MIRACLES: STAP Spectroscopy report (March 2023 – October 2024)

José Pereira, on behalf of the MIRACLES team*

Status and management

The MIRACLES instrument has started installation of the first components. Additionally, the cave will hold its SubTG3s in October 2024. The rest of the components are in the manufacturing phase (being manufactured, manufactured and with FAT tests ongoing or ready to be installed). Here is a list presented:

- Installed:
  - NBOA(2021)
  - BBGOA
  - In-bunker guide
  - In-bunker guide supports
  - BWI
  - Control room
- Manufactured (FAT ongoing or approved):
  - Out-of-bunker guide
  - D03 out-of-bunker guide supports
  - Scattering vessel
  - Choppers
  - Detectors electronics (front end)
- Manufacturing:
  - E02 & E01 Out-of-bunker guide supports
  - Analyzer
  - Detectors
  - Radial collimator
  - Get-lost tube/Beam stop
- Detailed design:
  - Cave
  - Sample area equipment
  - Slit
- Preliminary design:
  - Crane
  - Infrastructure (utilities, electrical, …)
  - Beam monitors

Additionally, the instrument team and the NSS worked on the replanning exercise of the MIRACLES project. The main milestones agreed are:

- Final TG3: 2024
- Completion of installation and beginning of cold commissioning: 2026
- TG5: 2027

A general overview of the status of the main work packages, and providers of the detailed design at this stage are depicted in Fig. 1:

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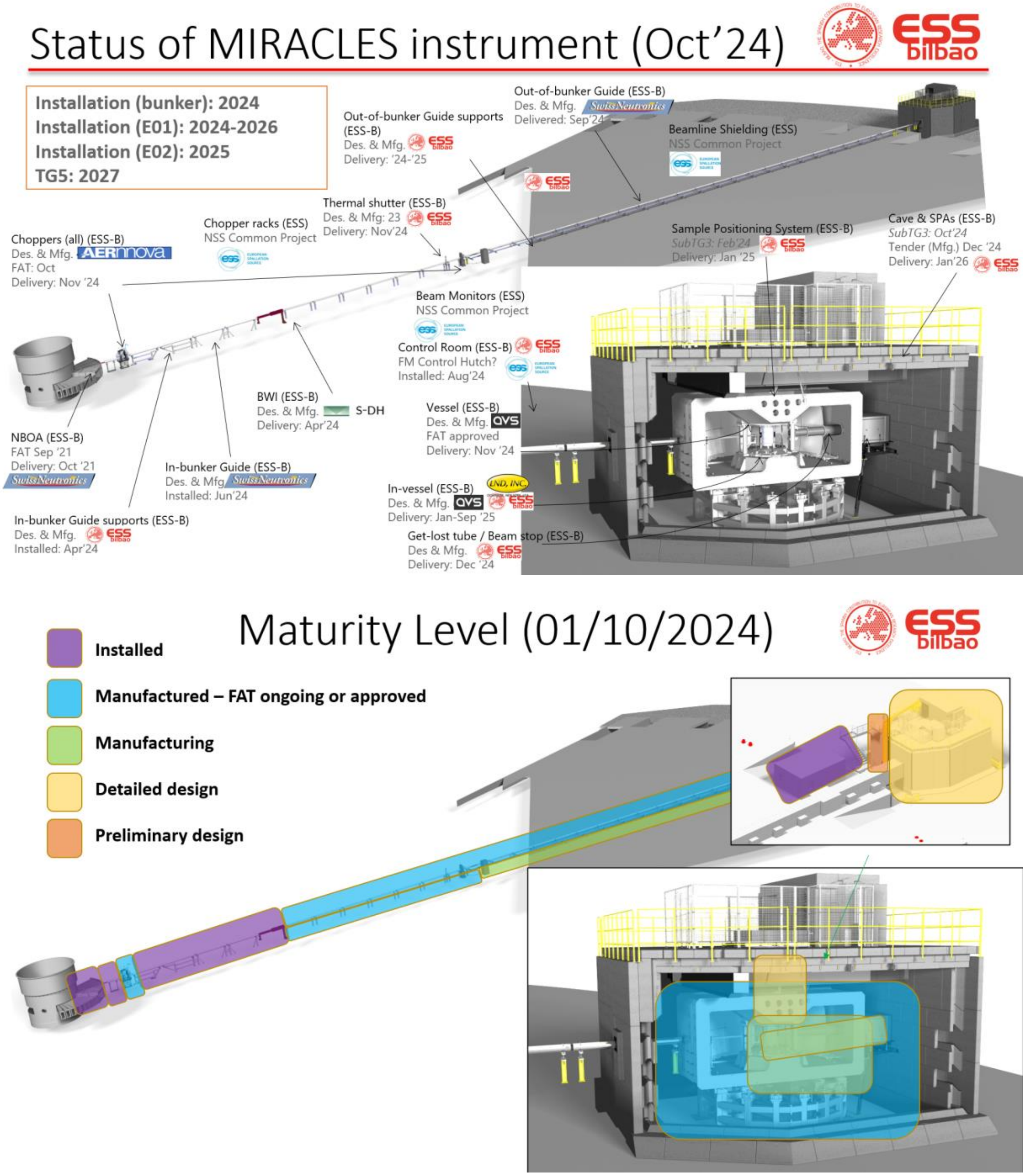

Figure 1 Illustration showing status, providers, and milestones for the different components of MIRACLES.

