MIRACLES Initial Operations and Staging Plan

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SUMMARY

The initial operations and staging plan describes the preliminary plan for the validation of the instrument function and scientific performance using spallation neutrons. This `hot commissioning` is beyond the scope of the instrument construction work package. This document also describes the potential upgrades beyond the allocated cost book value.

1. HOT COMMISSIONING

The hot commissioning of an instrument refers to the testing and validation tasks to prepare the instrument for the user program in the operations phase of the ESS. This phase must be carefully planned to address all the high-level scientific requirements. For the case of MIRACLES, a a series of McStas and MCNPx simulations will be performed prior to hot commissioning considering each new input received during the project timeline. This will help identifying possible issues.

1.1 Beam validation and flux measurement

The beam monitoring system provides diagnostics for neutron beam diagnosis at three different parts of the beam transport and conditioning systems (BTS). A first beam monitor (BM1, diagnosis) will be located prior to the last chopper at $L \approx 80$ m, used for inspection of the guide performance over time. Another beam monitor (BM2, normalization) will be located at the end of the beamline, between the guide and the sample, to measure the incident flux and the time of flight near the sample position. A third position-sensitive monitor (BM3, sample alignment) will be used for beam visualization (divergence).

Flux and pulse length will be measured for various wavelength bands:

- $\lambda \in [5.50, 7.05]$ Å: High elastic energy resolution extremely well adapted for quasielastic neutron scattering (QENS) measurements using the Si(111) reflection from the analyzer crystals. Offset of the elastic line allows for measurements of low-lying excitations.
- $\lambda \in [2.50, 4.05]$ Å: Range of the source spectrum with the highest flux, adapted for inelastic neutron scattering (INS) at the neutron energy-loss side. Accessibility to this range opens the upgrade path for installation of Si(311) analyzer crystals to extend the accessible observation time of the instrument.
- $\lambda \in [1.50, 3.05]$ Å: McStas calculations have confirmed that the accessible energy transfer for MIRACLES can be extend beyond 40 meV, since neutrons with $\lambda \approx 1.5$ Å are still transported. Thus the Si(333) reflection can also be used to extend the observation time provided by the instrument.

A proposed strategy for flux measurements can be outlined as below:

i) Place a neutron camera to evaluate the beam cross section.
ii) Replace the camera with a gold foil and put the monitor between the gold foil and the slit (just like our beam monitor BM2).
iii) Measure for hours, turn off the beam, and monitor the radioactivity of the foil in a gamma spectrometer.
iv) Measure a vanadium sample for analysis of the resolution function.
v) Repeat for all the PWD settings (all flux-resolution operation modes).
vi) For each setting, use the monitor measurements to get a relative spectrum in the wavelength range of interest, the gold foil measurements to establish

the absolute case and the vanadium sample to have the flux for each resolution.

1.2 Alignment of Si(111) analyzer

Previous analytical and McStas calculations will provide an ideal backscattering geometry with the position of the top and bottom analyzers, as well as the tilt of the detectors.

The analyzer consists of a number of panels (made of bent Si(111) crystals glued on a B4C-lined Al frame, and all panels supported by an Al frame structure). Once the panels have been installed, the panels will be aligned by means of laser track inspection to focus the backscattered laser beams on the cylindrical detector array. Every panel will be conveniently aligned, using independent manual positioners (3 for each panel: two rotations and one translation).

1.3 Background

MCNPx calculations will provide a detail theoretical map of the high energy background at the primary and secondary spectrometers, while background reduction will be a continuous effort for the entire period of the hot commissioning. Special attention will be paid to:

- Impact of gamma radiation from the sample environment equipment and the beam stop. Prevent this by making sure that the shaping time set in the detector electronics is appropriate for the MIRACLES instrument.
- Measurements of diverse sources of unwanted radiation: gamma rays, fast neutrons, thermal neutrons outside the selected bandwidth propagating in the scattering vessel.

1.4 Energy resolution

The elastic energy resolution is measured either with a vanadium sample (mostly to correct for detector efficiency) or with the sample at the lowest temperature (to correct possible broadening of the elastic line by the sample itself). The following measurements that will be performed:

- Obtain the line shape for the elastic resolution as a function of the PWD choppers configurations.
- Obtain the contribution of the sample size to the elastic energy resolution.

