



Diffraction & Imaging Division update

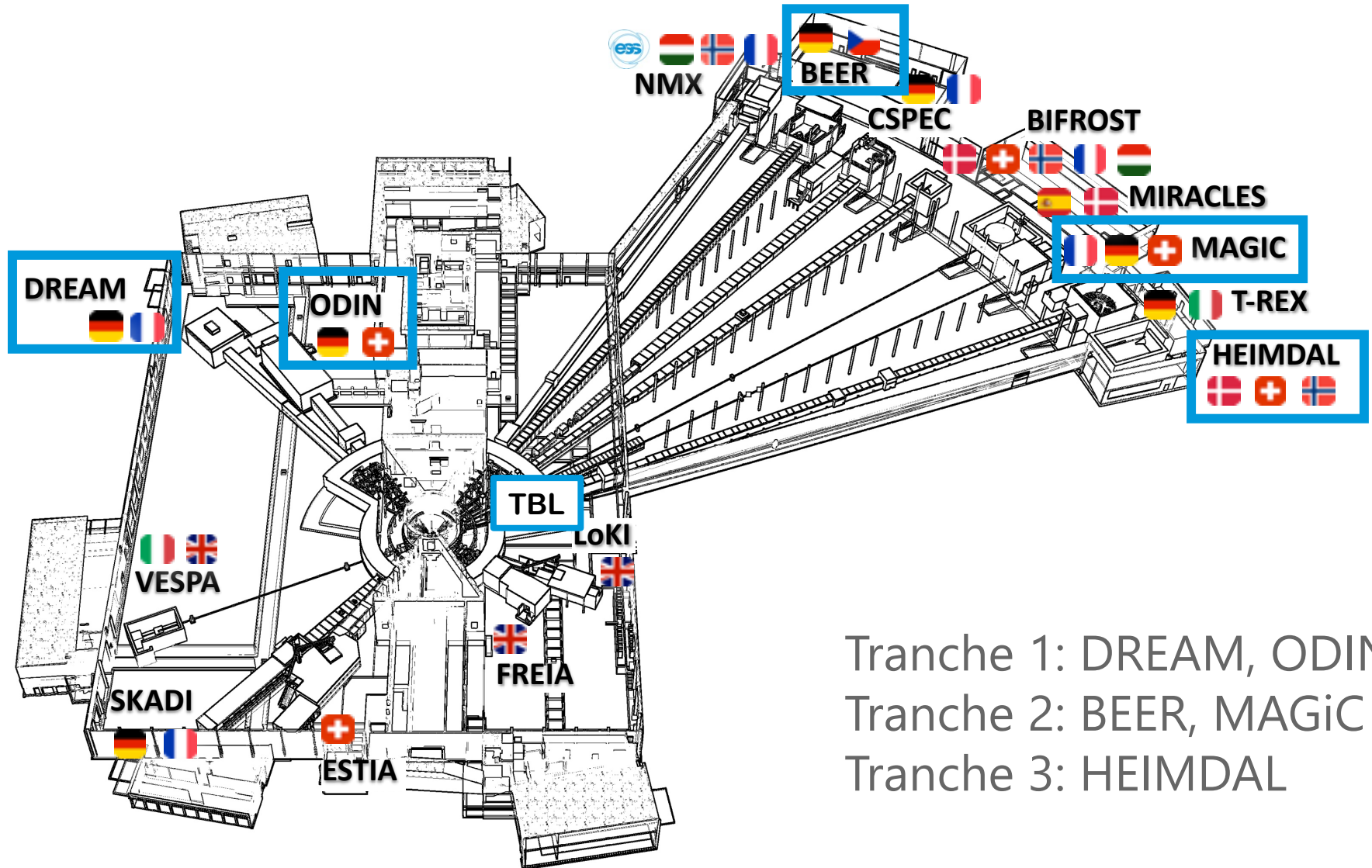
Mikhail Feygenson^{1,2,3}

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³ Jülich Center for Neutron Scattering, Forschungszentrum Jülich

Instruments



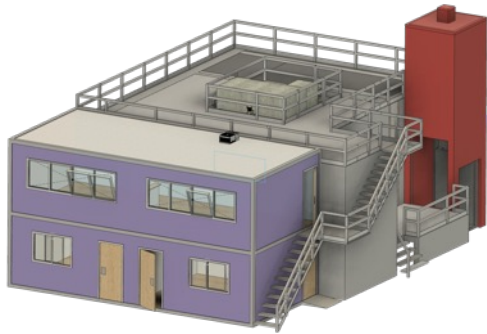
Tranche 1: DREAM, ODIN, TBL
Tranche 2: BEER, MAGIC
Tranche 3: HEIMDAL

Instruments



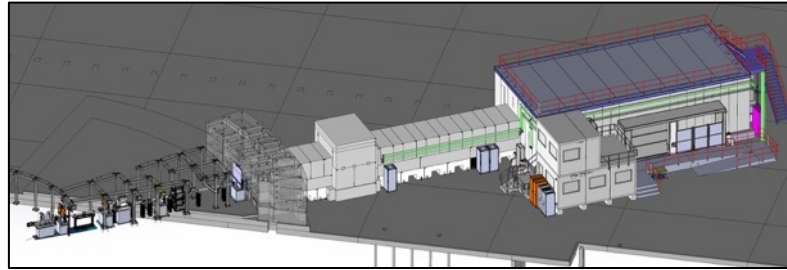
MAGiC

Denis Vasiukov*



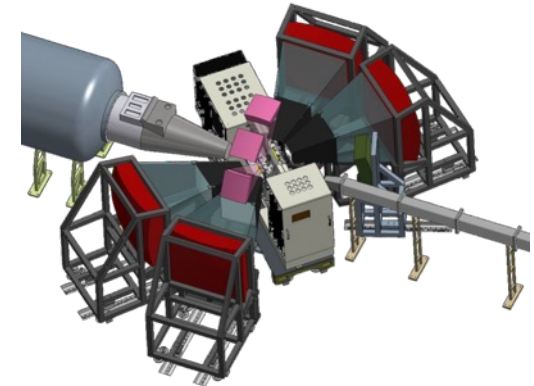
ODIN

Robin Woracek*
(robin.woracek@ess.eu)



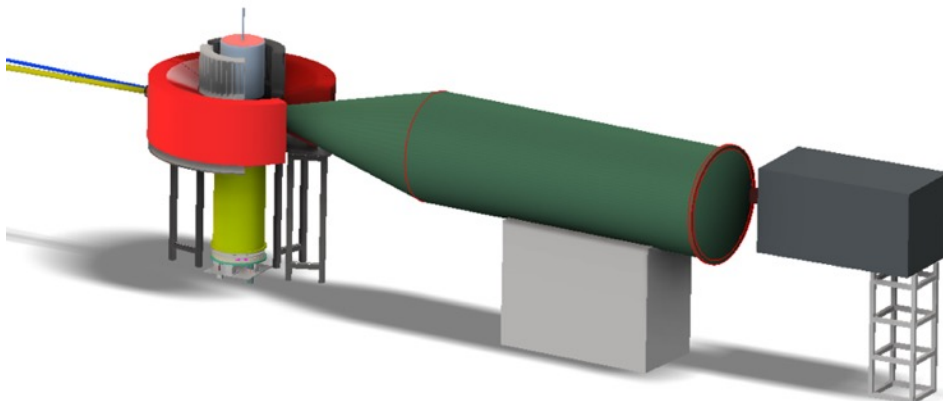
BEER

Premek Beran
(premysl.beran@ess.eu)



HEIMDAL

Dan Mannix
(dan.mannix@ess.eu)



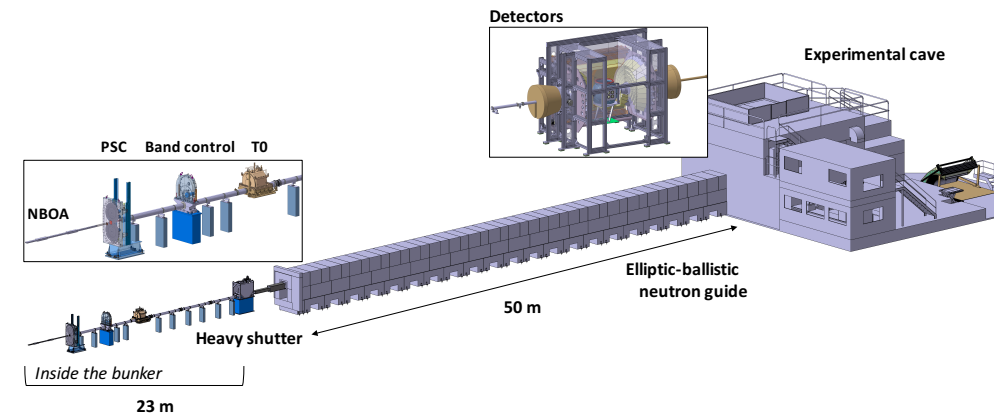
TBL

Thawatchart Chulapakorn
(thawatchart.chulapakorn@ess.eu)