Scattering System

Vessel

The design and manufacturing of the vessel has been completed (see Figure 2).

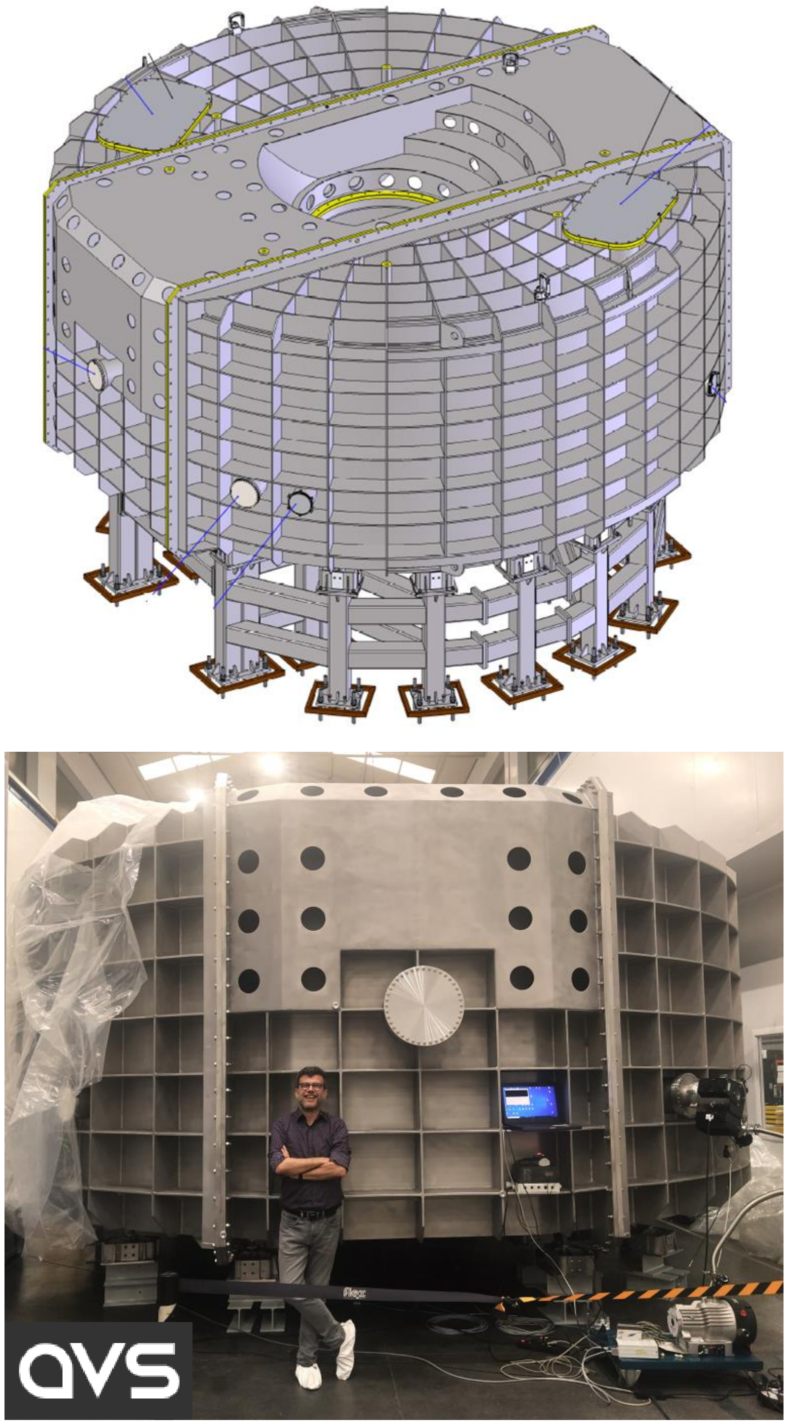

Figure 2 3D model and picture of the manufactured (steel 316L) MIRACLES vessel.

Analyzer

The mechanical assembly of the analyzer was manufactured, see Figure 3.

Figure 3 Panels and alignment supports of the MIRACLES analyzer system.

