The roadmap to the first science at DREAM

This document briefly outlines the plan for the first science at the DREAM instrument. It is a living document, which will be constantly updated to include most recent developments in the sample environment and power ramp up plan for ESS. Suggestions from Diffraction STAP will be added as well.

The first experiments at DREAM can be roughly divided into three categories (i) beamline characteristic studies, (ii) standard experiments and (iii) complex experiments. All of these experiments will be pursued in parallel. Each type of experiment has a different lead time and number of resources. The description of each category is provided below.

Beamline characterization studies (low risk, low impact)

This is the first type of experiments to be conducted at DREAM when the neutron beam is available. We plan to measure neutron powder diffraction standards, pair-distribution function (PDF) standards, known single-crystals and samples to tests polarized SANS capability of the instruments. These studies will be carried out at low, medium and high-resolution chopper settings to provide instrument resolution function for each setting. 2D Rietveld resolution function will be obtained as well. Using those functions will help to plan more challenging experiments. The beamline characterization studies require minimum sample environment. The results will be published in the instrument paper.
Samples: NIST Si and LaB_6 powders, $Y_3Fe_5O_{12}$, Cu, and Al single-crystals, NAC ($Na_2Al_2Ca_3F_{14}$), Vanadium rods of various diameters, zeolites A and X, diamond powder, NiO powder (magnetic at room temperature), silica nanoparticle to estimate resolution for SANS data and Fe_3O_4 magnetic nanoparticles to extract magnetic form factor using polarized neutrons
Sample environment: DREAM dedicated sample-changer or alternative sample changer at room temperature (ESS ongoing development). The goniometer for the single crystal measurements.

Standard experiments (low risk, intermediate impact)

In this category, we will choose the samples that were already measured with neutrons at other facilities. We would like to confirm the results of previous studies and capitalize on the DREAM specific features, such as the highest resolution for powder diffraction. The results can be published as standing-alone scientific papers in journals with an intermediate impact factor.
Samples: NiO nanoparticles that show rhombohedral distortion below 523 K, that could not be resolved on the POWGEN beamline, but it was visible in synchrotron data. MOFs, cobaltite and nickelate powders. Zeolite MFI (SiO_2 silicate-type) with the cell parameters a = 19.90 Å, b = 20.04 Å, c = 13.38 Å (for high-resolution mode), deuterated MOF MIL-53(Al), (Co)MOF-74-1 and (Co)MOF-74-2 (collaboration with ESS Deuteration Lab), RE-Fe-B magnets with prepared using additive manufacturing techniques, high-entropy alloys, metal hydrides: H_3S, CaH_6, and LaH_{10}, water
Sample environment: DREAM sample changer, vacuum furnace, ILL-type cryostat, magnet, gas injection, pressure cells

Complex experiments (high risk, high impact)

This is the most challenging type of experiments. Not only new samples within a complex sample environment will be measured, but also simultaneous data analysis of the neutron diffraction, PDF and SANS data will be attempted. The experiments will be focused on unique capabilities of the instrument, that are not available elsewhere. Success of the experiments will rely heavily on the stable neutron beam and performance of the sample environment. The samples will be synthesized specifically for these experiments. For example, the electrochemical cells will be used to study magnetic nanoparticles as a function of lithiation with polarized neutrons (scope of the RAC proposal). The data analysis will be challenging, but results have a chance to be published in high-impact journals

<u>Samples:</u> cubic and spherical Fe_3O_4 nanoparticles within the electrochemical cell, samples with complex magnetic structure (incommensurate), solid electrolyte: Rb/Cs H_2PO_4, HKUST-1 Cu_3(benzene 1,3,5-tricarboxylate)$_2$(H_2O)$_3$

<u>Sample environment:</u> DREAM sample changer, pressure cell, furnace, electrochemical cell, gas handling system (up to 200 bar)

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