DREAM

Florence Porcher*
(florence.porcher@ess.eu)



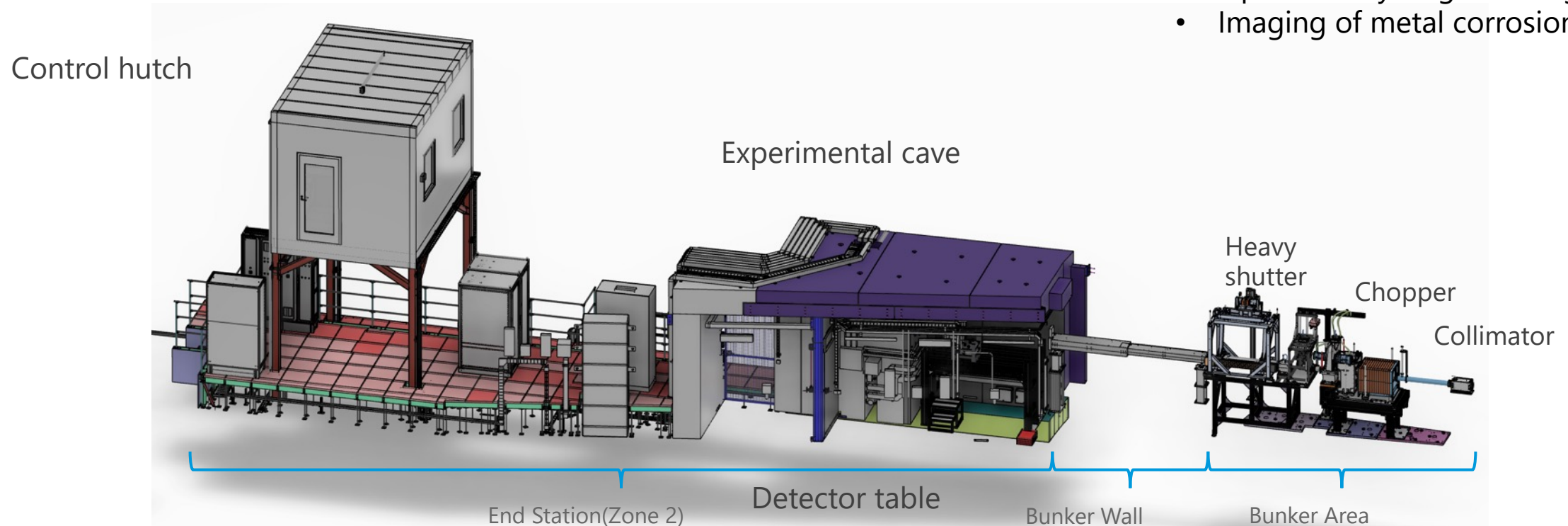
ESS Test Beamline



- Characterization of the ESS moderator system
- Proton beam stability/Moderator stability
- Spatial distribution of neutron beam
- Fast neutron flux measurements
- Pulse-shape of cold-thermal neutrons
- Detectors and data processing systems
- Sample (e.g. single crystal) alignment
- Simple imaging and diffraction experiments

First Science

- Low-resolution transmission (e.g. parahydrogen)
- Operando hydrogen storage
- Imaging of metal corrosion



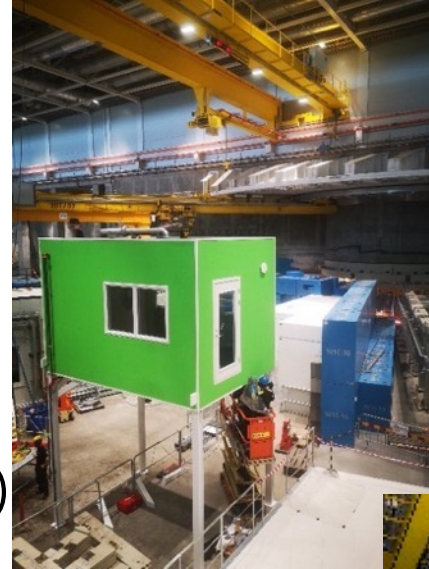
Status

- Replacement of lead IS is ongoing
- Second IS position will be open
- IOE recruitment is ongoing
- In-bunker supports installed
- CEP infrastructure installed
- False floor installed
- All racks installed (except for Beam Monitor rack)
- Detector table installed
- All Sub-TG3s are completed

Issues

- IOE has resigned
- Limited resources (since Oct 1 mech. Eng. + 1 IS)
- Late in-house collimation system manufacturing
- All collimators are delayed until Dec. 2024
- Many parallel QG for in-bunker components
- ToF detector integration (also for ODIN)

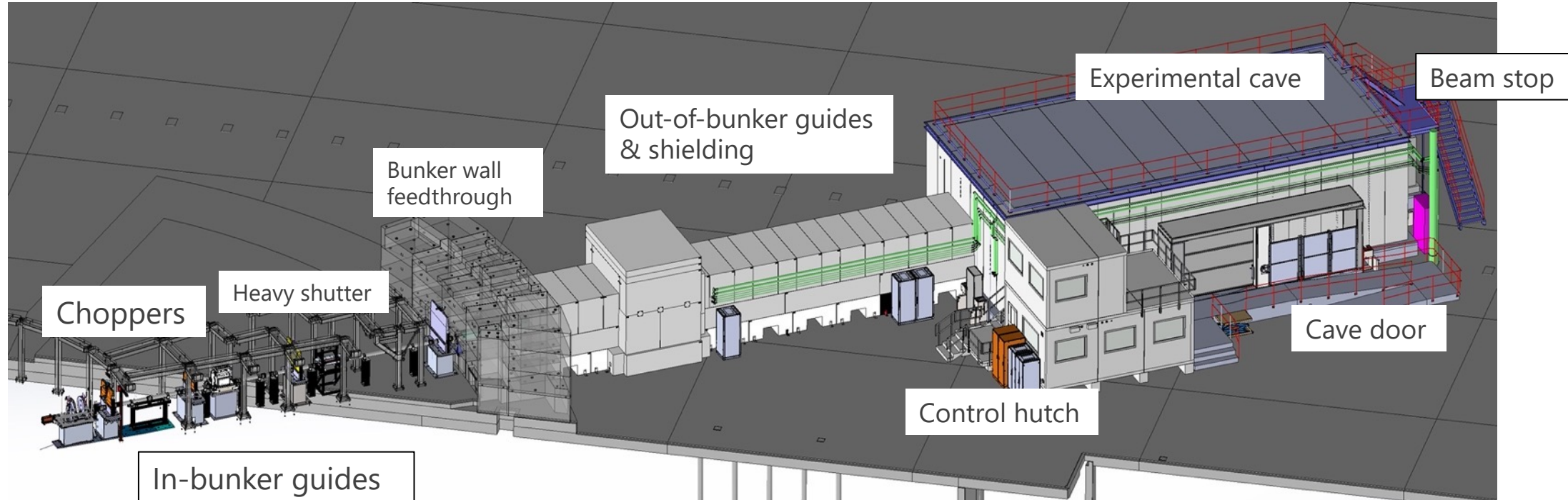
Hutch



Cave



Optical and Diffraction Imaging with Neutrons



- Spatial resolutions down to the μm -range
- Tailored wavelength resolution
- Variety of imaging techniques, including x-rays (full scope)

Applications

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

Status

- IS is hired (Robin Woracek)
- Second IS is hired (Stefanos Athanasopoulos)
- IOE is hired (Richard Ammer)
- Internal & external doors installed
- Slits and fast shutter inside the cave installed
- Cave interior & sample stages are being installed
- Re-installation of choppers will be completed in January
- Installation readiness review (IRR) for PSS completed

