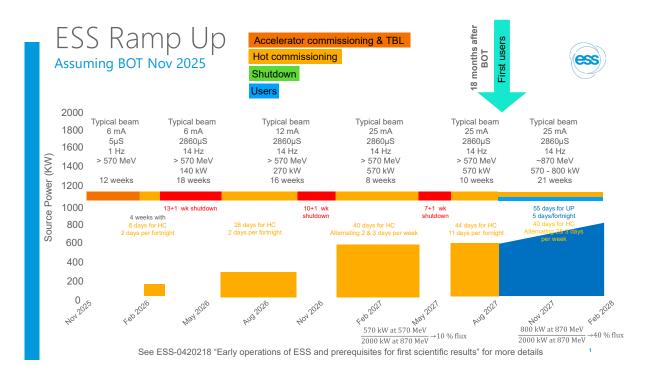
First Science DREAM - technical aspects (STAP April 2025)

Here we discuss the technical prerequisites provided by ESS in order to evaluate further the current First Science plans for DREAM, see link,

DREAM first Science is conditioned by availability of "good quality" beam at the instrument, fruitful hot commissioning validating instrument performance, sufficient data reduction flow and possibility to deploy the sample environments required for the science itself.

1. ESS Neutron production Ramp-up and expected schedule on DREAM



The present estimation of ESS BOT is now end of November 2025 as the Dream TG5 (end of cold commissioning) milestone. The 3 following months can be considered as a buffer period when the beam characteristics (pulse frequency) will not be suitable for advanced commissioning activities. This period will be used for the Safety Readiness Review (validating the PSS) leading to Instrument SAR milestone and for basics instrument characterizations on detector (efficiency) and chopper (basic checkup of the configurations). One can expect the validation of instrument performance with reference samples to start in February 2026 for 1 month before a more than 3 months shutdown until June-July 2026. This could be the starting date of First Science in an optimal scenario. The following 4 active months until August 2027 will come with an increase in beam energy and flux, however, with time needed for additional instrument commissioning.

For First Science, we may consider - after the commissioning phase 0 - three phases of beam operation before user operation, with increasing beam power from 270kW to 570kW and increasing reliability and matureness. We assume readiness for powder diffraction after commissioning in phase 0, based on approval with test samples, data reduction, availability of sample environments for DREAM, which is all as described in the Appendix below.

We categories the <u>proposed experiments</u> according to the three beam phases with respect only to feasibility, by Y or. N or scaled from 0-9, and propose the phase to start.

Experiment	Importance/ Interest	Feasibility Instrument/Sample/ SE	Phase 1	Comment
4.1 Transition metal monoxides		9/?/Y	1	High resolution should work Small basic cells
4.2 Zeolites and MOFs		6 / Y / Y (MFI) 8 / Y / Y (MIL-53	3	Low Q coverage is poor
4.3 Electrode materials in pristine state		7/?/Y	2	Medium resolution, Sample size?
5.1 Perovskites and complex oxides		9/?/Y	2-3	Idem 4.1
5.2 Small samples with cation disorder		4 / ? / Y (Temperature only)	3	Sample size/ Neutron flux is critical. Low Q coverage for complex magnetic structure
5.3 Hydrogen- containing samples		5 / ? / Y for [CH ₃ NH ₃][Co(COOH) ₃] 4 / ? / ? for Mn _x (OH) ₂ (C ₆ H ₂ O ₄ S)y	3+	Background level critical. Polarisation options not ready on time?
5.4 Energy materials		8/?/Y NMC 3/?/Y HKUST-1	2-3	Ex situ on NMC: should work Low Q coverage needed for HKUST-1 + 1H background
5.5 Incommensurate magnets		6/?/Y	2-3	Low Q coverage needed (MnGe :Q~3nm)

Appendix

Phase 0 Commissioning / Reference Measurement and test samples

The procurement of reference samples for the calibration of the Tranche 1 instrument will allow to calibrate the main instrument parameters (geometry and resolution) and the data reduction flow for powder diffraction/pdf and SANS.

Sample	Availability	Test
V-rods various diameters	ESS	Detector homogeneity
NAC	ESS+order	Powder
Y_2O_3	ESS	Powder
Diamond	ESS	Powder
Silver behenate	ESS	Powder
(AgC22D43O2		
Silica spheres	ESS	SANS
Al oxide spheres	ESS	SANS
LaB ₆	June2025	Powder
Al ₂ O ₃ (Merck0	ESS	
YIG single crystals	Ordered	
NIST Si	unclear	
NIST Al ₂ O ₃	unclear	

Data flow and reduction/analysis

The data management has been focused up to now on tools for live instrument control, and data reduction (mainly for powder diffraction) through python scripts (Jupyter notebooks). The VISA platform for users remote access is under development.

Data Reduction (C. Durniak, IDS)	Status
Generic reduction tools Loading, reduction, masking (detectors coordinates or physical units) Saving as xye, cif, converting to units (tof, Q, d-spacing, wavelength) Normalization by monitor or proton charge, normalization by Vanadium, filtering, strip vanadium peaks, grouping by wavelength bands and detector banks Plots in 1,2,3 D (detector and physical quantities)	
Powder Diffraction Reduction and conversion of 4D ToF data to 2D data (theta, lambda) to (theta,d-spacing) and integration to 1D data (d-spacing) Sample Sample 10-5 10-7 dspacing [Å]	Done (1D)

PDF	In progress
	(60 % done)
Polarization (with A. Stellhorn)	In progress
	(just started)
SANS	Not started
Adapt workflow done for LOKI	
Single Crystal Diffraction	Not started
Collected requirements specific to DREAM (done by CD)	
Responsibility of IDS to be recruited	

Commissioning tools	Status
Live visualization: NICOS and beamlime	In progress
User access (VISA)	Status
 VISA desktop and Jupyter lab available after submitting "DREAM proposal" 	Done
- Diffraction analysis software available on VISA : easydiffraction, FullProf, GSAS-II, MAUD, DISCUS, RMCProfile, Mag2Pol, SScanSS	Done

Availability of sample environment and polarization options for DREAM

Dry cryofurnace (pool)	2025	6.5T magnet	2025
He-cryofurnace (pool)	End 2025	8T magnet	End 2026
Dilution fridge(pool)	2026		
Heat gun/cryojet + changer	End 2025	Cold Polarizer (Dream, RAC)	Mid 2026
Vanadium furnace	End 2026	SANS Analyzer	2026
		Wide angle analyzer	End 2026
HP cryostat	2025		
PE press	2024	Gas manifold (3 gas, 0-30b)	2025
Gas pressure cells	2024	I-sorb cell for gas injection	Design
Clamp cells	2025		
Liquid pressure cells	2024	Potentiostat (electrochem.)	2024
DAC	2027	Cells (electrochem.)	Design