Two prototypes of the analyzer were manufactured to validate the Gd paint coating procedure and the gluing procedure as well as to evaluate the effect of different fabrication conditions of the Si crystals (method, etching) and thickness for the Si(111) crystal reflectors. A systematic analysis of Si(111) wafers with different parameters was performed using the backscattering spectrometer IN16B at the Institut Laue-Langevin (ILL). Figure 4.

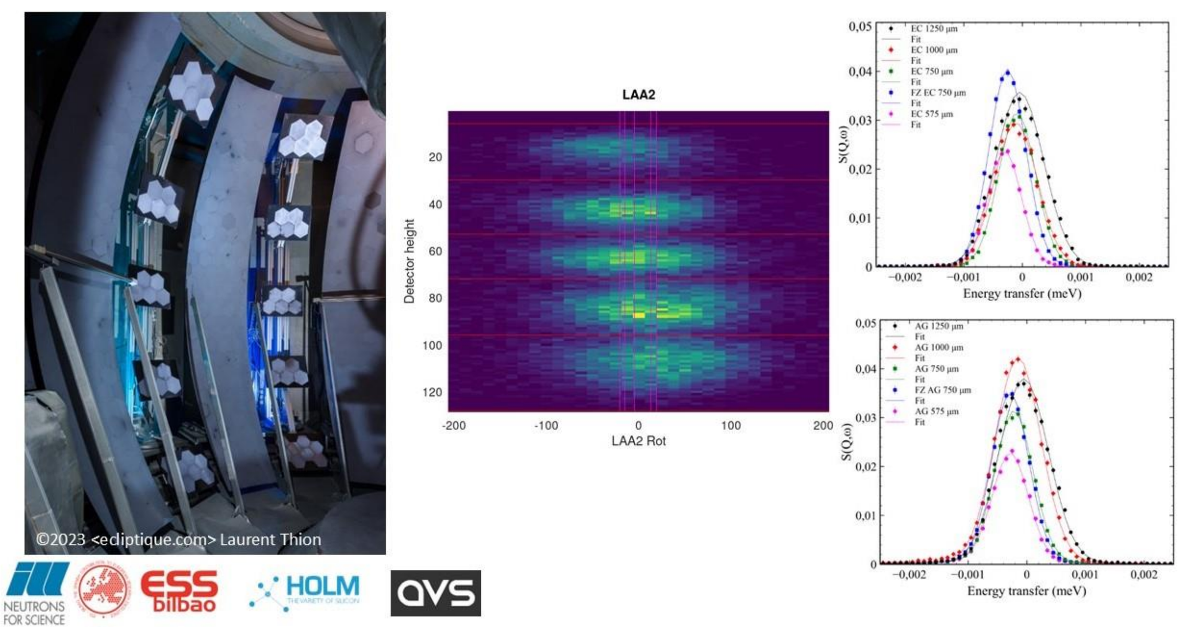

Figure 4 Panels prototypes with different Si crystals samples tested in IN16B.

Based on the results of flux (area), growth method, and thickness, the Si (111) crystal with a thickness of 1000 µm, etched, and grown using the floating zone method, was selected for the MIRACLES analyzer system. A publication with the complete analysis of the results is in review for to be submitted.

A purchase order for 1100 Si units has been placed, and the first batch has already arrived. Meanwhile, the gluing and painting station was developed and tested at ESS Bilbao. To optimize and speed up the panel manufacturing process, new gluing stations, including a table and pneumatic pressing system, are to be built. These activities are scheduled to begin in November 2024.

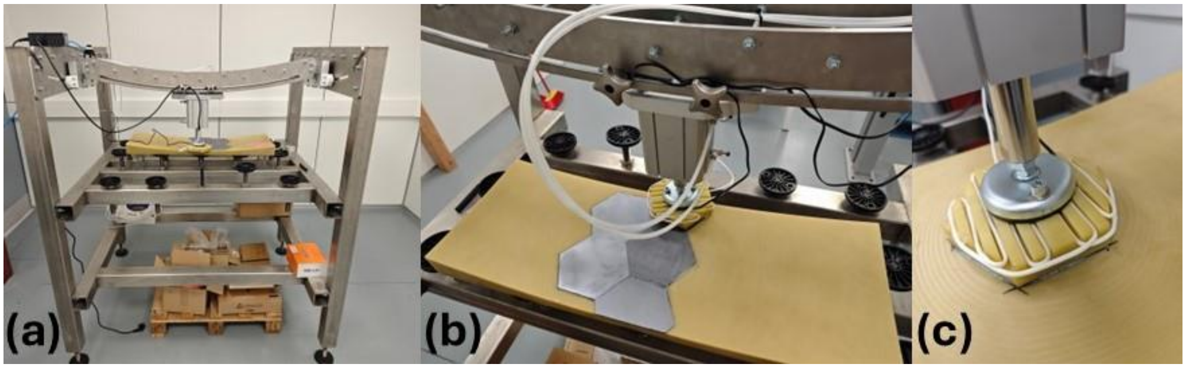

Figure 5 (a) Station for bending and gluing the Si crystals; (b) Pneumatic press; (c) Stamp head with a heating wire for keep temperature constant during the curing process of the glue.

