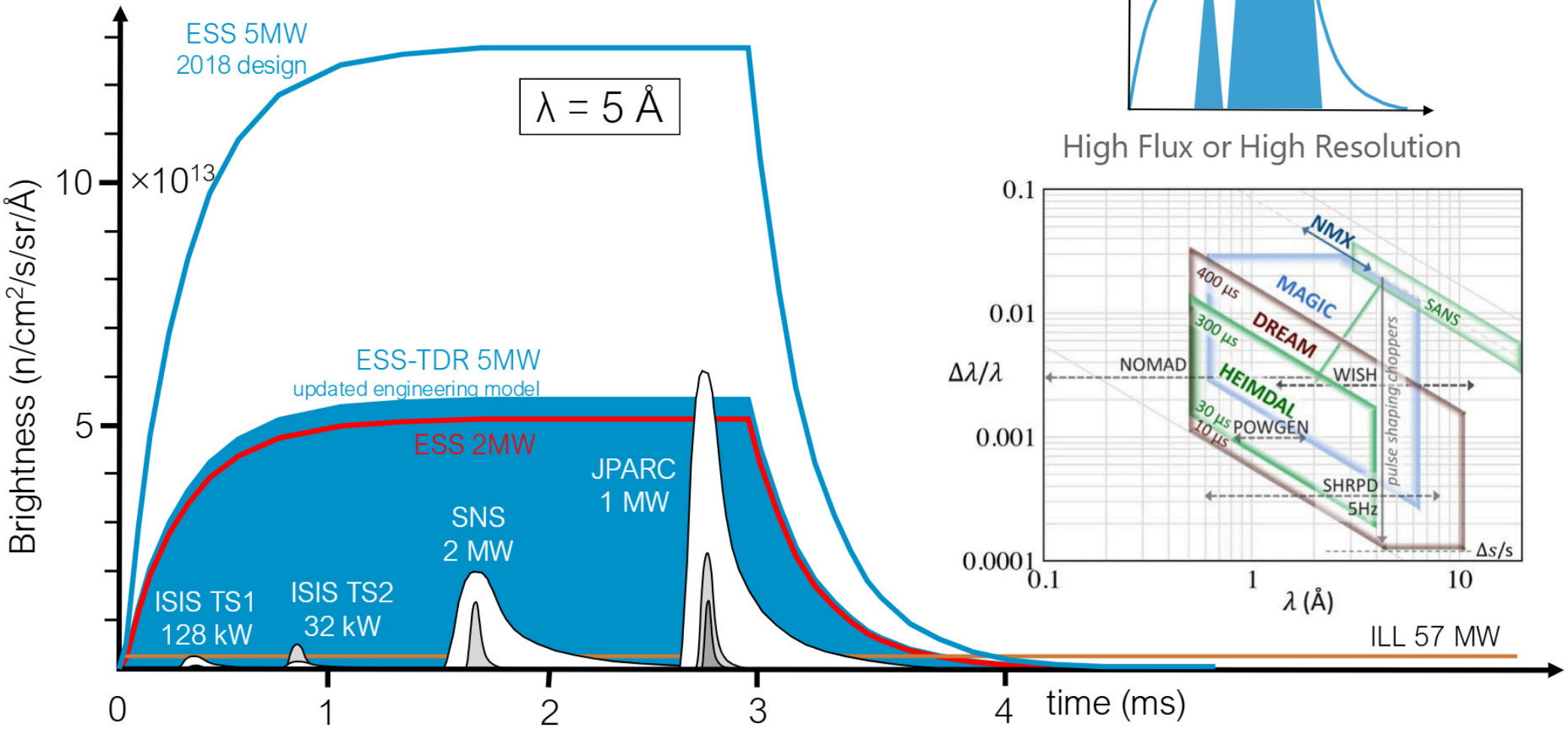
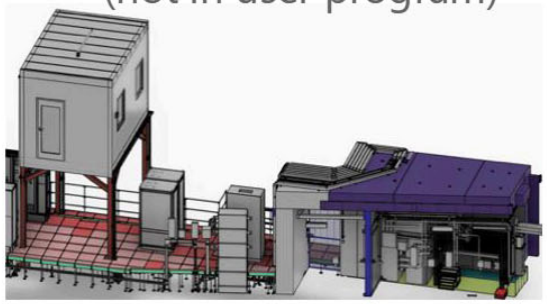
Long-pulse Performance and Flexibility



Possibilities of pulse shaping

High Flux or High Resolution

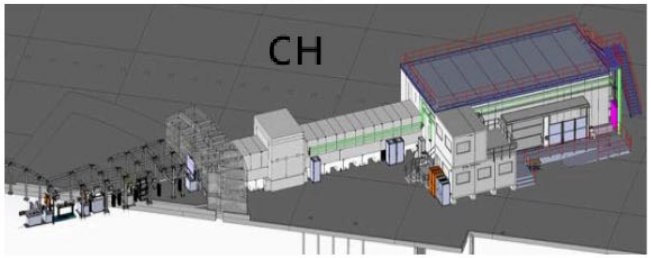
TBL (2025)
Test beamline
(not in user program)



ODIN (2025)
Neutron imaging

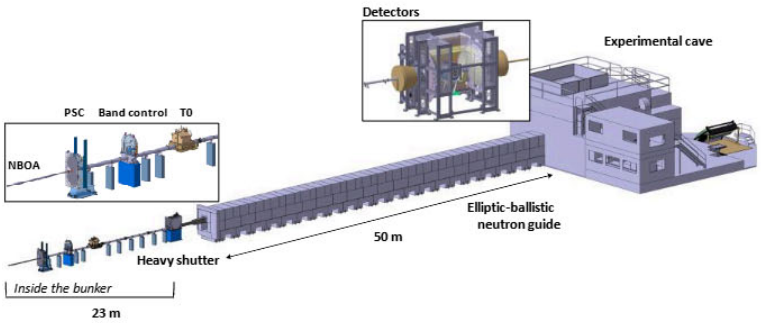
DE

CH



DREAM (2026)
Powder diffractometer

DE FR

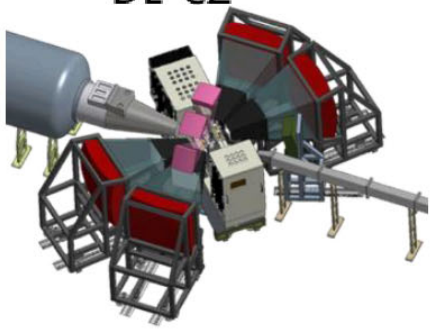


MAGiC (2027)
Polarized diffractometer

DE FR CH

BEER (2027)
Engineering diffractometer

DE CZ



HEIMDAL (2027)
Multiscale diffractometer

DK CH

NO

TBL, 2025

ODIN, 2026

DREAM, 2026

MAGiC, 2027

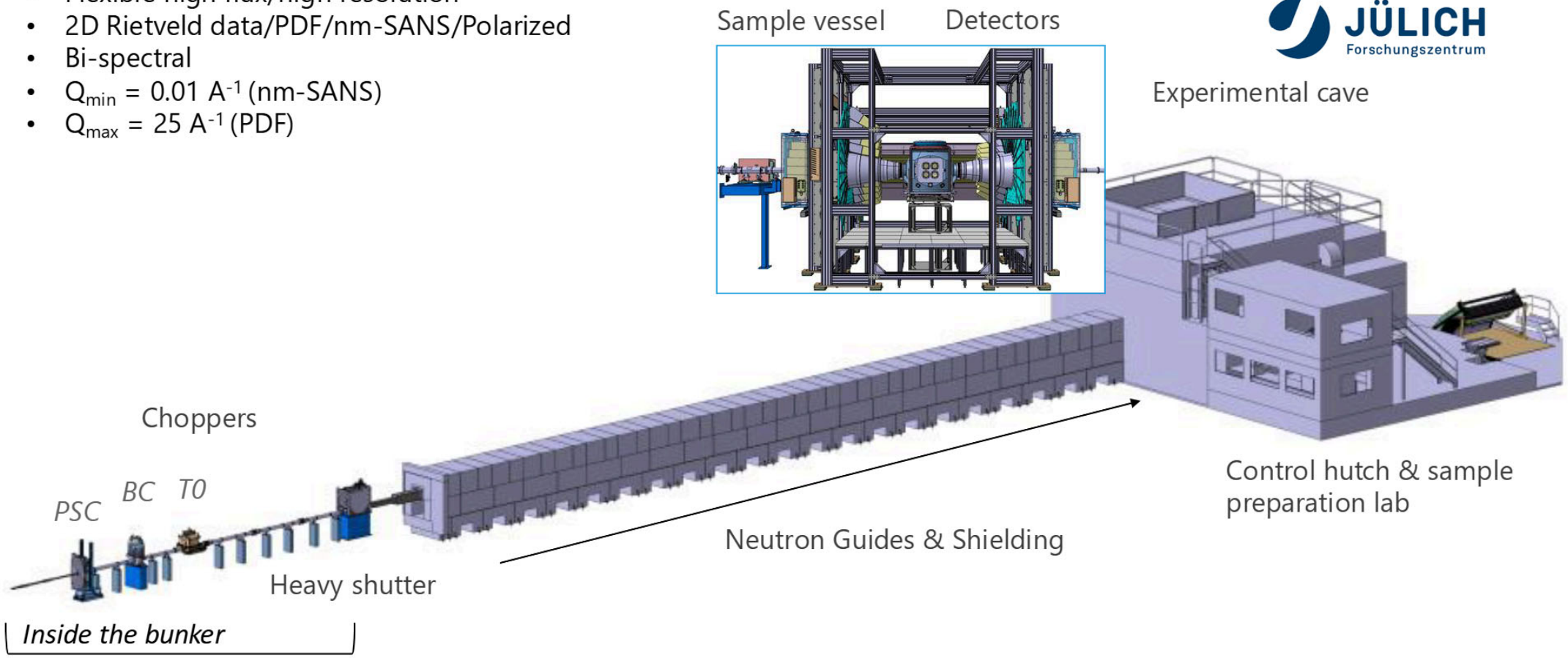
BEER, 2027

HEIMDAL, 2027

DREAM Cold commissioning completed : Q1, 2026

Diffraction Resolved by Energy and Angle Measurements

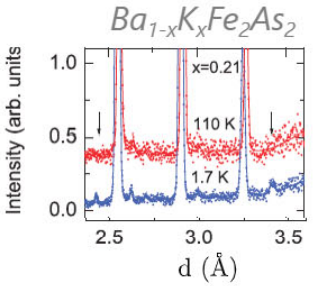
- Powder diffraction
- Flexible high flux/high resolution
- 2D Rietveld data/PDF/nm-SANS/Polarized
- Bi-spectral
- Q_{min} = 0.01 A^{-1} (nm-SANS)
- Q_{max} = 25 A^{-1} (PDF)