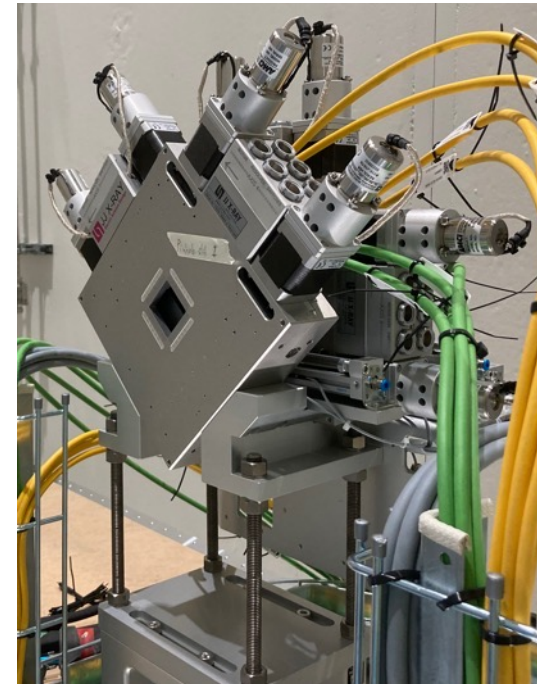
Challenges

- Neutron guides & chopper system interfaces
- Beam stop misalignment
- Integration of ToF detector into ESS pipeline
- Data analysis is key for success of imaging
 - data reduction not yet implemented in scipp
 - data analysis resources are limited
- Lead engineer coming back to BEER this year

Cave and hutch



Slits



Sample stage



DREAM Cold commissioning completed : Q2, 2025

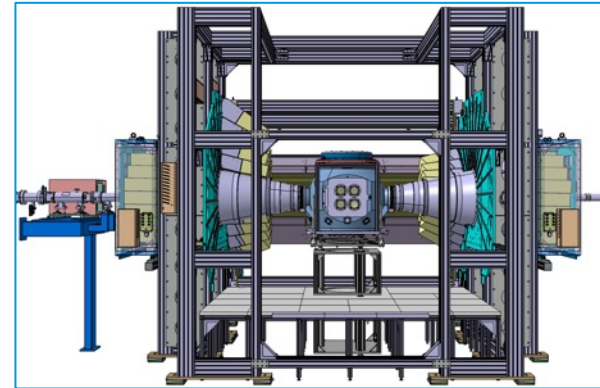
Diffraction Resolved by Energy and Angle Measurements

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

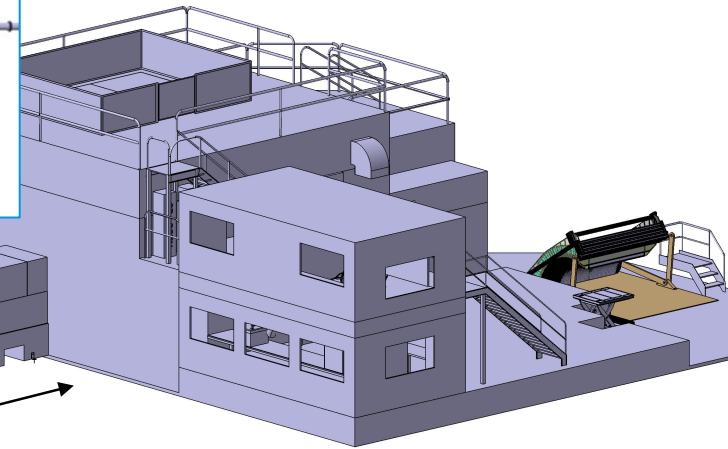


Sample vessel

Detectors



Experimental caves



Control hutch & sample preparation lab

Choppers

PSC BC T0

Heavy shutter

Neutron Guides & Shielding

Inside the bunker

Status

- New lead IS (Florence Porcher)
- Second IS recruitment is ongoing
- IOE recruitment is ongoing
- All choppers are delivered and installed (SAT tests in Nov 2024)
- CUP & CEP installations completed
- PSS & ICS installations ongoing
- Beam monitors tested with neutrons and delivered to ESS

Issues

- Cave energization
- Delay in mantle detector delivery
- Firmware re-installation for installed detectors
- Gas mixing solution for detection gas
- Problems with cryofurnace sample changer procurement