Detectors

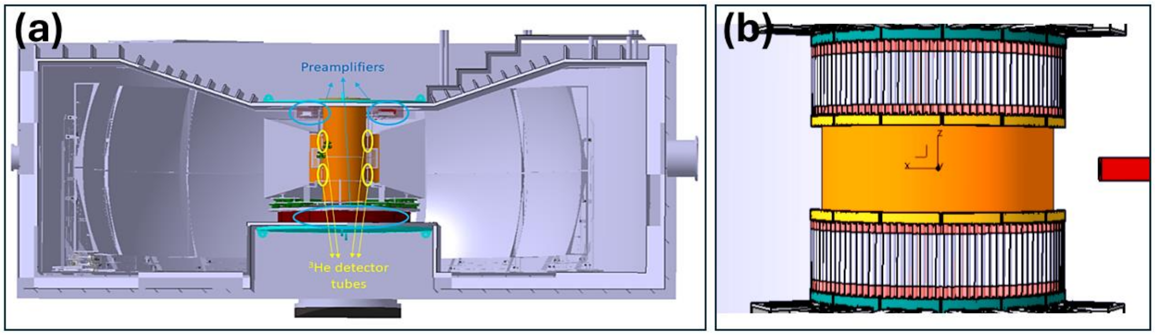

Figure 6 (a) Scattering system and (b) Detectors layout of the MIRACLES backscattering.

The neutron detector system of the MIRACLES instrument consists of 96 ^{3}He tube detectors, arranged in two arrays of 48 tubes, configured in a semicylindrical layout around the sample environment (see Figure 6) with a cylinder radius of ~230 mm, above and below the sample plane (vertical gap sample plane detectors: ~95 mm). The detectors were ordered and are in the manufacturing stage.

Based on the conceptual design of the MIRACLES scattering characterization system, the 96 tube detectors will be arranged in 48 doublets, 24 in the upper bank and 24 in the lower bank covering a scattering angle (*2q*) from 9.5º to 165º. The tubes in the doublet are connected in series, forming a U-shape; this connection is in the extreme closer to the sample plane.

An experimental plan was drafted as an approach to have a preliminary validation of the detection system of MIRACLES. To this purpose, a doublet assembly formed by two ^{3}He tubes were design and manufactured to check the robustness of the U-shaped connection in terms of thermal stability, ground and RF isolation; two preamplifier modules were also tested. Finally, integration tests between the electronic devices included different cable lengths.

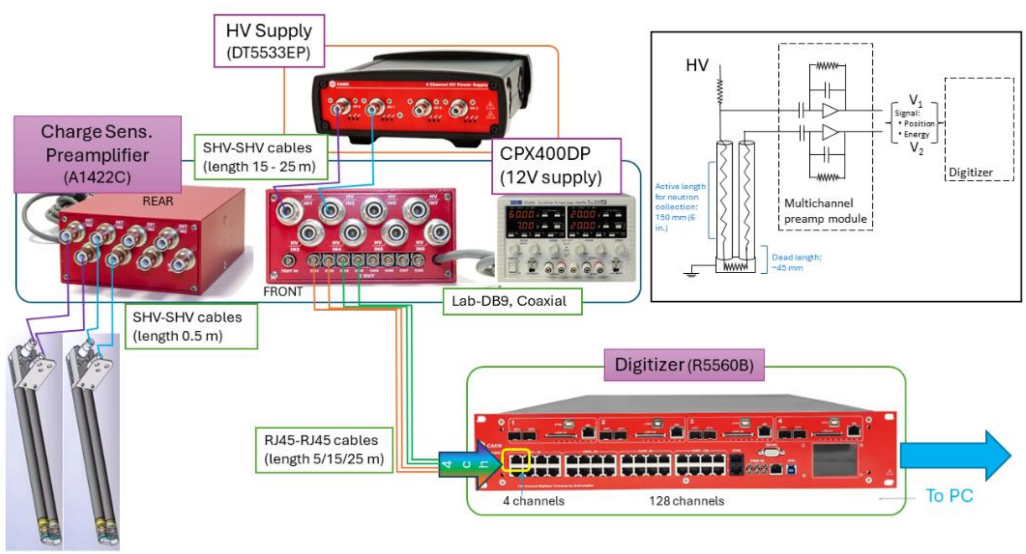

Figure 7 Basic layout of the experiments and test.