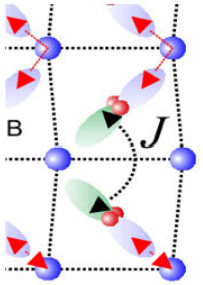


powders
single-crystals
nanoparticles
alloys
liquids

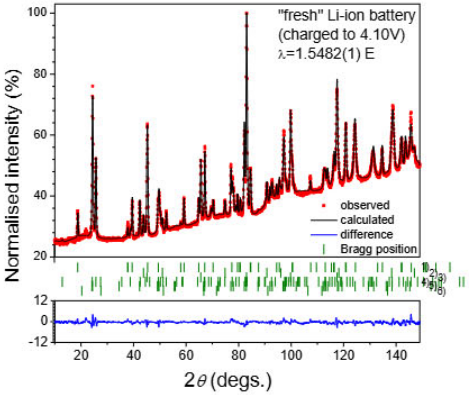
Magnetism



weak moments
phase diagrams of
superconductors
multiferroics



orbital ordering
charge ordering
distortion
magnetic exchange

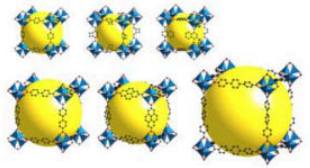


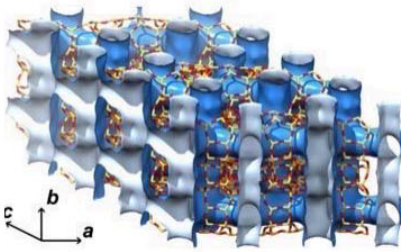
Energy Materials

multiphase
catalysts
in-operando
batteries

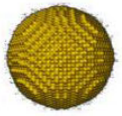
Large Unit Cells

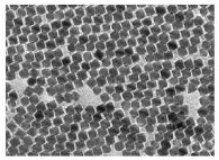
MOFs
thermoelectrics
molecular sieves
H_2 - storage





Nanostructures



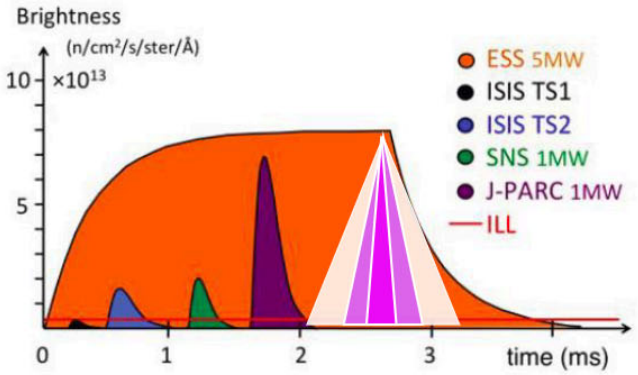


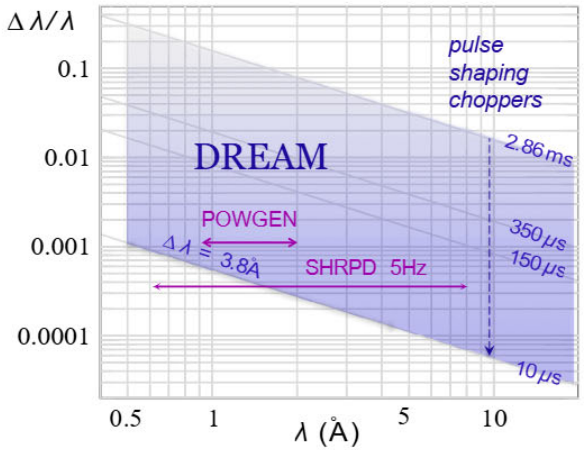
many novel samples come in np
magnetic nanoparticles
core-shell structures
self-assembly
synthesis

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

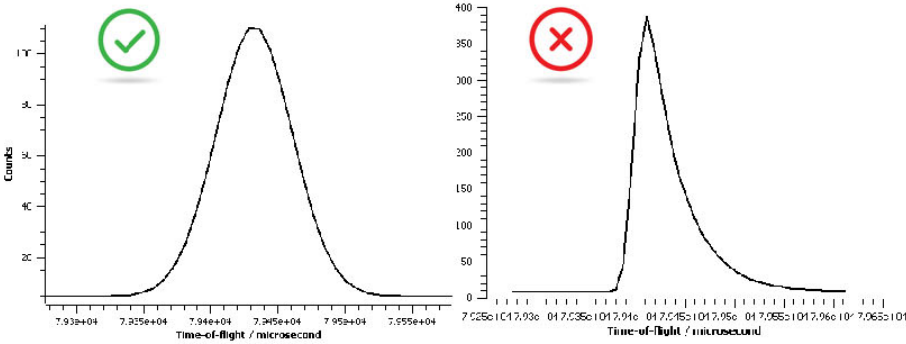
Röntgen Ångström Cluster

Pulse-shaping: high flux & high resolution flexibility

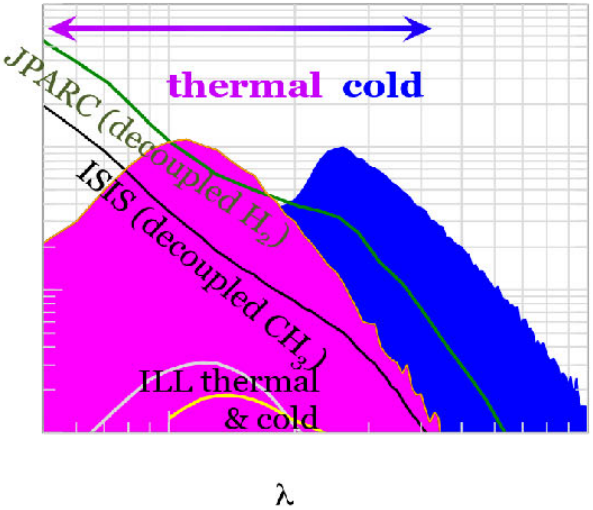




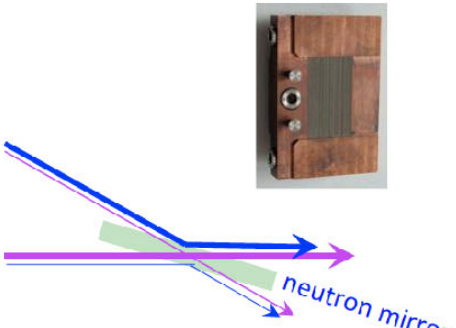
trivial peak profile

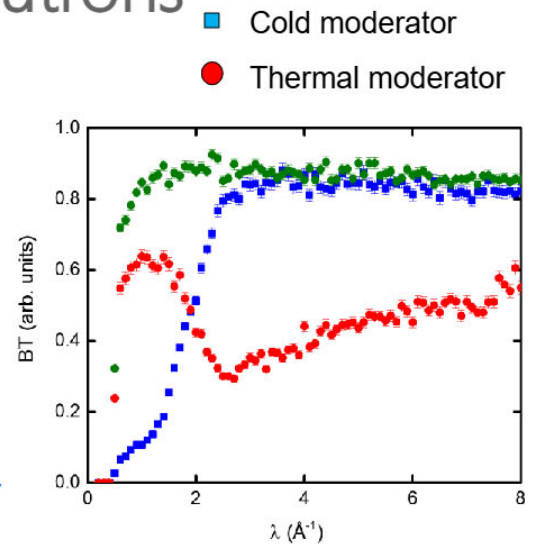


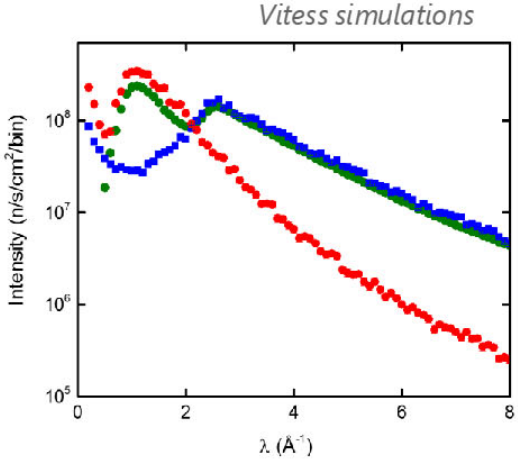
Combination of thermal and cold neutrons



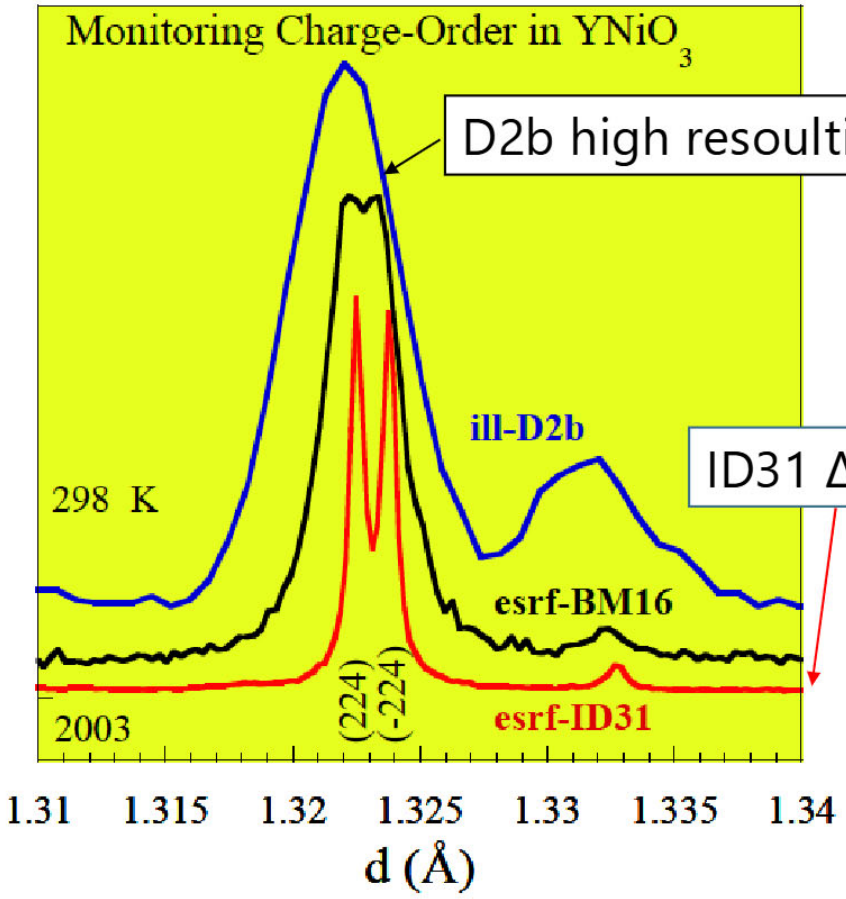
Bi-spectral switch







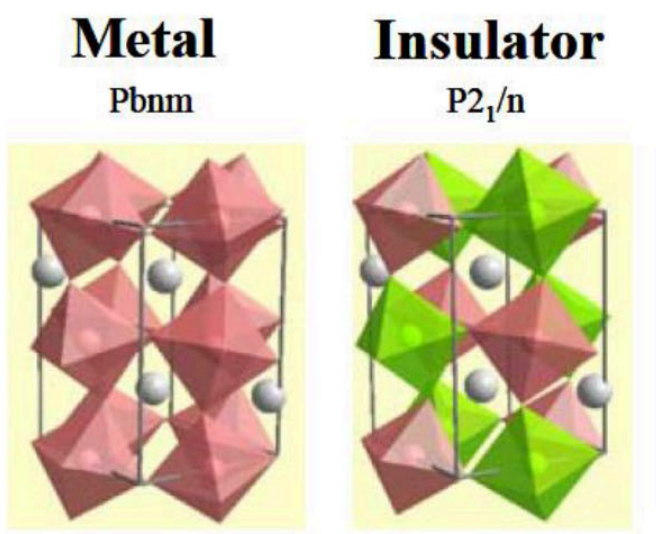
High Resolution: Subtle Phase Transitions