PSS racks



Motion racks



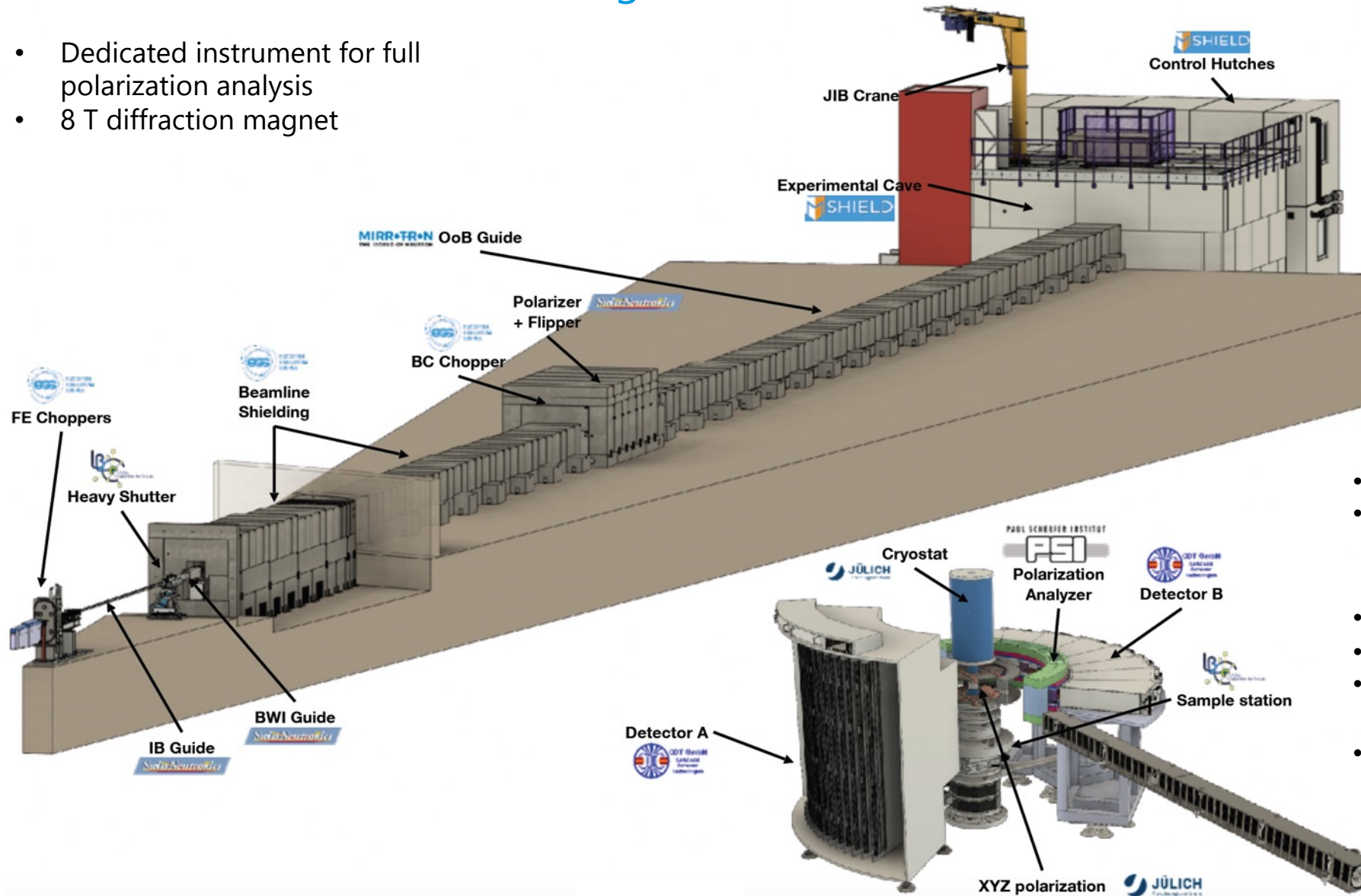
Cave and hutch



MAGiC Cold commissioning completed: Q1, 2027

Polarised Diffractometer for Magnetism

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



- 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

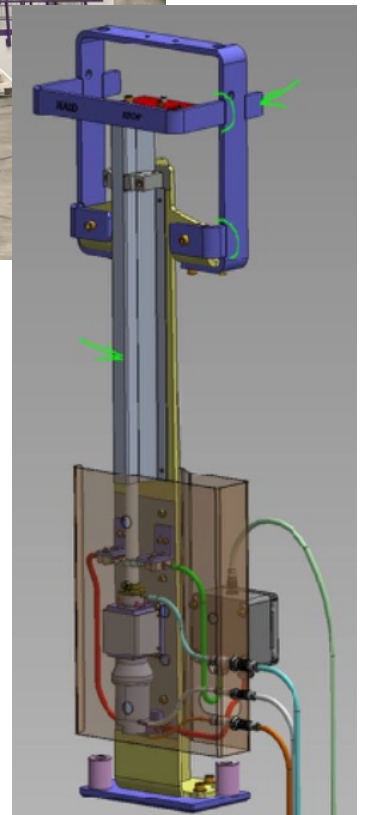
Status

- New lead IS (Denis Vasiukov, Dec. 1st)
- New engineer started at ESS (Moritz Braun)
- Engineering support (Daniele Erbi)
- Cave & hutch installed
- Replanning is completed
- CEP/CUP requirements agreed
- New hub for PSC is manufactured
- Beam Monitors are successfully tested with neutrons (for MAGiC & DREAM)

Cave and control hutch



Solid state bender



Issues

- Solid state bender delivery delayed to Dec 2024 (long lead time for missing motor)
- Vacuum housing redesign to be agreed with quality at ESS

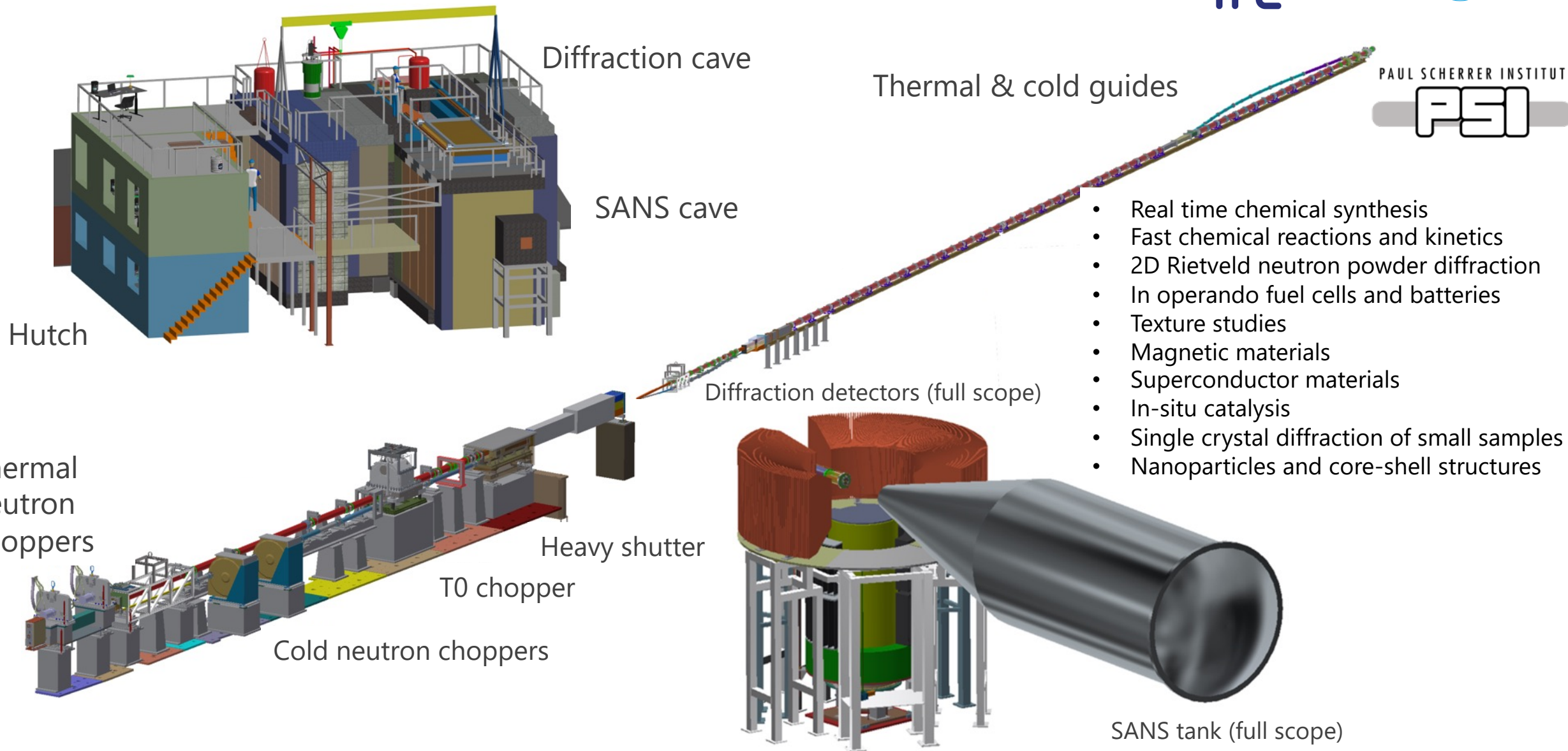
New PSC hub



HEIMDAL

Cold commissioning completed : Q2, 2027

Hybrid Diffractometer: Combined Diffraction and SANS and Imaging



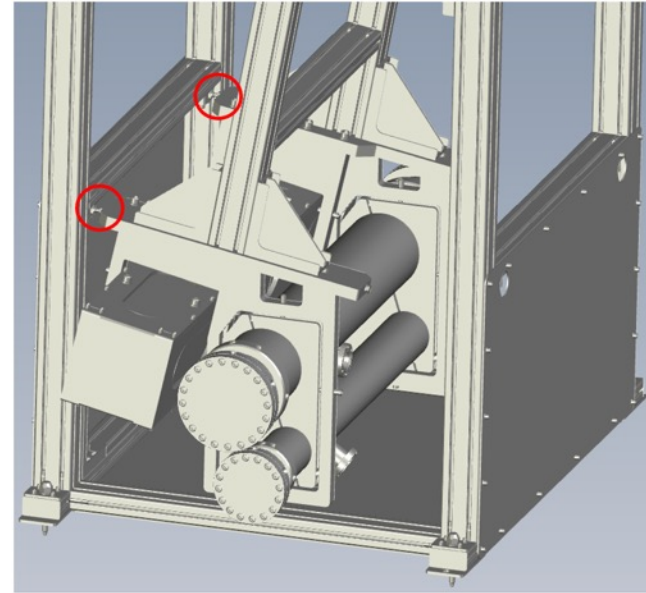
Status

- New lead engineer at ESS (Siamak Kianzad)
- Technical writer to be provided by a partner
- Cave structure PDR in November 2024
- Detector procurement completed
- IDR of detector completed
- IDR of heavy shutter completed
- Replanning to be completed in Nov 2024
- New design of the cold guide accepted
- BWFI installed

Issues

- Still limited engineering resources
- Interfaces for final detector design have to be provided by partners and ESS
- Delay in SubTG3 of the detectors
- No offers yet from CUP, CEP, MCA, BM