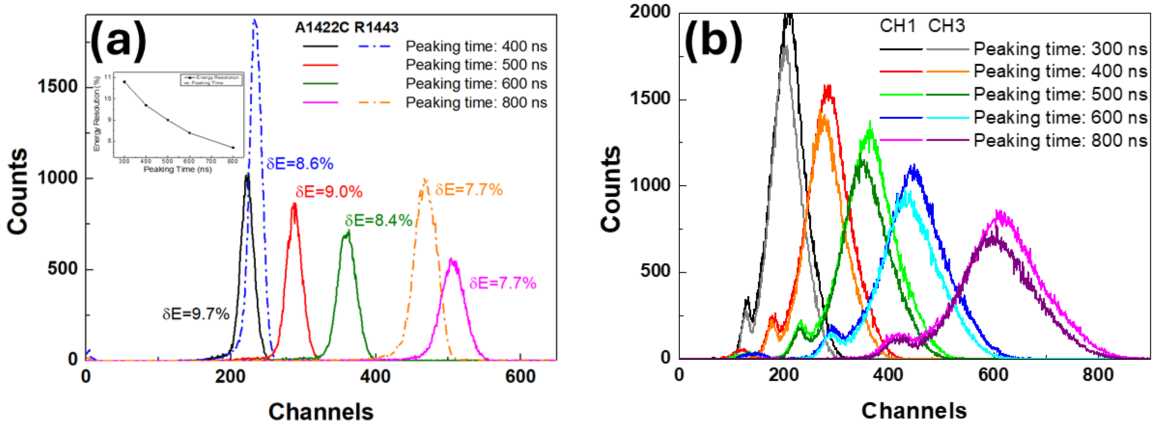

Figure 8 Pulsed height spectra vs peaking time using the A1422 preamp module as a function of peaking time (a) in the counter configuration, including results from the R1443 preamp for comparison (inset: evolution of the energy resolution with peaking time); (b) in the position sensitive configuration.

In these tests, two types of preamp module were evaluated: on one hand, an 8-channel CAEN A1422C module, with preamp gain of 2 V/pC; on the other hand, the 32-channel CAEN R1443A, recently developed, with a preamp gain of 2.25 V/pC. Both preamp modules are suitable for 3He doublet detection, showing an energy resolution ~10%. However, the difference in the height of the raw signal and the significant difference in the decay time confirms that the R1443 device is more suitable for the high-count rates expected in MIRACLES with respect to the A1422 one. The processing parameters such as peaking time and the working HV bias for the front-end detection system, in terms of gas gain and space charge effects, have been optimized. Results suggest an adequate operative bias ranging between 1500 and 1600 V. Finally, the position sensitive measurements show at large a good linearity; however, it also provides useful insight into the optimization of the U-shaped connection resistivity for the MIRACLES spectrometer. A paper with the results has already been submitted for publication.

Experimental end station

Cave

The main building for scientific activities (roof), giving access to the sample position, hosting the sample preparation areas and handling / moving sample environment equipment.

The cave has a design completed with the integration of the utilities, also considering development and planning related to operational aspects, that includes what type of experiments can be performed, where people will be during experiments/maintenance, where access points are and which doors need PSS interlocking, moving parts, etc