ID31 $\Delta d = 4 \times 10^{-4}$ Å (x-rays)

New ID22: $\Delta d = 0.8 \times 10^{-4}$ Å

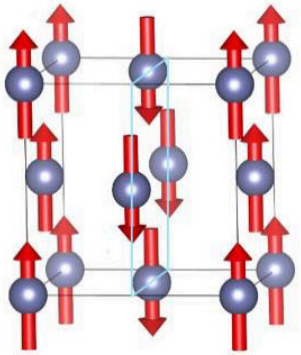
Symmetry breaking in nickelate



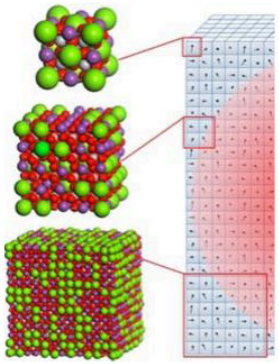
DREAM: $\Delta d = 3.0 \times 10^{-4}$ Å
in dedicated backscattering detector

The new world record in high resolution neutron diffraction during the first days of operation, even with a low flux

Combination of
thermal & cold neutrons



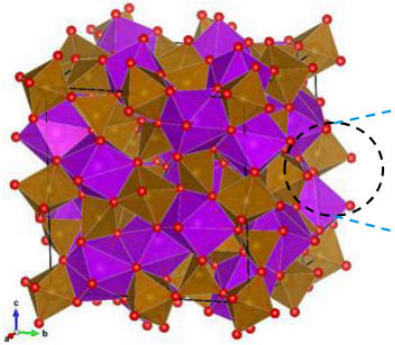
magnetism
(cold neutrons)



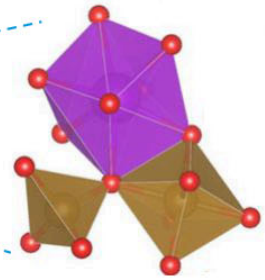
local structure
(thermal neutrons)

small samples
(thermal + cold neutrons)

Wide Q-range for
powder diffraction:
0.01 – 25 $Å^{-1}$



crystal structure
(highest resolution)



local structure
(PDF)

morphology
(nm-SANS)

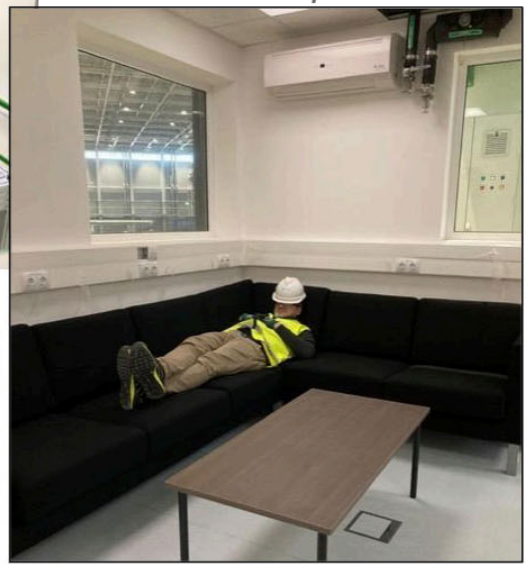
one shot!

Installation completed
Integrated tests ongoing

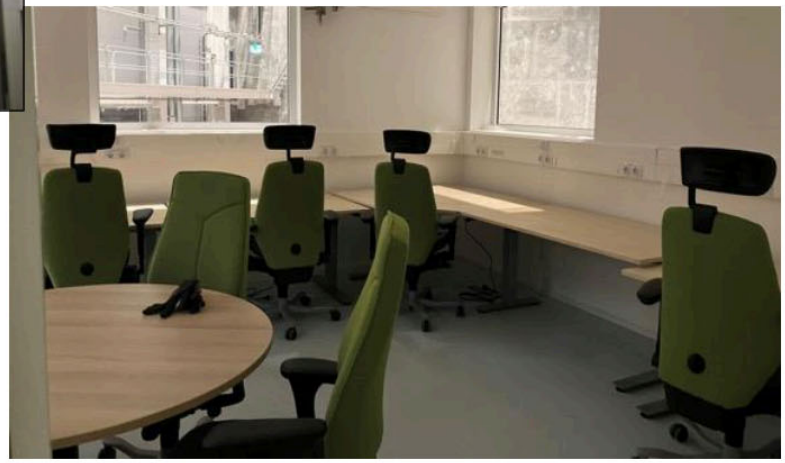
Mantle detector installation

Sample vessel

Couch Site Acceptance Tests



Control room



Choppers

DREAM

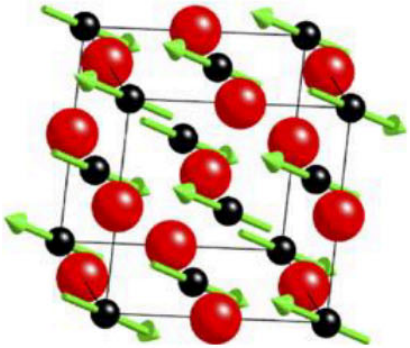
First Science

- **Pulse-shaping (flux vs ΔQ resolution)**
- **The highest resolution in backscattering**
- Pair-distribution function with Q_{max} = 25A^{-1}
- nm-SANS down to 0.01A^{-1} + cold neutron polarization

Transition metal monoxides
Zeolites and MOFs
Electrode materials in pristine state
Perovskites and complex oxides
Small samples with cation disorder
Hydrogen-containing samples
Energy materials

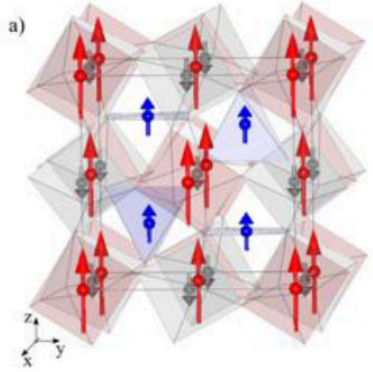
Mix of new science and "classic diffraction" materials

Transition metal oxides NiO



E. Ressouche et al., Physica B: (2006).

Double-double perovskites $CaCuFeReO_6$

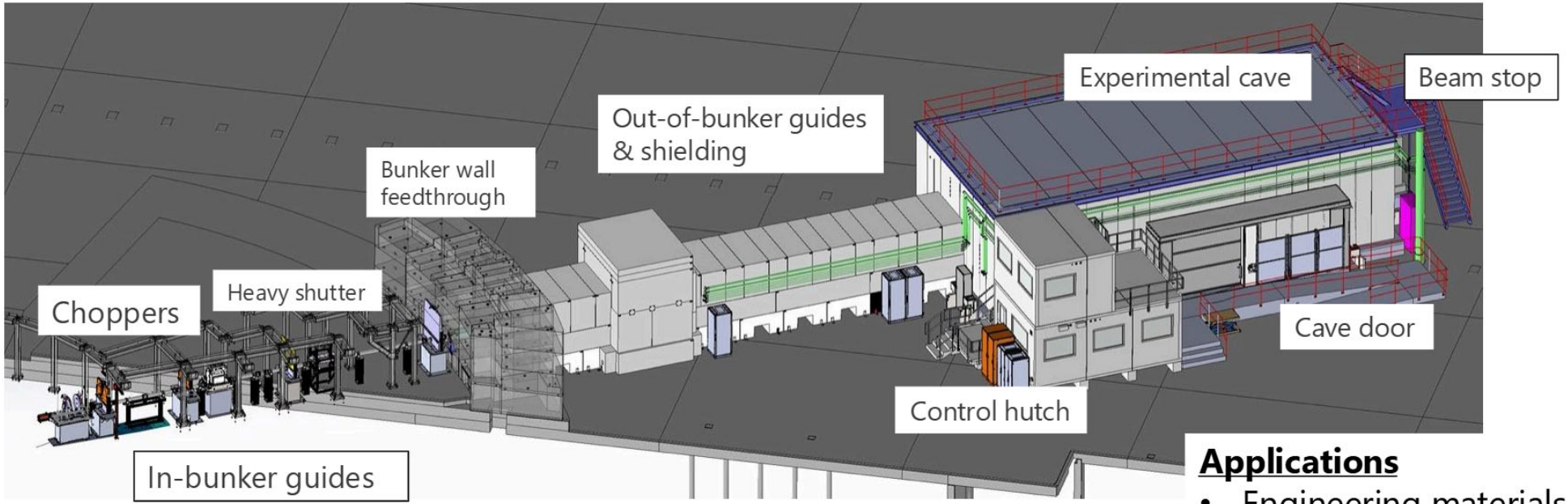


E. Solana-Madruga et al. Angew. Chem., 61 9497 (2022)

ODIN

Cold commissioning completed : Q4, 2025

Optical and Diffraction Imaging with Neutrons



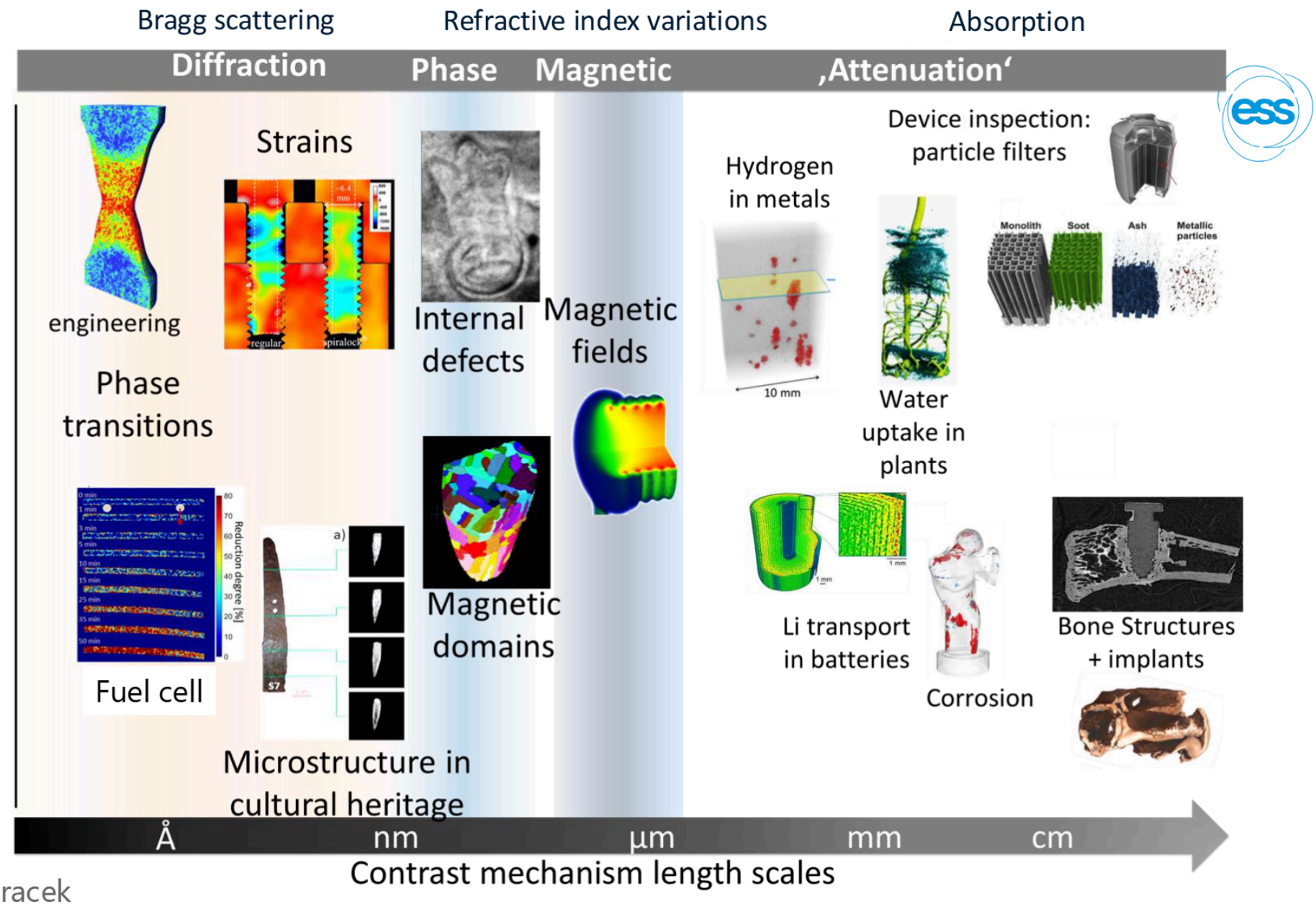
- Bi-spectral extraction
- Direct line-of-sight (T0 chopper)
- Tailored wavelength resolution
- Variety of imaging techniques, including x-rays (full scope)