Heavy shutter

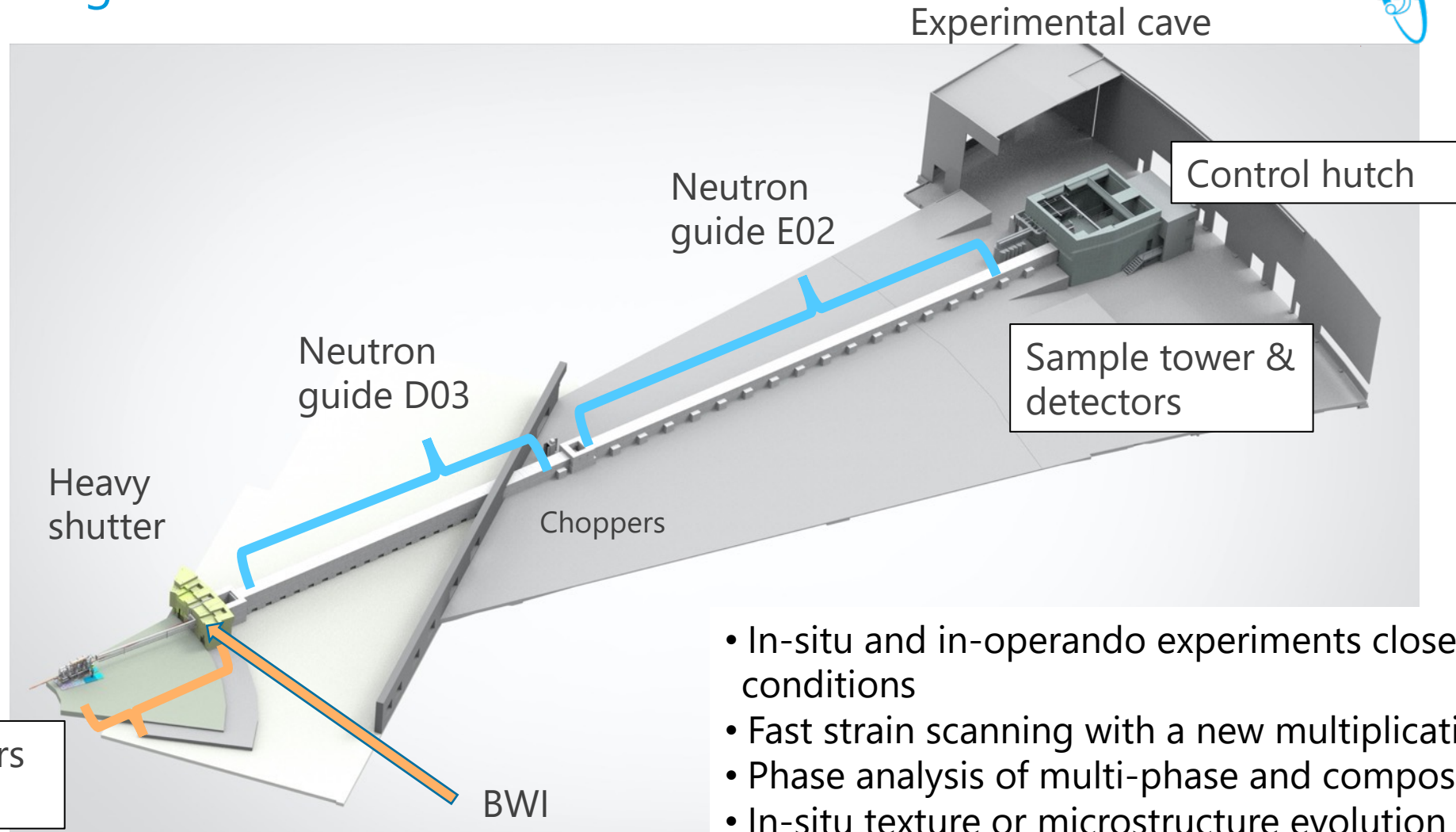


Bunker wall feedthrough insert is installed



BEER

Cold commissioning completed : Q4, 2026
Engineering & Material Science Diffraction



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

Status

- Second IS recruitment will start soon
- SubTG3 for Robot/Hexapod/Stage completed
- Hexapod & Rotary Stage delivered to ESS
- 6-axis Robot Arm and BBG delivered to ESS
- Replanning completed
- BWI & Choppers in manufacturing
- Bi-spectral switch neutron tests completed
- Cave IDR completed
- CEP requirements are being finalized

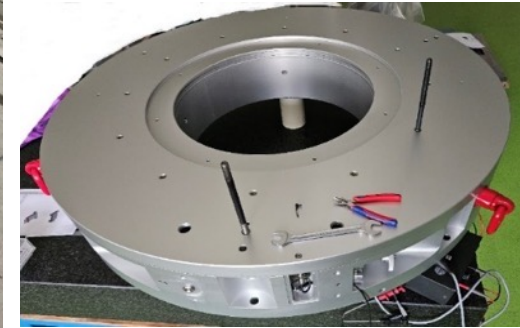
Issues

- Temporary loss of the lead engineer
- Risk of delaying in-bunker installation due to limited resources
- Design of chopper section guides delayed due to lack of resources at supplier
- Not enough information from CUP
- Current PSS design interferes with user operation

Robot



Rotary stage



Bridge beam guide (BBG)



Hexapod



Other updates

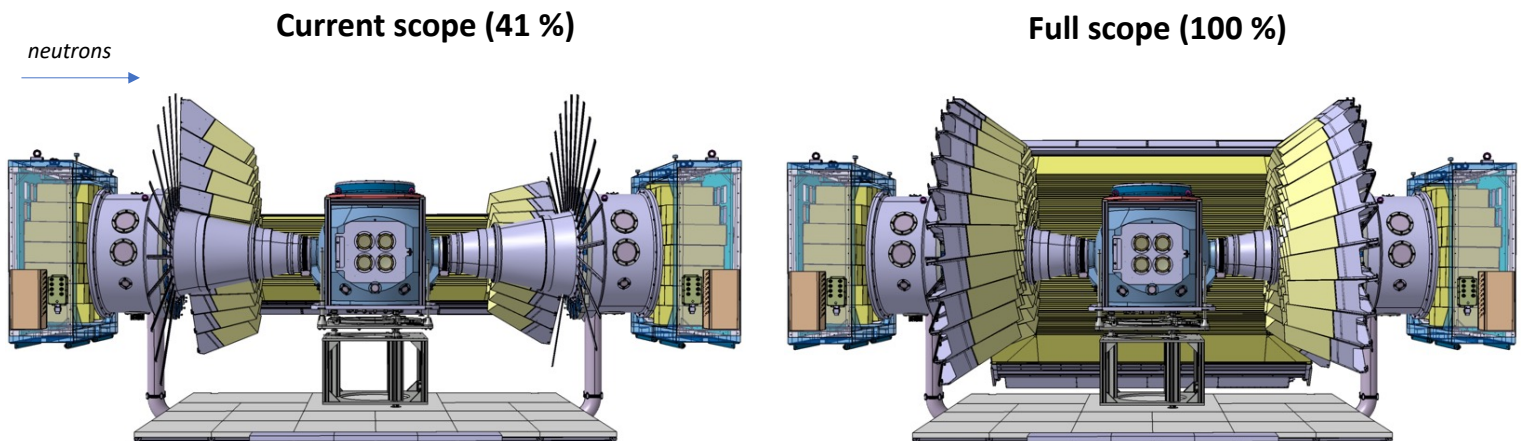
- Re-planning exercises provided more realistic end-of-completion dates
- Two division-relevant conferences in Lund (NEUWAVE-12, IUCr high pressure workshop)
- Visit to JPARC and interactions with tests and imaging beamlines
- Three instruments to be completed next year: practical and day-to-day challenges
- Regular meetings with NSS, DetG and SSD heads to address short-term challenges
- External funding proposals: more careful selection with SSD and DMSC
- Good experience in developing the DREAM first science paper with STAP (detailed science cases, planning of samples synthesis, preliminarily studies)