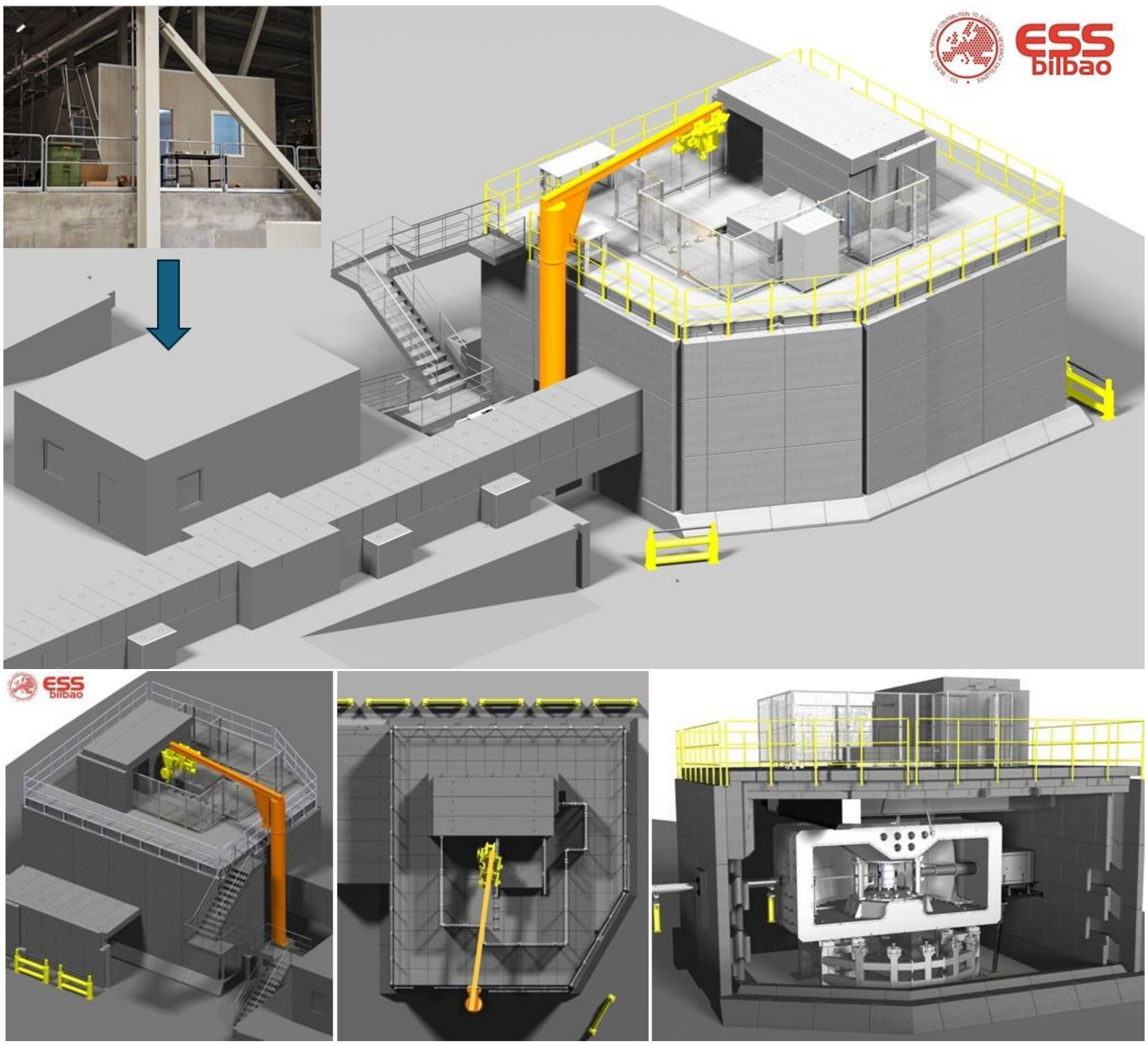

Figure 9 Views of the MIRACLES end station.