- 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

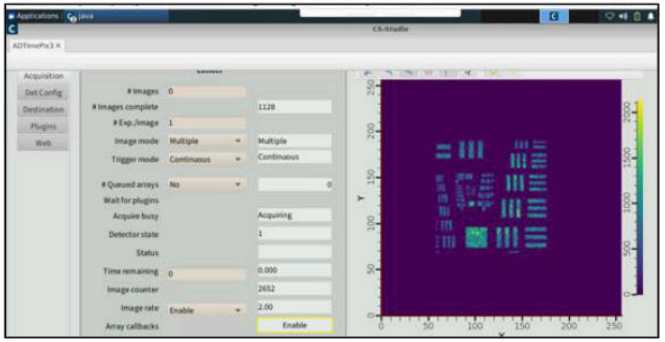
Applications



Slide by R. Woracek

Installation completed
Integrated tests completed

TPX3 image



Cave and hutch

Cave interior

Slit system

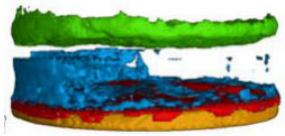
Motion stage

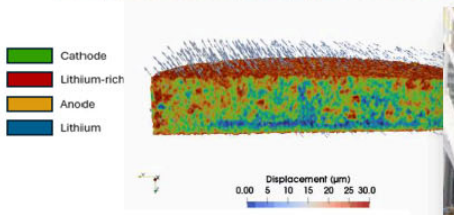
ODIN – 1st Science Strategy

Active involvement in in-kind partners/STAP/ In-house collaborations

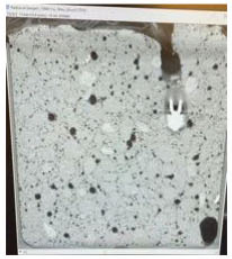
Hydrogen embrittlement
- ReHeart (2 Postdocs, KTH+LU/ESS)
- ISOTOPE (1PhD, KTH, defending soon)
- ILL-ESS-KTH PhD (starting 2026)

Solid State Batteries
- ANISSA (1 Postdoc, 3PhDs, UU, LTH, HZB, UM)



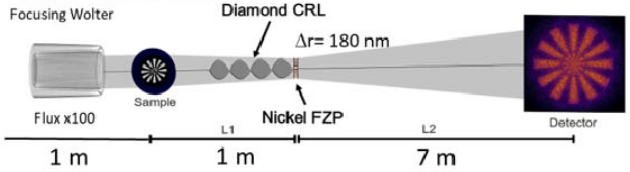


Freezing mortar
- Malmo, LTH (ongoing, MS project LTH)

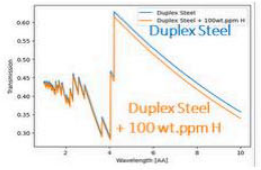


Thermography/Sand Batteries
- LTH (ongoing, LU postdoc project)

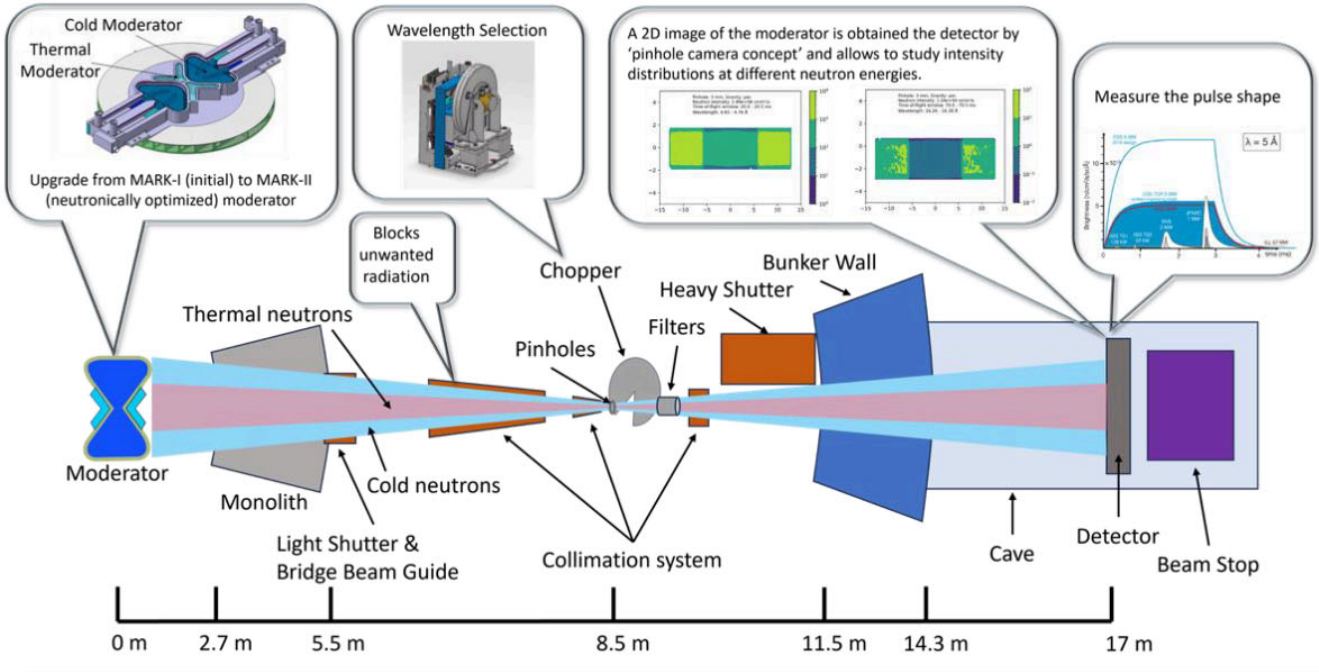
Wolter optics (1st step towards a neutron microscope)
- 1 PhD,1 postdoc at DTU (starting 2026)



Improving quantitative neutron transmission interpretation
- Collaboration with ESS Spallation Physics Group & DMSC

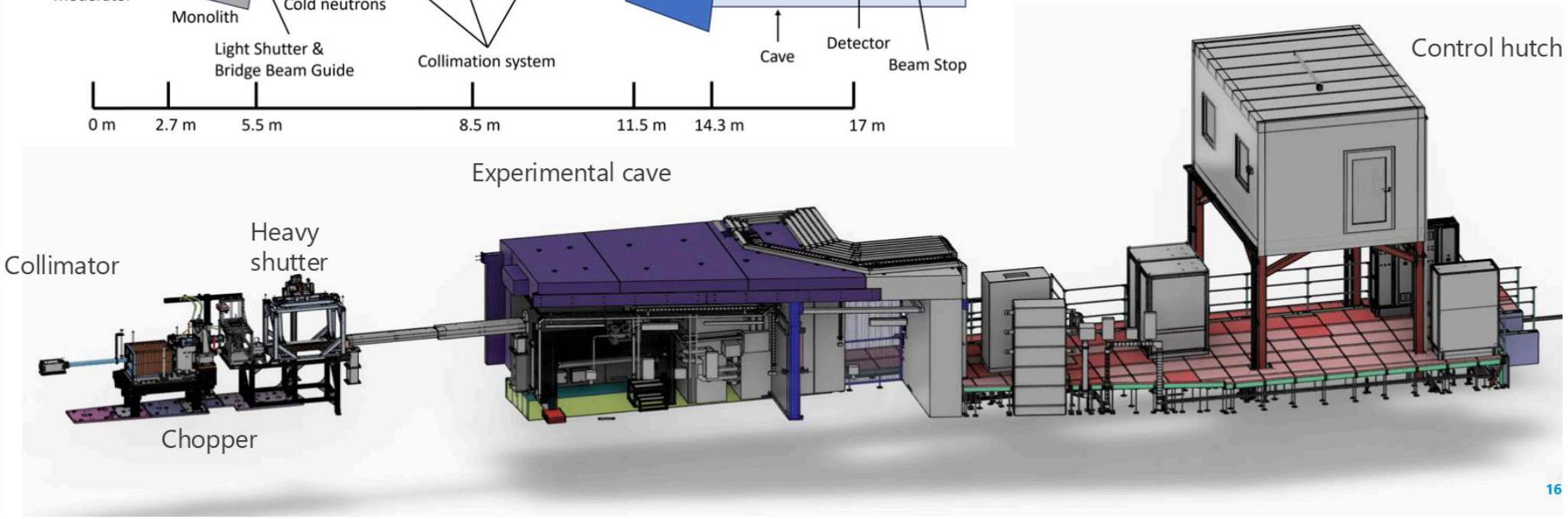


TBL Cold commissioning completed



ESS Beam-on-Target Milestone:

- Measured reasonable thermal and cold neutron spectra on the Test Beam Line
- Completed a first estimation of the yield of thermal and cold neutrons per proton as measured on the Test Beam Line



Installation completed
Integrated tests completed
Safety readiness ongoing

Control room with stairs!