1.5 Detector calibration

Detector calibration focuses on reproducibility and calibration and will be scheduled following these two steps:

- Tests with a radioactive neutron source will be carried out prior to installation in a laboratory at ESS-Bilbao.
- Tests during hot commissioning will be carried out, using a vanadium sample. In both spectrometer and diffractometer tubes, use a Bragg peak to test the detector count rate, and subsequently rotate the detector out of the Bragg condition, and confirm stability of the count rate.

1.6 Scientific performance

To verify that the instrument is ready for data collection, well characterized samples will be measured:

- A vanadium sample (rod) to quantify the elastic line.
- A soft matter sample (water) with well-known evolution of the quasielastic elastic signal as a function of resolution and scattering vector.

2. STAGING

MIRACLES will be a world-leading instrument on Day 1 of its user program. In addition, several upgrade tasks will be carried out during the operations timeframe, that will have an immediate impact on the scientific performance.

2.1 Full analyzer-detector coverage

It is envisaged a ½ analyzer-detector coverage (150°, left side) will be installed on Day. Once the instrument is fully operational, the first priority will be its full coverage (left and right sides). The idea is to extend the observation time covered by the instrument. To this purpose, the following strategy is planned:

i) To carry out the commissioning experiments with the Si(111) analyzer. This will also allow to verify if the Si(333) harmonic reflection (E~19 meV; λ=2.08 Å) can be explored to extend the instrument capabilities. The incident beam elastic energy resolution as well as incident energy will be tuned using the choppers cascade.

ii) If the use of Si(333) reflection gives satisfactory results, here we note that the Si(333) reflection although intense is quite narrow, the full coverage will be carried out with Si(111) crystals. This will allow a double counting rate, and considerable extension of the observation time provided by the instrument.

iii) If the results from (ii) are not satisfactory, the upgrade path will be oriented to cover the other half of the tank with Si(311) analyzer crystals. So, the final layout will be ½ coverage for E=2.08 meV (elastic energy resolution from ??? to ??? μeV) and ½ coverage with more thermal neutrons (E=7.63 meV).

2.2 Diffraction detector

The project scope on Day 1 provides only one ^{3}He tube for diffraction detection. At the beginning of operation, the complete diffractometer will be developed. A conical frame around the focusing guide (ensuring a diffraction angle range around 168°-172°) will host an array of either ^{3}He position sensitive detectors or boron-lined straw detectors. Collection of Bragg peaks with this detector will be very useful for first inspection/characterization of polycrystalline materials, as well as for monitoring phase transformations due to temperature or other factors.

2.3 Be filter

The beryllium filter is used to get rid of the peak harmonics at higher energies. A significant increase of the signal-to-noise background ratios in the quasielastic region has been demonstrated in OSIRIS with this filter.

Tests to validate the performance of the Be filter will be carried out with a vanadium sample at room temperature. The Be filter will be retractable in order to take out of the neutron pathway when the Si(333) reflection is used.

2.4 Exchangeable focusing guide

The focusing guide concepts developed during the preliminary design phase are oriented towards a versatile beam size at sample position enabling measurements on samples of different dimensions, from 3x3 cm^2 to 1x1 cm^2. A possible upgrade, that will take shape only after a couple of years of full operation with users (e.g. on demand) will consist in the development of an exchangeable focusing guide optimized for smaller samples (~5x5 mm^2). This will extend and update the scientific portfolio of the instrument.

2.5 Sample environment

Since MIRACLES is one of the last instruments to enter into operation, provision of sample environment equipment was shifted to the operations budget. This will include (instrument dedicated or part of the pool):

- Dedicated cryofurnace (from 2 K to 700 K).
- Dedicated multiple sample changer
- A high-temperature furnace (up to 1200 K).
- Dilution insert (down to 20-50 mK)
- A humidity chamber.
- Magnets reaching 3 T and 5 T.
- Gas reaction/pressure chamber for catalysis
- Laser pump-probe (IK from Estonia; ready, dimensions adaptable to MIRACLES)
- In-situ Raman spectroscopy
- In-situ electric field control for membrane protein studies (IK from Italy; ready, dimensions adaptable to MIRACLES)