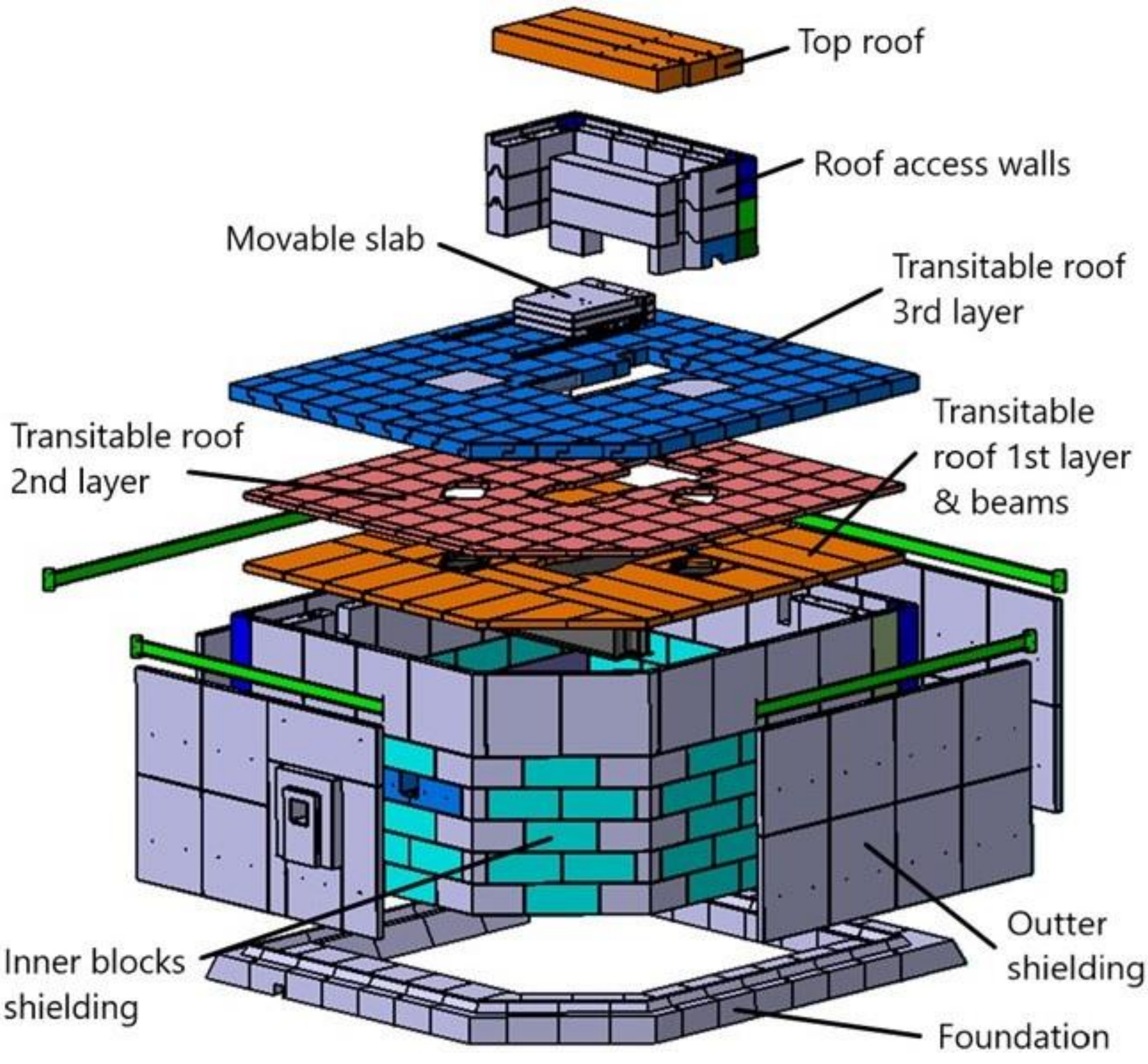

Figure 10 Detailed view of the MIRACLES cave.

<u>Access to hatch and sample loading area</u>

The idea of MIRACLES is to provide suitable and ergonomic experimental areas so that the workflow when carrying out experiments is fluid, safe and efficient (trying to avoid jumping, juggling or acrobatic positions). This implies for instance a sample loading area with easy access (the user must go comfortably down to the flange level).

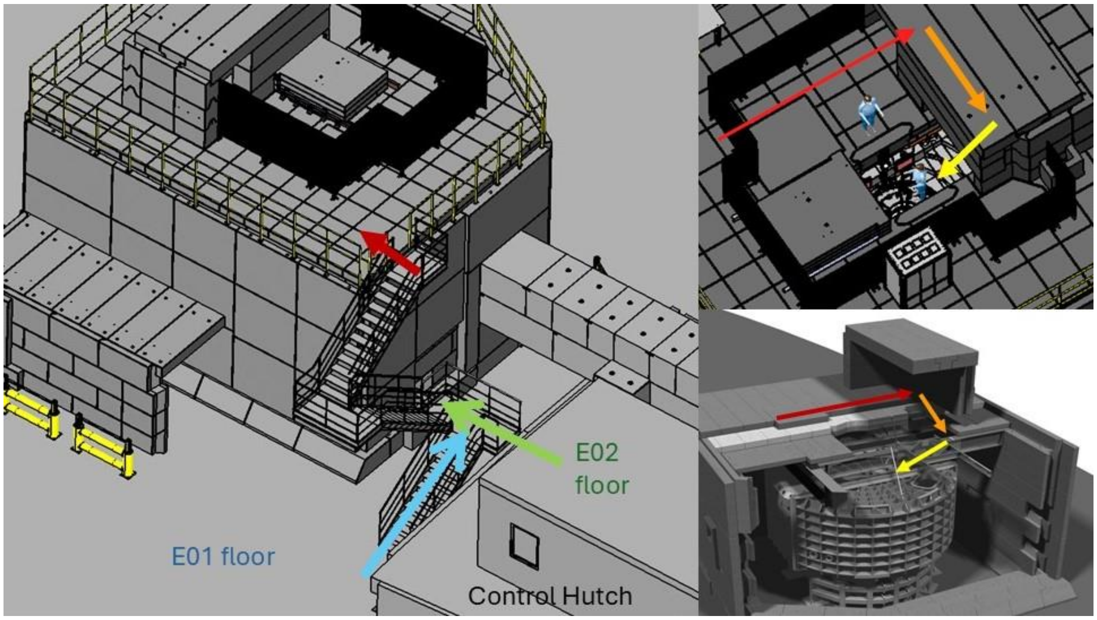

Figure 11 Access to the sample position from E01 and E02 floors (control room).

The sample hatch has opening dimensions of 2000 mm by 1460 mm, allowing for the loading of MIRACLES sample environment equipment onto the sample flange. A two-position stick holder will be fixed to the roof of the cavern blocks to enable ergonomic transfer of the stick to and from the roof, facilitating the rapid release of activated samples.