Instrument safety readiness review

In-bunker view

Test Beamline

Early Science Ideas – beyond the source characterization

Idea 1

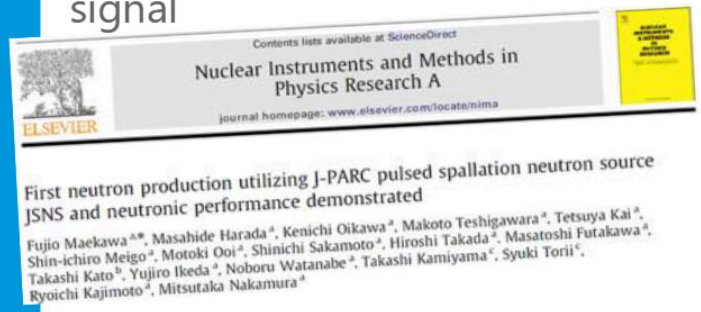
Validation of unique neutronics design features of ESS

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

- **potential collaborators:**

other neutron sources

- **requirements from DMSC:** 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[d]

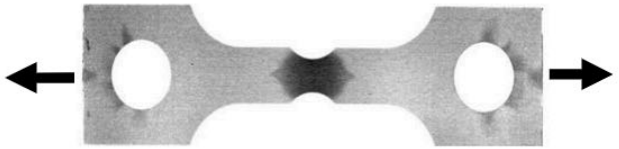
Idea 2

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



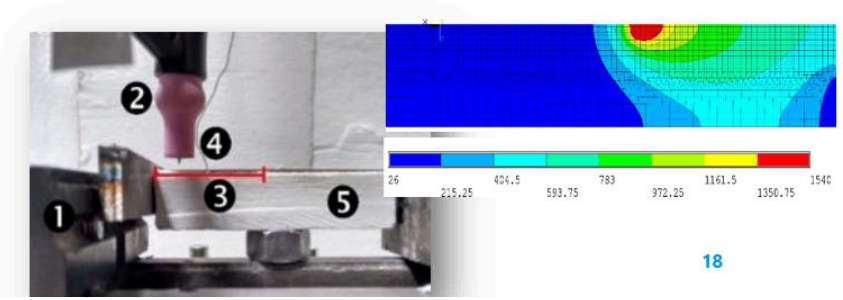
Idea 3

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

- **current collaborators:** BAM (Berlin), HZB

- **potential collaborators:** Industrial network within Sweden

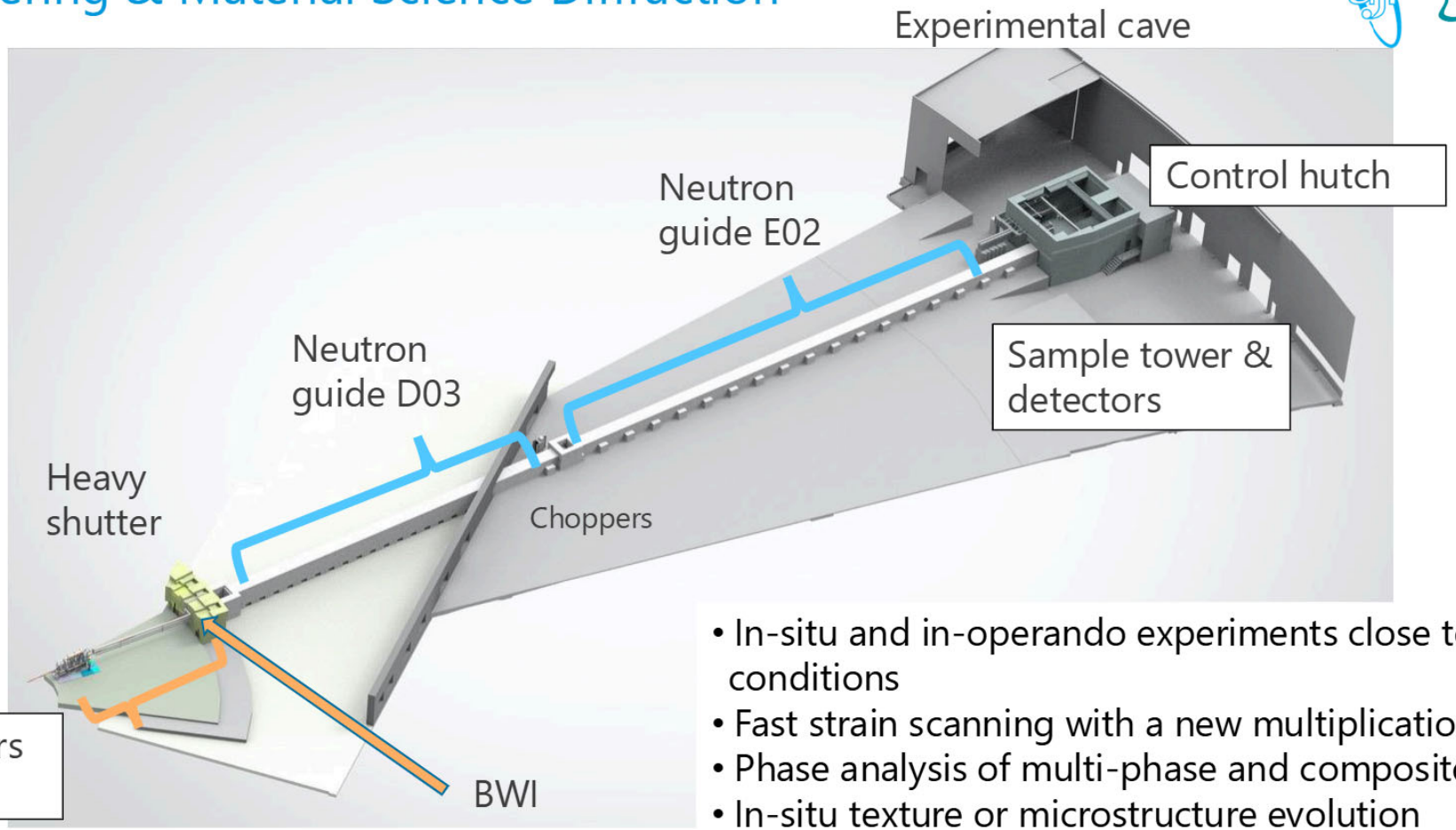
- **requirements from SE/DMSC/external developmental needs:** Welding device available and control/DAQ linked



BEER

Cold commissioning completed : Q1, 2027

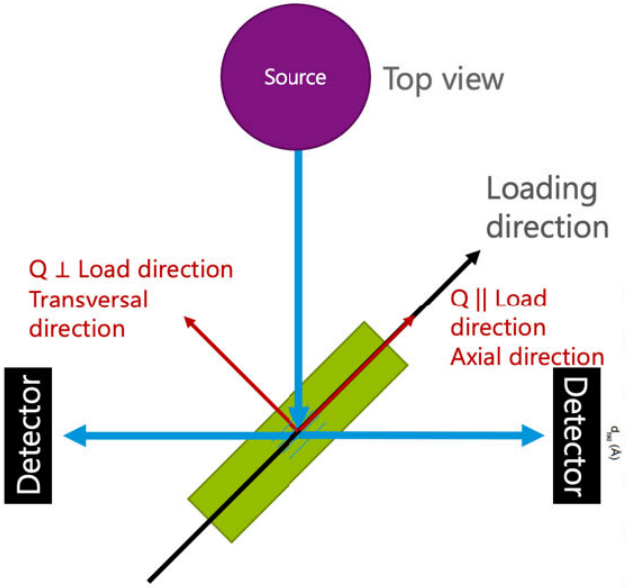
Engineering & Material Science Diffraction

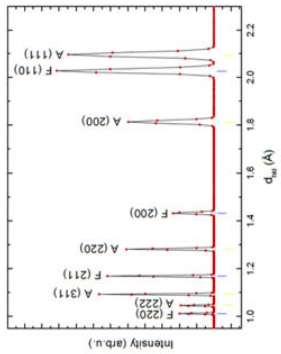


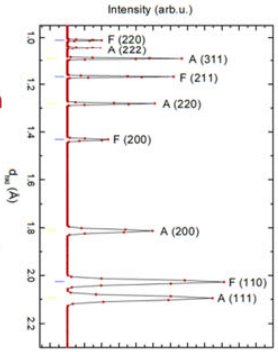
- In-situ and in-operando experiments close to the real conditions
- Fast strain scanning with a new multiplication technique
- Phase analysis of multi-phase and composite materials
- In-situ texture or microstructure evolution
- Multi-scale characterisation
- Long term experiments

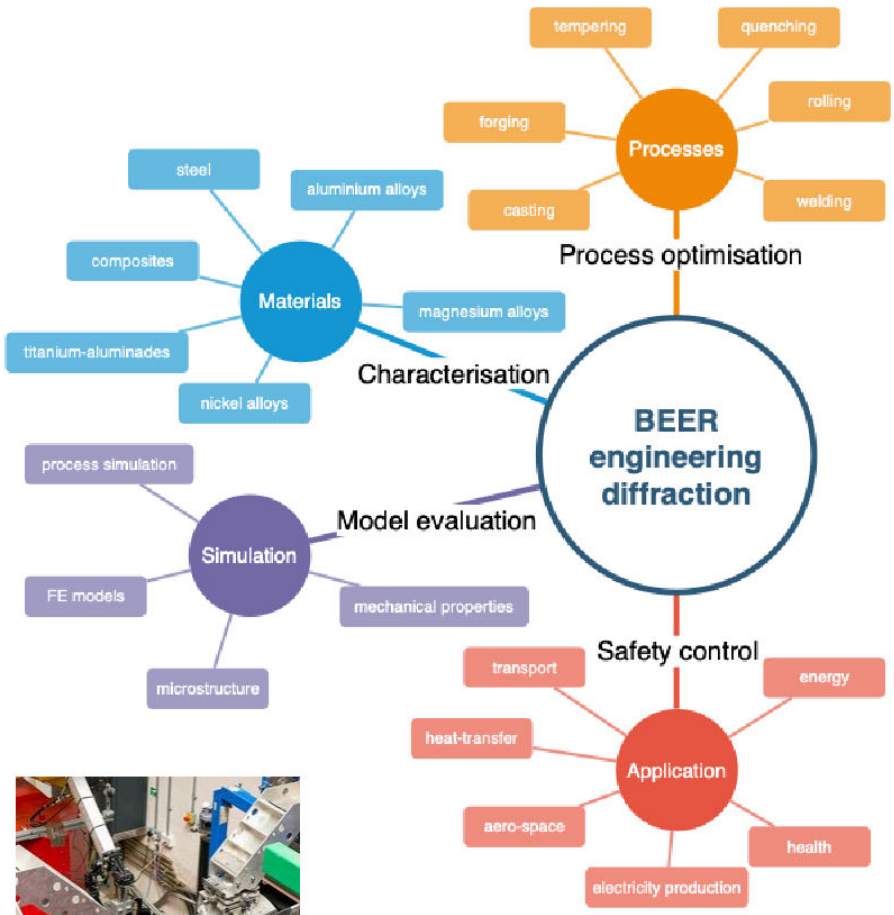
ToF Engineering diffraction

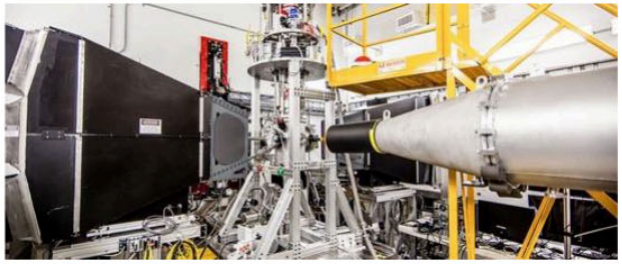
- Incident beam and 2 detectors at ±90°
- Load axis along 45° with respect to the incident beam
- Full pattern at once, no need to move the detector
- Measurement of two perpendicular components at once:
  - Axial direction: Q || load axis
  - Transversal direction: Q ⊥ load axis











Courtesy of P. Beran

Biggest Cave at ESS !