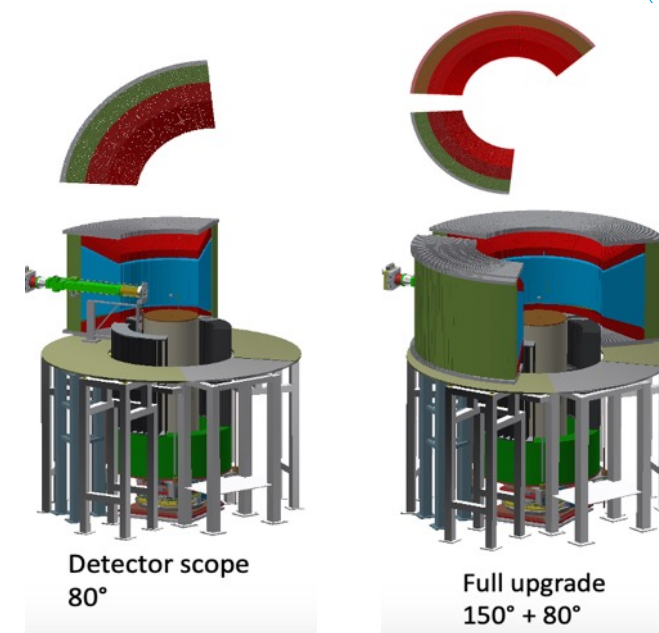
Rescoping priorities

1. Complete detector coverage for diffraction suite

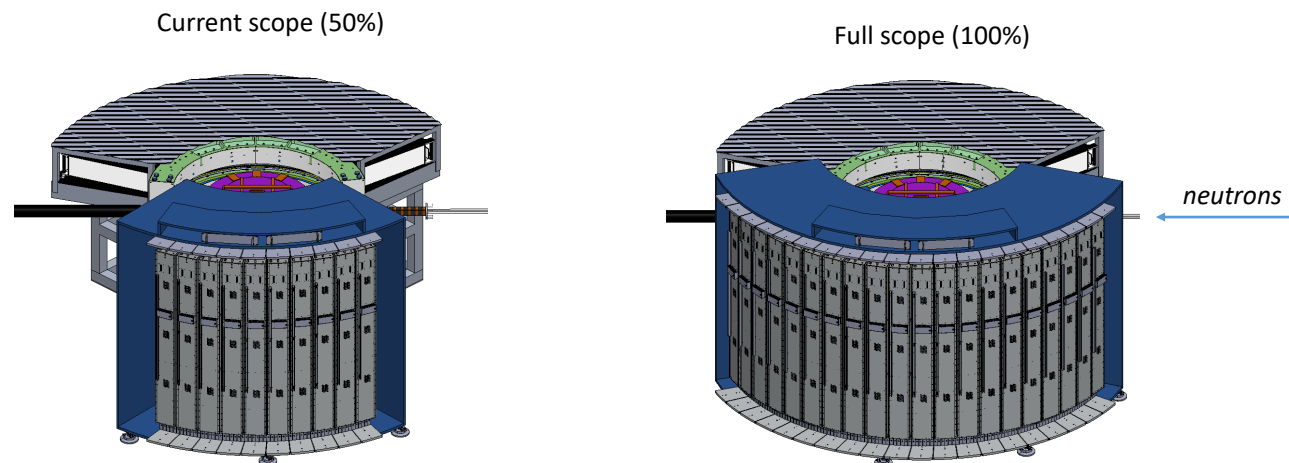
DREAM



HEIMDAL



MAGiC

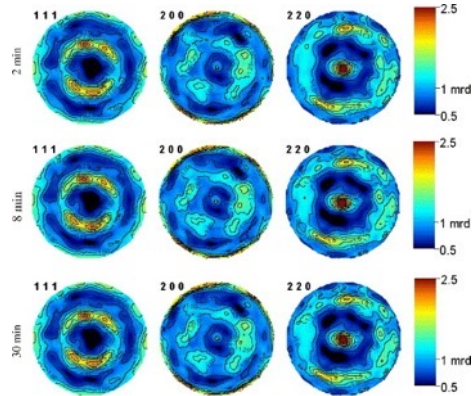


- To be competitive on day 1
- Low risk: same technology
- Experience with DREAM & MAGiC units
- Careful considerations of manufacturer resources

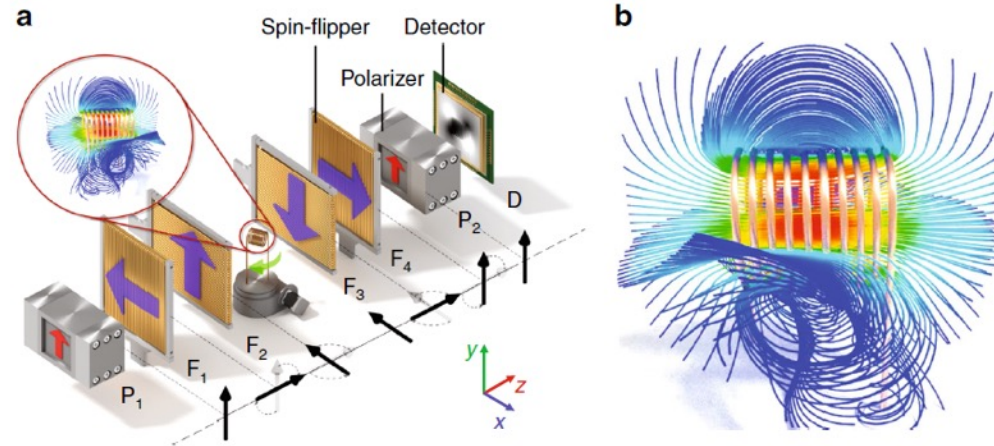
2. Recovering capabilities in engineering diffraction and imaging



BEER texture detectors & choppers

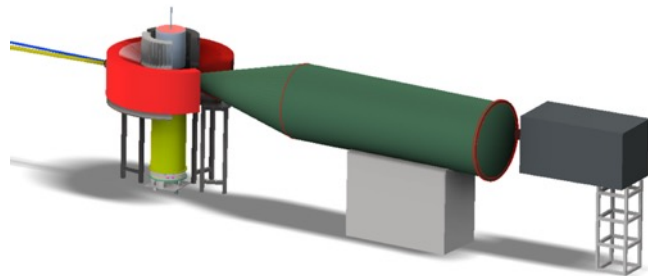


ODIN 3D Polarimetric Neutron Tomography

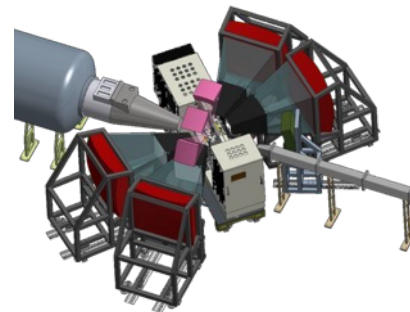


3. Recovering SANS options for HEIMDAL and BEER

HEIMDAL



BEER



4. Remaining scope: MAGiC spectroscopy chopper, BEER SEE handling, HEIMDAL imaging option, ODIN:diffraction detectors, SEMSANS and high-resol. setups

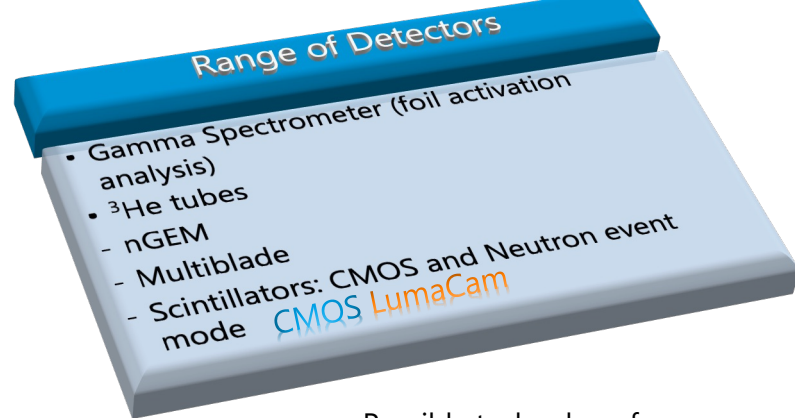


First Science ideas for DREAM, ODIN and TBL

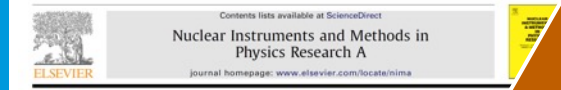
Test Beamline

First Science

Slide by Thawatchart Chulapakorn & Robin Woracek



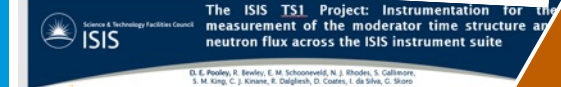
First neutron production utilizing J-PARC pulsed spallation neutron source JSNS and neutron performance demonstrated
 Fujio Maekawa^{a*}, Masahide Harada^a, Kenichi Oikawa^a, Makoto Teshigawara^a, Tetsuya Kai^a, Shin-ichiro Meigo^a, Motoki Ooi^a, Shinichi Sakamoto^a, Hiroshi Takada^a, Masatoshi Futakawa^a, Takashi Kato^a, Yujiro Ikeda^a, Noboru Watanabe^a, Takashi Kamiyama^a, Syuki Torii^a, Ryoichi Kajimoto^a, Mitsutaka Nakamura^a
 Nuclear Instruments and Methods in Physics Research A 600 (2009) 333–337