Neutron guides & shielding

Hutch

Collimators

Hexapod

Detector base plates

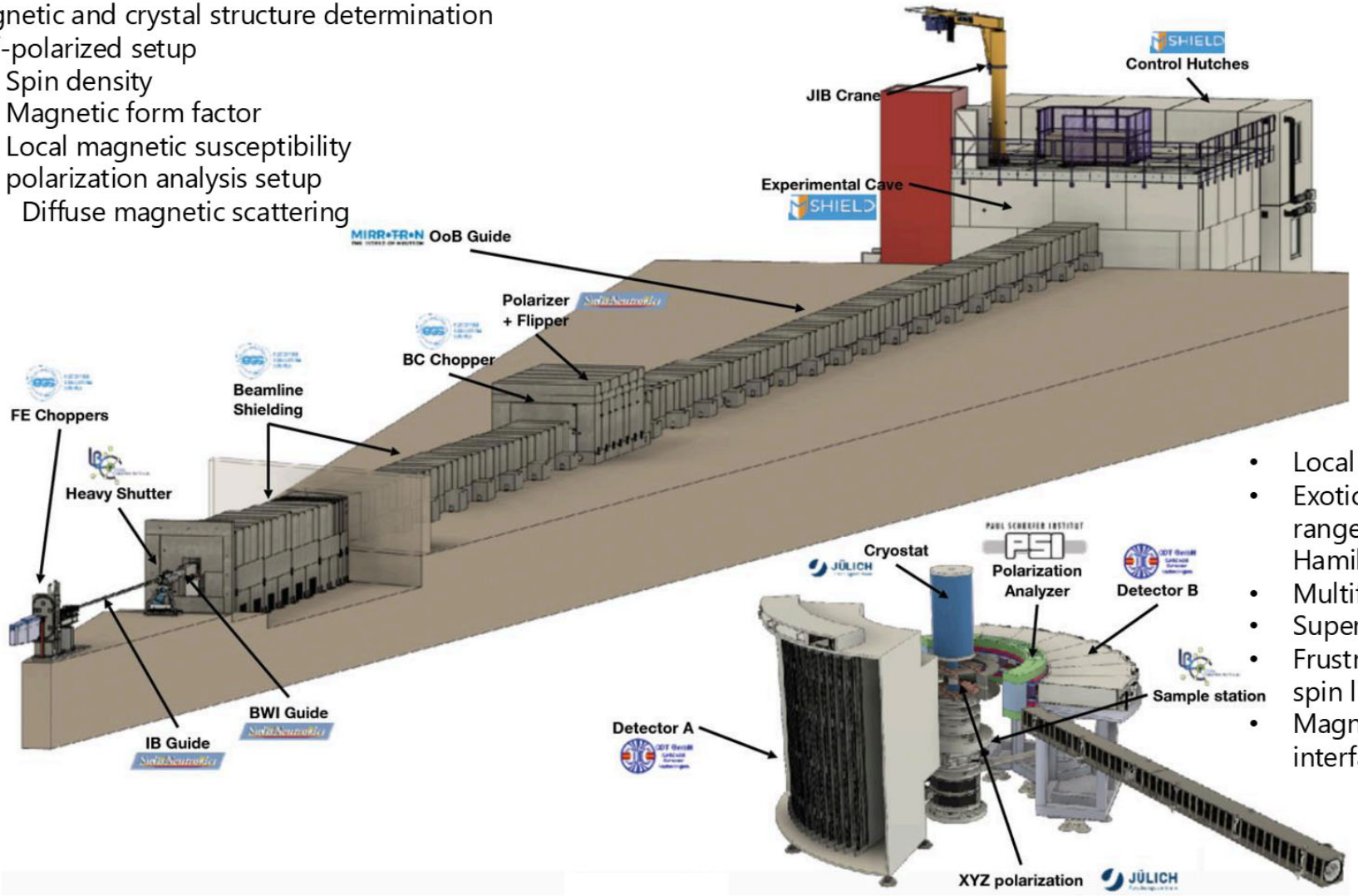
Fast chopper disks

MAGiC Cold commissioning completed: Q2, 2027

Polarised Diffractometer for Magnetism

Magnetic and crystal structure determination
Half-polarized setup
- Spin density
- Magnetic form factor
- Local magnetic susceptibility

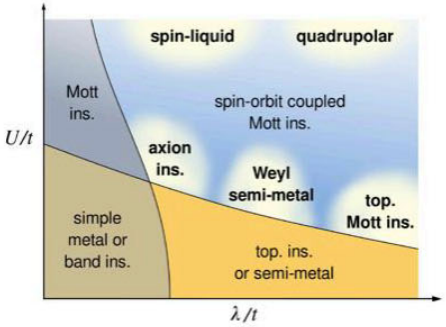
XYZ polarization analysis setup
- Diffuse magnetic scattering



- 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

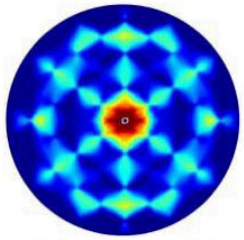
W. Witczak-Krempa et al
Ann Revi Cond Matt Phys 5 57 2014



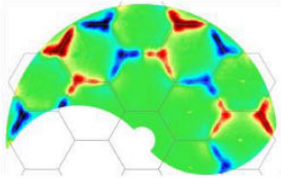
MAGIC proposal

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

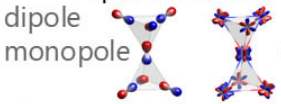
Frustrated magnetism spin-liquid



Spin-Ice model



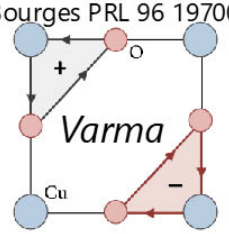
Chirality
PRX 12 021029 202 2



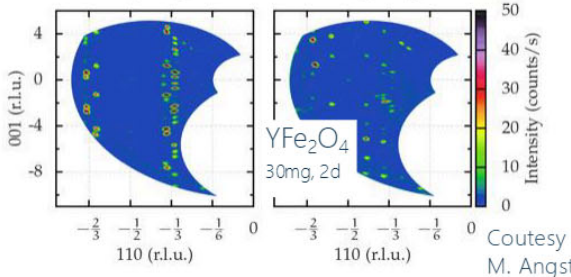
Fennell, Science 2009
Sibille, Nature Physics 2020

Superconductivity

Loop current order
P. Bourges PRL 96 197001 (2006)



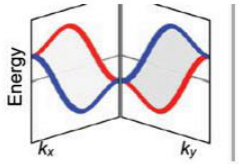
Spin and charge order



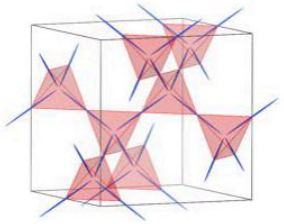
Coutesy of M. Angst

Spintronics

PRX 12 040501 2022

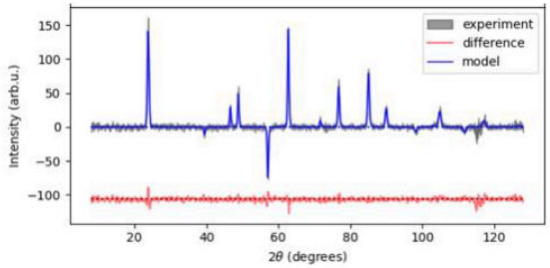


Spin anisotropies



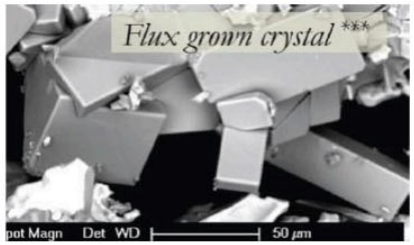
Iurii Kibalin & Arsen Gukasov
PRB 2019

from powders



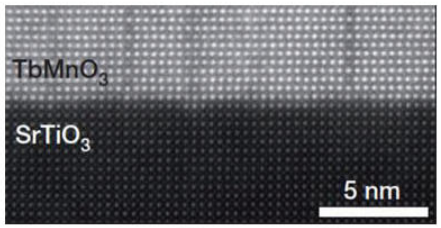
small moments S=1/2

small crystals

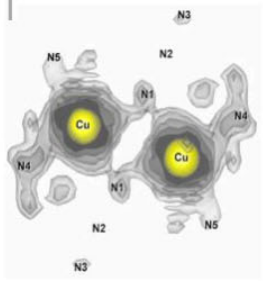


M. Valldor

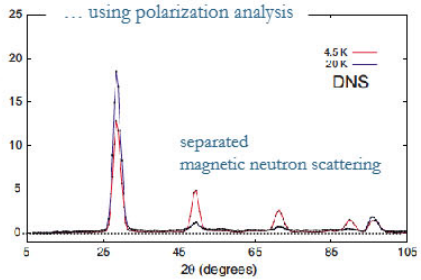
small structures

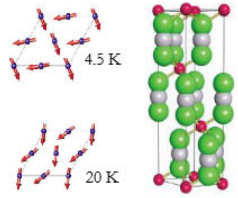


S. Farokhipoor et al
Nature Materials 515 , 379 (2015)



Molecular magnets





MnNCN

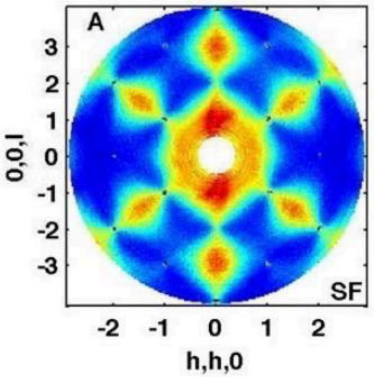
Background suppression

hydrogeneous materials
Li, Na- batteries

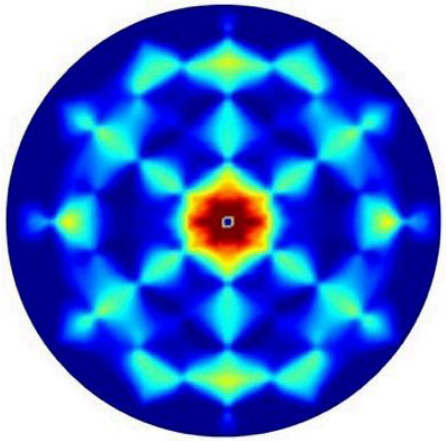
Courtesy of W. Schweika

$Ho_2Ti_2O_7$ Single-crystal

Data: D7

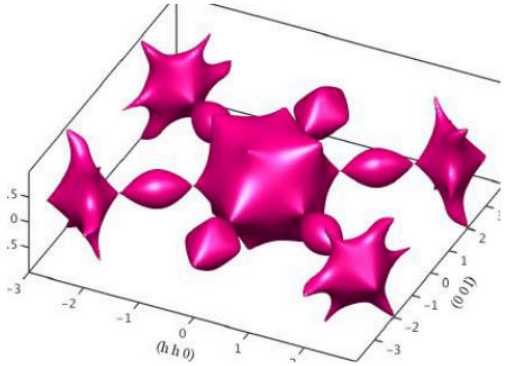


Simulations: MAGiC



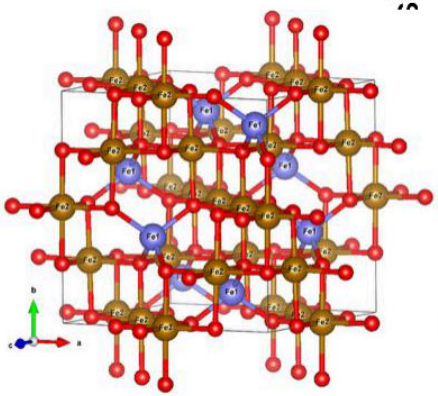
T. Fennell et al., 2009

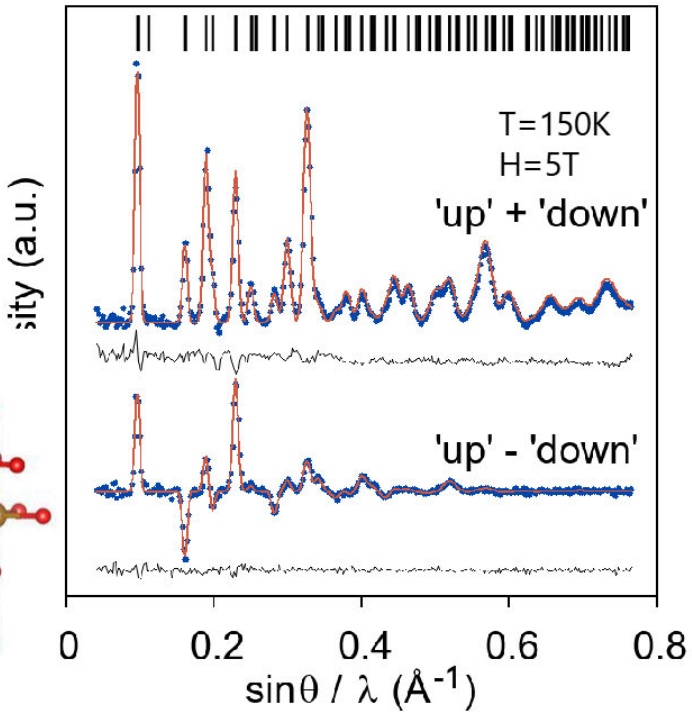
Spin-ice



Fe_3O_4 powder

CrysPy





moment of Fe_1 is antiparallel to magnetic field

Fe_1 = -4.03(1) μ_B

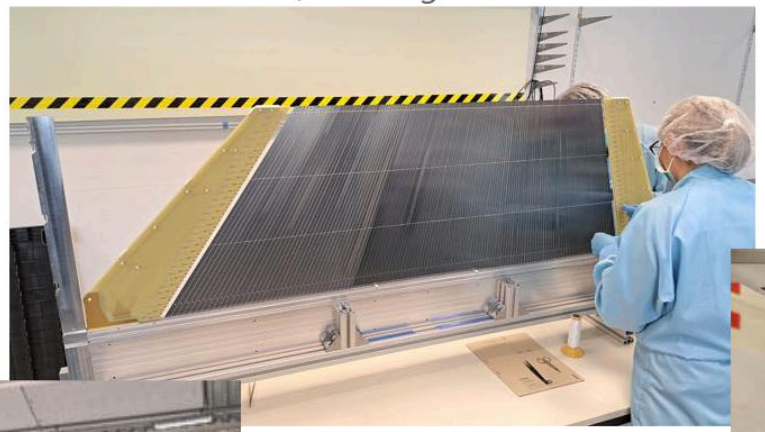
moment of Fe_2 is along magnetic field

Fe_2 = 3.95(1) μ_B

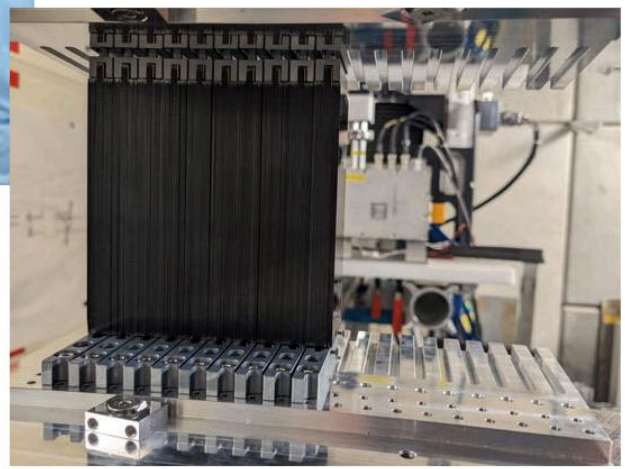
I. A. Kibalin et al, 2019

Manufactured in-Bunker Vacuum Housing

Detector A manufacturing



Analyzer prototype



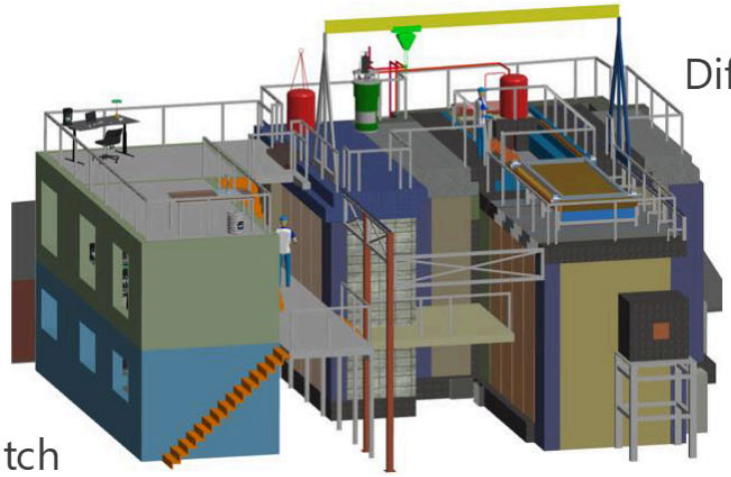
Cave and control hutch

Detector B

HEIMDAL

Cold commissioning completed : Q2, 2027

Hybrid Diffractometer: Combined Diffraction and SANS and Imaging

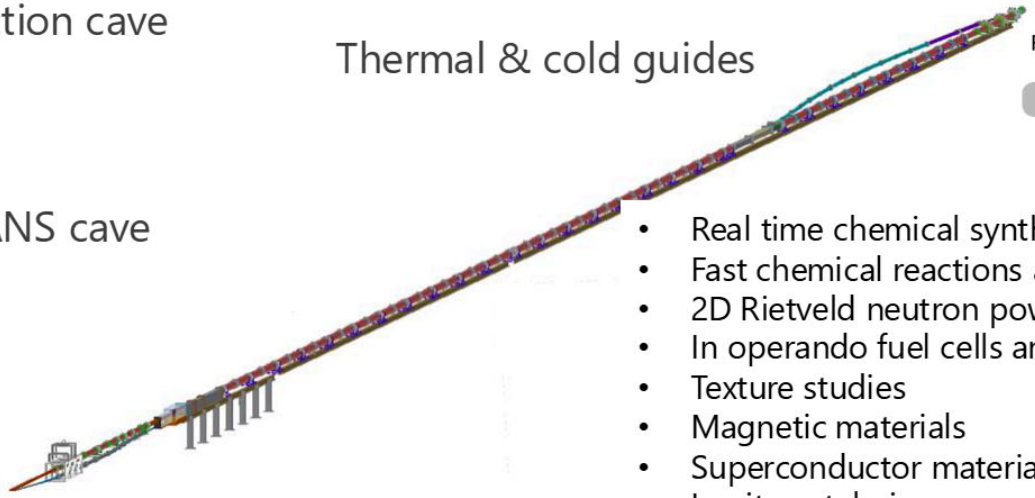


Diffraction cave

SANS cave

Hutch

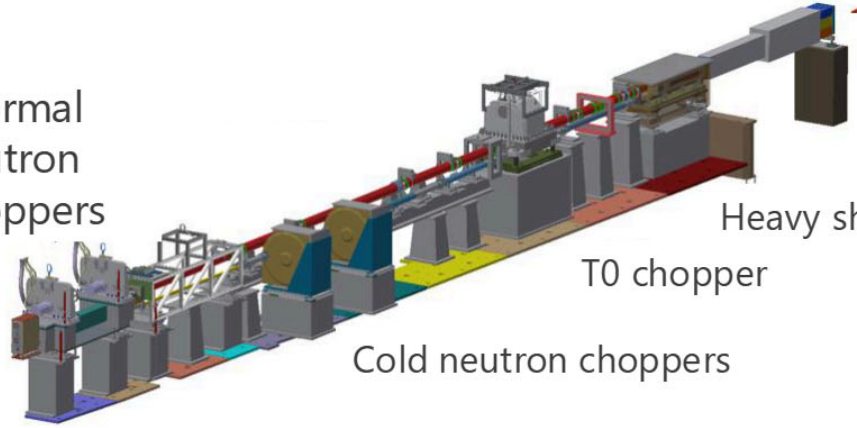
Thermal & cold guides



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

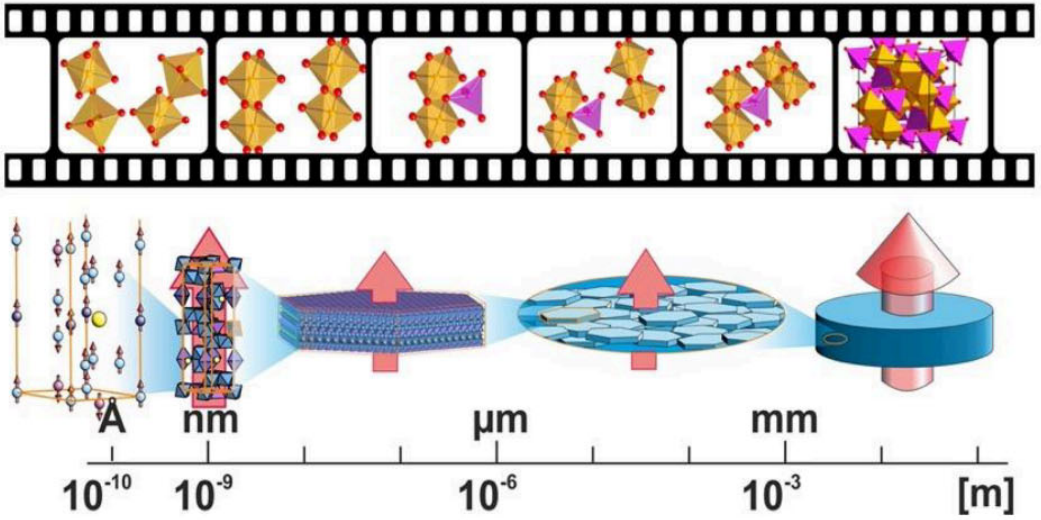
T0 chopper

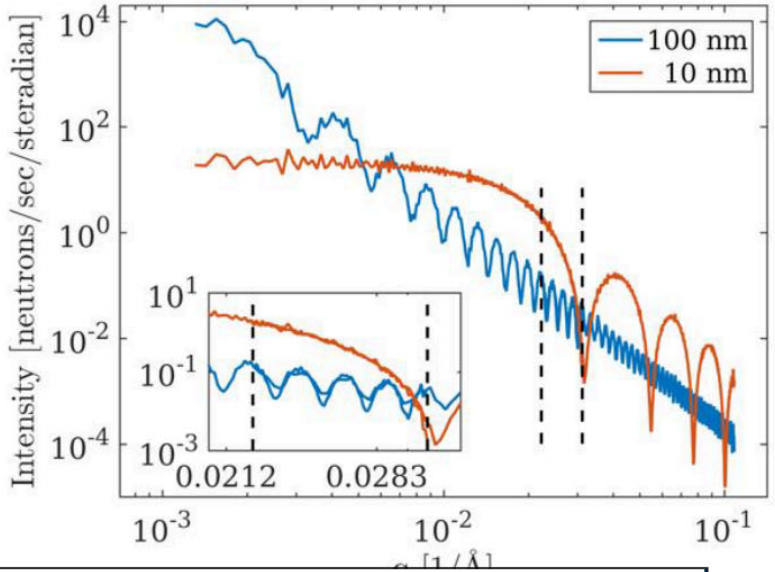
Cold neutron choppers

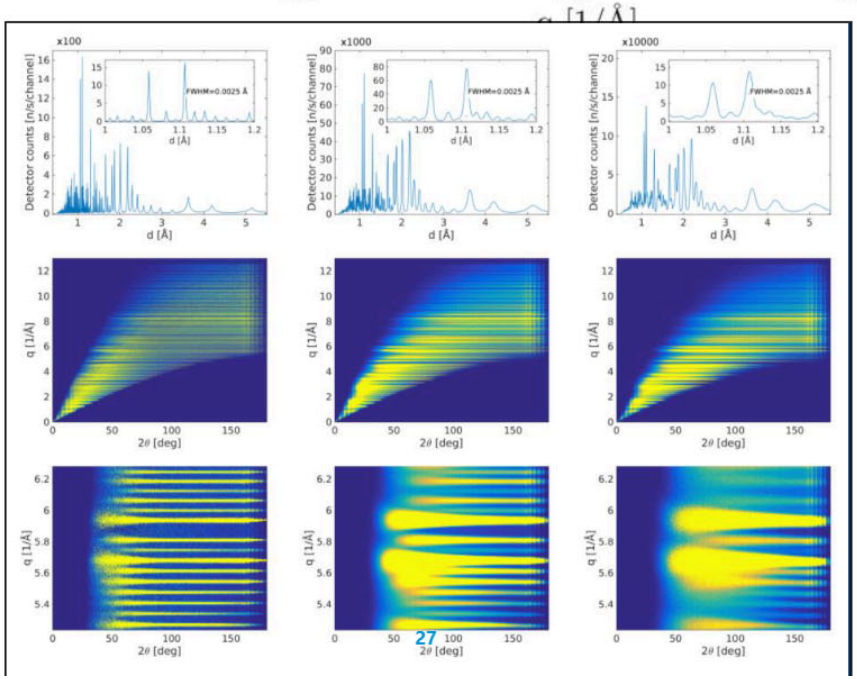
SANS tank (full scope)

Science case

By combining diffraction and SANS HEIMDAL probes an extended q-range of
10^{-3} Å^{-1} < q < 25 Å^{-1}







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

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

Chopper cascade & Dan Mannix

Neutron guides at ESS

Chopper

Chopper base plate at ESS

First installation in hall starts Dec. 2025

First Science workshop in 2026

First Science Activities

Swedish Research Council workshops

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

A **DREAM** come true – Sustainable and functional materials from local resources (Uppsala 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

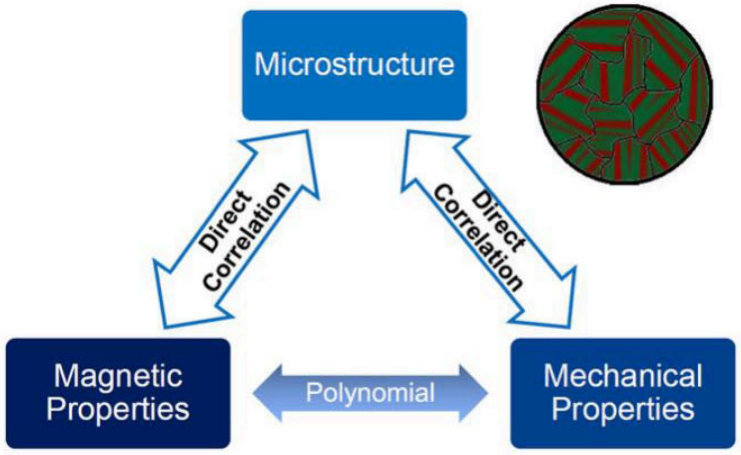