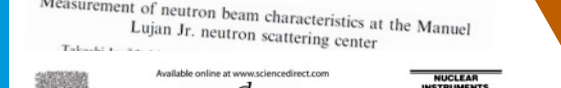
NOBORU: J-PARC BL10 for facility diagnostics and its possible extension innovative instruments
 F. Maekawa^a, K. Oikawa, M. Harada, T. Kai, S. Meigo, Y. Kasugai, M. Ooi, K. Sakai, M. Teshigawara, S. Hasegawa, Y. Ikeda, N. Watanabe
 Nuclear Inst. and Methods in Physics Research, A



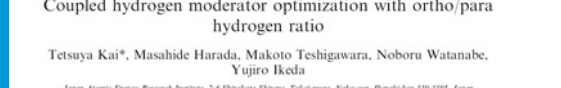
Experimental validation of the brightness distribution on the surfaces of coupled and decoupled moderators composed of 99.8% parahydrogen at the J-PARC pulsed spallation neutron source
 Masahide Harada^{a,b*}, Makoto Teshigawara^a, Motoki Ooi^a, Esben Klankby^{b,c}, Luca Zanini^b, Konstantin Batkov^b, Kenichi Oikawa^a, Yonkai Tobi^a, Atsushi Kimura^a, Yujiro Ikeda^a
 * Japan Atomic Energy Agency, 2-4 Shinohara Shimo, Takatori, Nakagun, Haraki-ken 319-1195, Japan
^b European Radiation Source (ERS), Box 176, 3-231 00 Lund, Sweden
^c Technical University of Denmark, DTU North, Roskilde, Denmark
 Nuclear Instruments and Methods in Physics Research A 523 (2004) 496–510



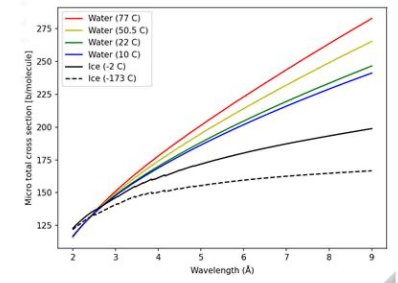
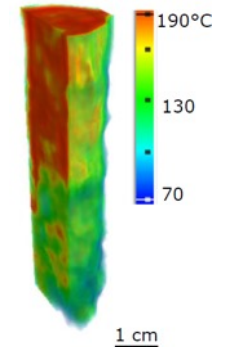
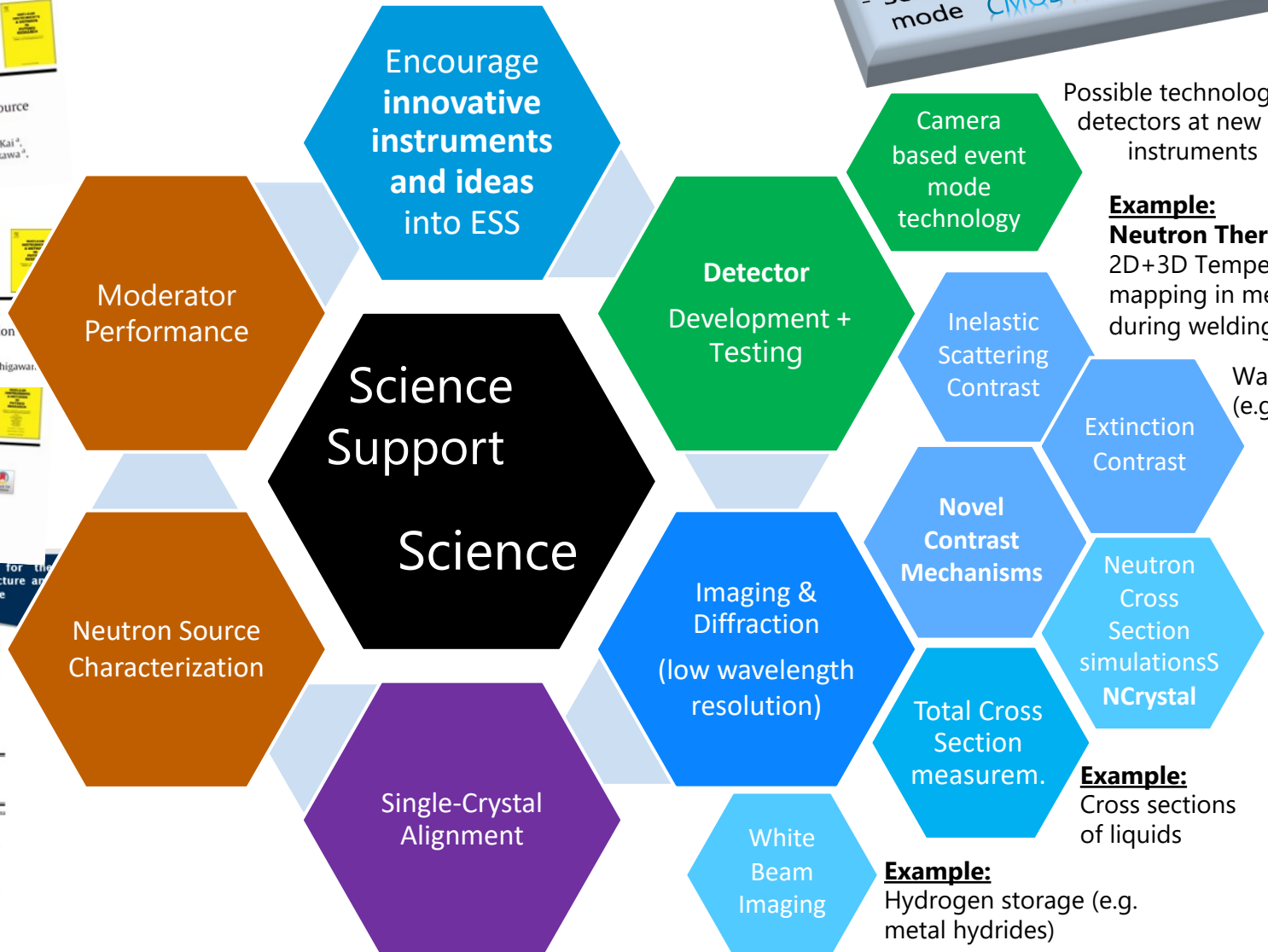
Measurement of neutron beam characteristics at the Manuel Lujan Jr. neutron scattering center
 Available online at www.sciencedirect.com
 SCIENCE @ DIRECT®
 NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH A
 ELSEVIER Nuclear Instruments and Methods in Physics Research A 523 (2004) 398–414



Coupled hydrogen moderator optimization with ortho/para hydrogen ratio
 Tetsuya Kai^a, Masahide Harada, Makoto Teshigawara, Noboru Watanabe, Yujiro Ikeda
 Japan Atomic Energy Research Institute, 2-4 Shinohara Shimo, Takatori, Nakagun, Haraki-ken 319-1195, Japan
 Received 31 May 2003; received in revised form 30 October 2003; accepted 28 November 2003



Received 31 May 2003; received in revised form 30 October 2003; accepted 28 November 2003



Example: Plastic deformation in metals

Example: Cross sections of liquids

Example: Hydrogen storage (e.g. metal hydrides)

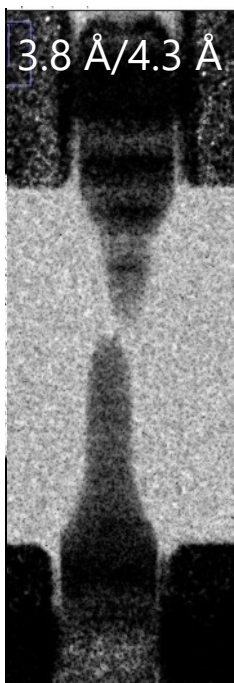
ODIN

First Science

Slide Robin Woracek

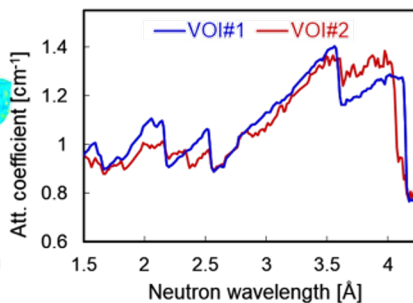
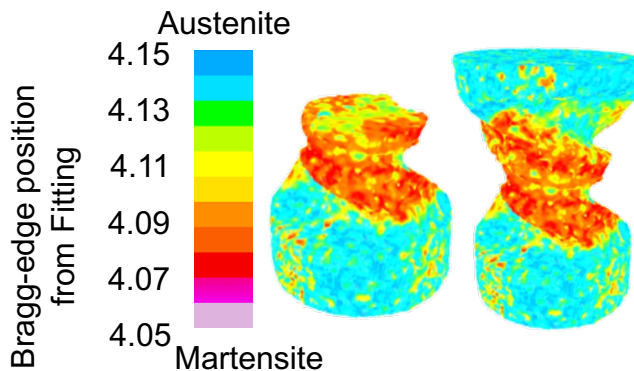
In-situ tensile testing of AM materials:

Texture, Strain, Phase



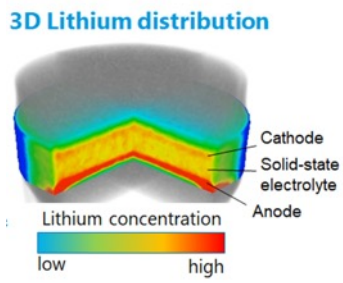
LumaCam

Spectral Tomography e.g. 3D Phase Mapping in Metals



LumaCam

Li transport in solid state batteries



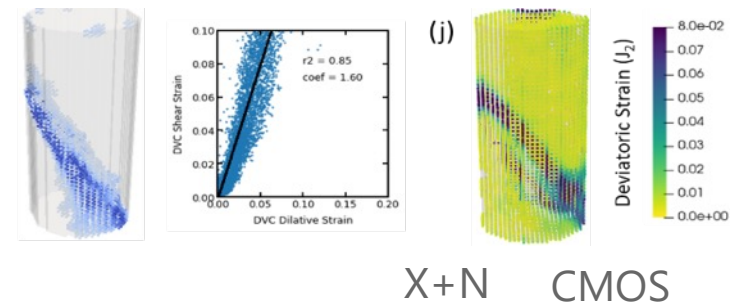
X+N
LumaCam
CMOS

Cultural Heritage



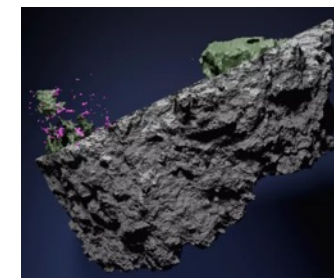
X+N
LumaCam
CMOS

Mechanics and flow through granular media



X+N CMOS

Planetary Sciences



ScienceAdvances

X+N
LumaCam
CMOS



DREAM

First Science

- Pulse-shaping (flux vs ΔQ resolution)
- The highest resolution in backscattering
- Pair-distribution function with $Q_{\max} = 25\text{\AA}^{-1}$
- nm-SANS down to 0.01\AA^{-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

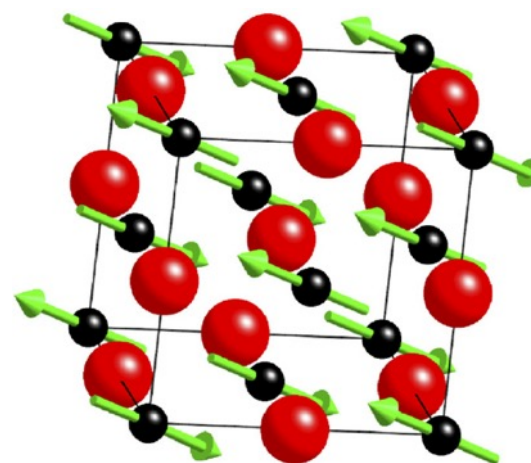
Energy materials

**Mix of new science and
“classic diffraction” materials**

EUROPEAN SPALLATION SOURCE		Document Type	Document Number	Date	Revision	State	Confidentiality Level	Page
			ESS-0456238	Oct 1, 2024	1	Preliminary	Internal	1 (5)
<hr/> DREAM INSTRUMENT FIRST SCIENCE <hr/>								
	Name	Role/Title						
Authors	Sibille Romain Franck	Paul Scherrer Institut						
	Florence Porcher	DREAM Lead Instrument Scientist						
Owner	Florence Porcher	DREAM Lead Instrument Scientist						
Reviewers	Martin Sahlberg	Uppsala University						
	Manuel Angst	Forschungszentrum Jülich						
	Gwenaëlle Rousse	Sorbonne Université						
	Reinhard Neder	Friedrich-Alexander-Universität Erlangen						
	Helen Playford	ISIS Neutron and Muon Source						
	Werner Schweika	Forschungszentrum Jülich/ESS						
Approvers	Mikhail Feygenson	Head of Diffraction & Imaging Division						
	Giovanna Fragneto	Science Director of ESS						

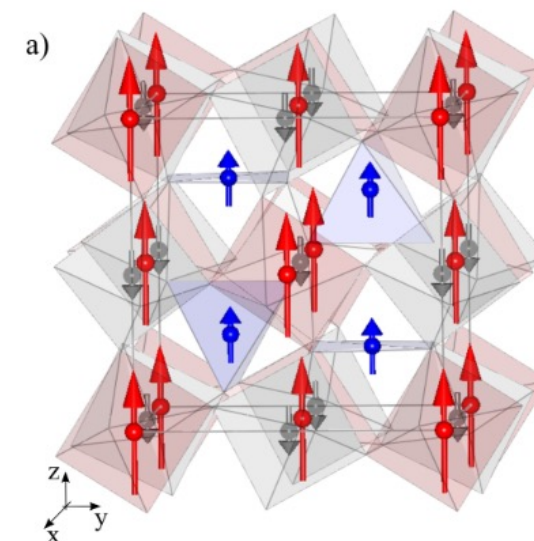


Transition metal oxides NiO



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

Double-double perovskites CaCuFeReO₆

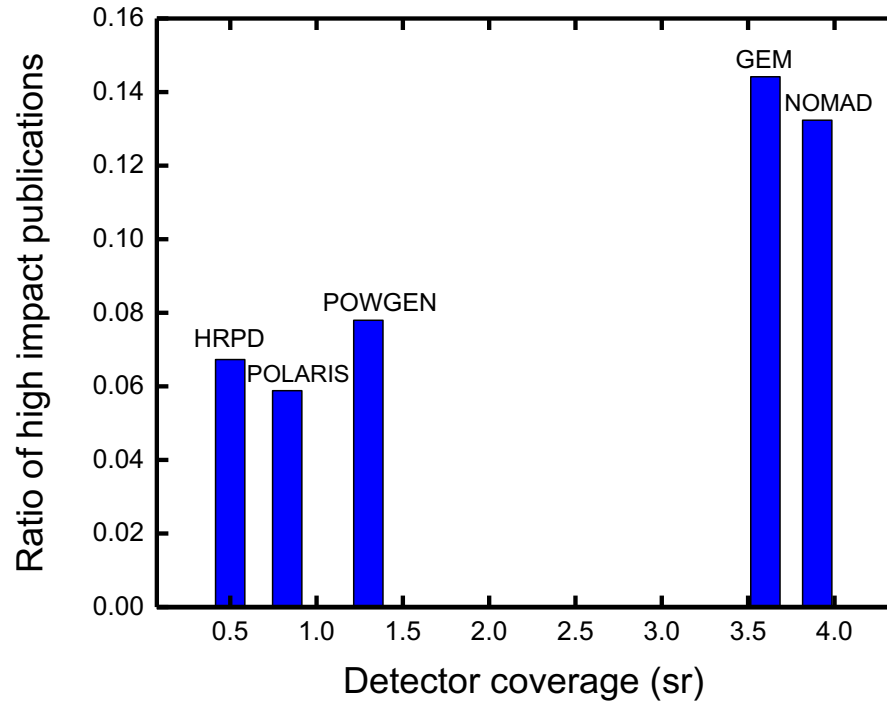


E. Solana-Madruga et al. Angew. Chem., 61 9497 (2022)

More detector coverage isn't about faster measurements; it's about enabling new science!



DOE high-impact journals list (2011-2016)



TITLE	CITED BY	YEAR
Deviation from high-entropy configurations in the atomic distributions of a multi-principal-element alloy LJ Santodonato, Y Zhang, M Feygenson, CM Parish, MC Gao, RJK Weber, ... Nature communications 6 (1), 5964	664	2015
The nanoscale ordered materials diffractometer NOMAD at the spallation neutron source SNS J Neufeind, M Feygenson, J Carruth, R Hoffmann, KK Chipley Nuclear Instruments and Methods in Physics Research Section B: Beam ...	401	2012



Aerodynamic levitator setup at NOMAD (SNS)