Hyperspectral, multidimensional Imaging with Neutrons to explore material processes and processing for a sustainable society (Lund University)

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

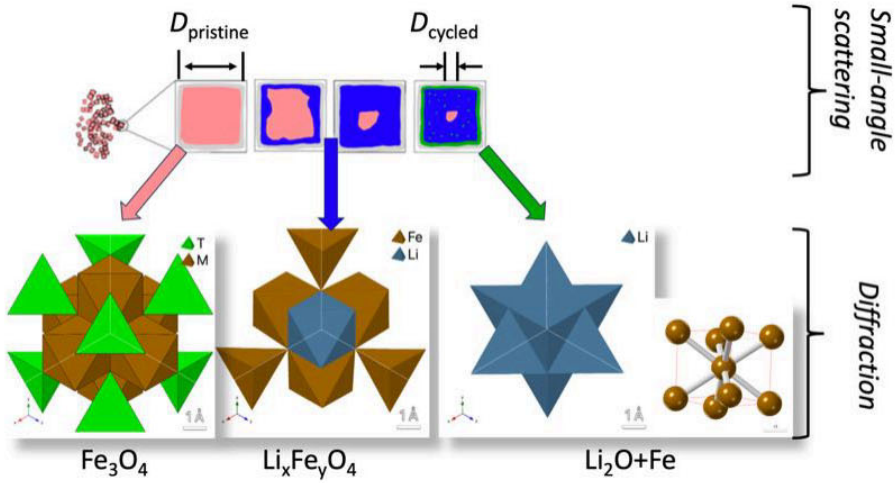
ODIN: Microstructural Characterization of Ferritic Alloys by Neutron Time-Of-flight and Grating Interferometry for Improved Materials



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

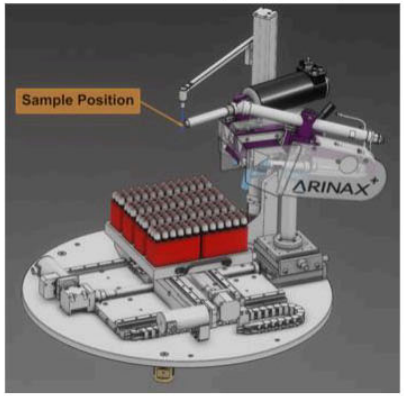
Supervisor: M. Feygenson

Diffraction & Imaging Sample Environment

Low temperature/magnetic fields

- **DREAM Electrochemistry Cryofurnace ready**, FAT organised
- **Helium recovery installed E03** SE workshops + dewar stations
- **High-Pressure Cryostat**, SAT completed
- **CryoStream sample changer** (DREAM and HEIMDAL), integration ongoing
- **8T for Diffraction** for MAGIC, manufacturing ongoing
- **1T Electromagnet** for DREAM, integration ongoing

Sample changer



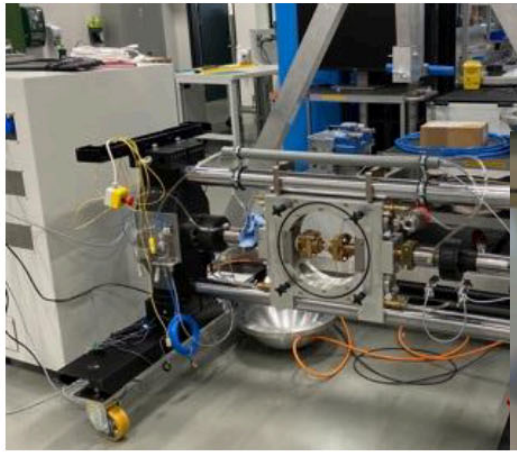
Courtesy of C. Curfs

HP cryostat

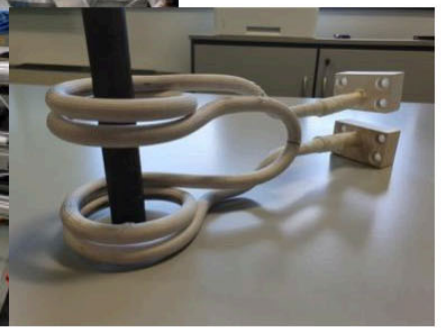
Mechanical processing & High T

- **NPI stress rig** for BEER, integration ongoing
- **Dilatometer** for BEER, procurement starting
- **Torsion/rotation rig** for ODIN, integration ongoing
- **UHT furnace** for BEER, in development
- **Induction furnace** for BEER, in development
- **ILL-Type furnaces** (DREAM and HEIMDAL):
  - Refurbished from LLB (delayed)
  - Dedicated with V tail, procurement ongoing

NPI stress-rig



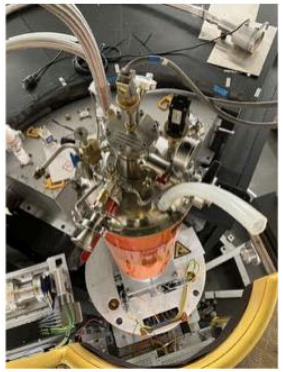
Induction coil



ILL furnace

Lower temperatures/Pool equipment

- **3 wet + 3 dry cryostats, 3 wet + 1 dry cryofurnace** for **MAGIC,** BIFROST, LOKI, SKADI, **DREAM, HEIMDAL,** T-REX and MIRACLES
  - Kicked off cryostats DREAM, SKADI, LOKI, BIFROST, T-REX
  - CDR for "WET" CRYOFURNACE (DREAM) is done. Manufacturing is in process



- **Cryostat for MAGIC** (2nd hand from FRMII)
  - Leakage in the glue joint of the tail has been fixed.
  - Control using the Mercury ITC temperature controller from Oxford Instruments (parts ordered).

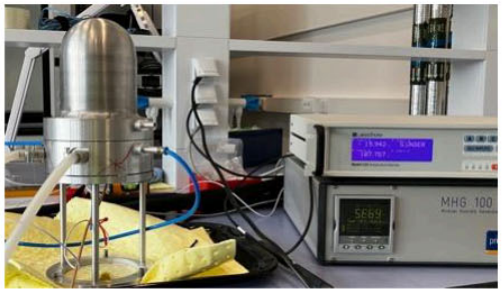
Courtesy of H. Wacklin-Knecht

Electrochemistry / Gas

- **Humidity chamber**,
  - 90 % relative humidity
  - tested and improved
  - Control integration ongoing

- **Electrochemistry/Battery cells**,
- Cells for Spectroscopy and **Diffraction** tests and development ongoing
  - Trigger box for potentiostat available
  - Cell tested at SNS (Vision)

- **Gas manifolds** (**Diffraction** / Spectroscopy)
  - Automatic up to 200 bar
    - tested with extended sample stick
    - tests ongoing for use in-situ experiments
  - Manual up to 20 bar
    - for flow and small pressures
    - prototype built, parts ordered for second one.



Thank you!

Mikhail.Feygenson@ess.eu