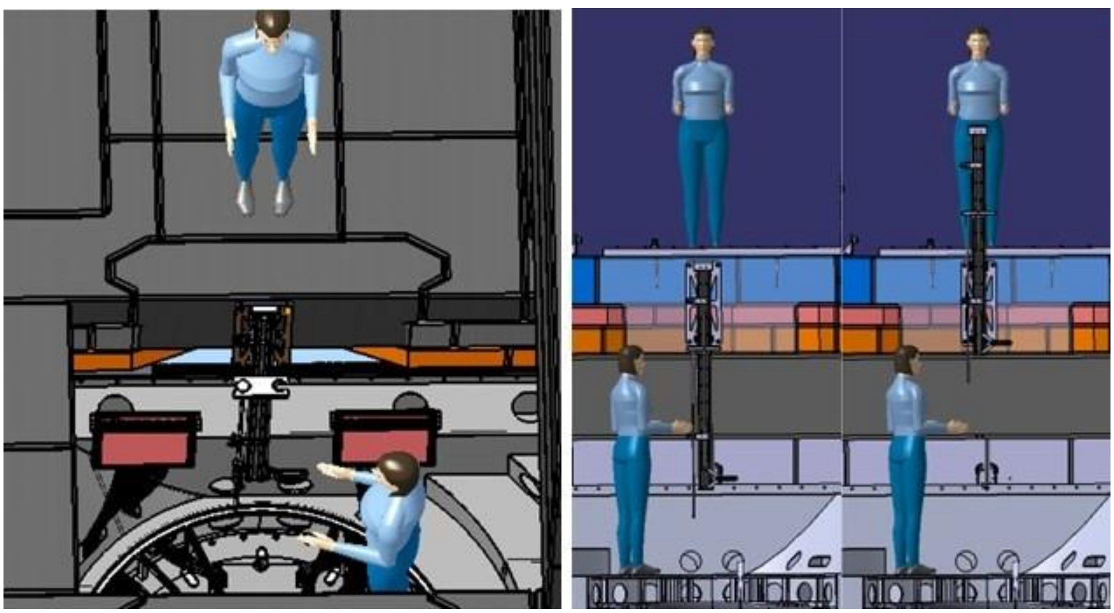

Figure 12 Telescopic stick holder for ergonomics at the sample loading area (top vessel).

Control hutch

After several meetings with ESS Facility Management related to the potential delivery of the Control Hutch by ESS, a final version of the control room was agreed, and now is under construction stage.

Figure 13 Picture of the control room (under construction).

Instrument Hazard Analysis

Instrument Hazard Analysis (IHA) workshop done, and Oxygen Deficiency Hazard (ODH) document uploaded into CHESS (MIRACLES ODH assessment ESS-5487918).

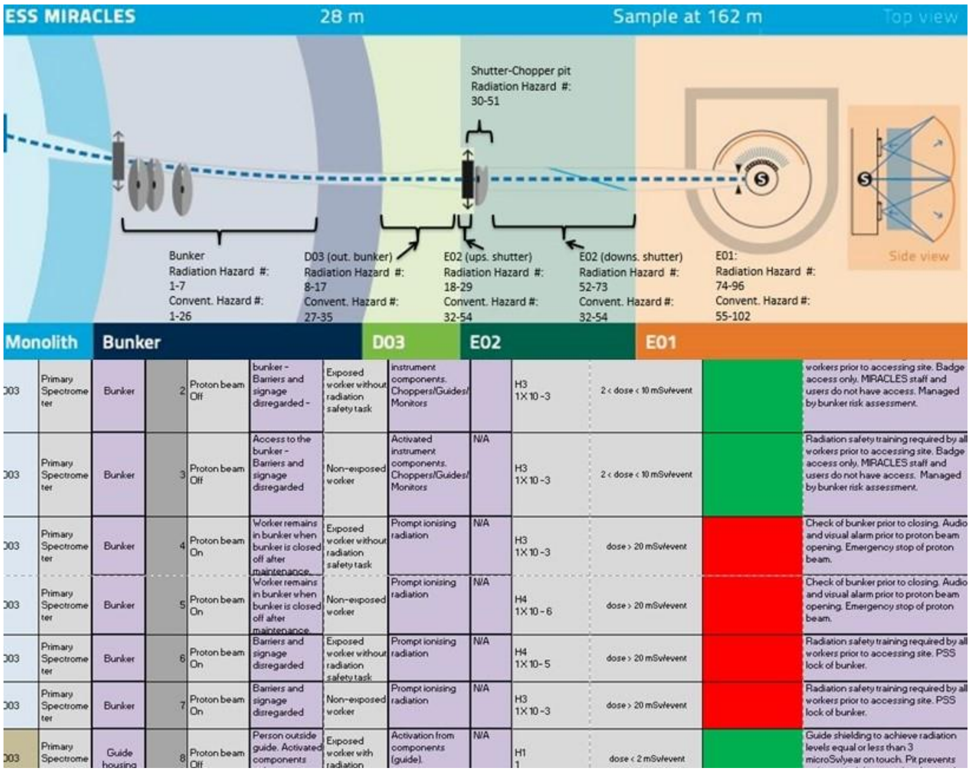

Figure 14 ESS-3235273 IHA MIRACLES.

Infrastructure NSS common projects

<u>Utilities</u>

MIRACLES is part of the Common Utility Project. The utility board is located in the E01/E02 transition, to the right side of the guide (main skid to be decided), and will provide (i) fluids and gases (water, helium and compressed air) to the utility boards distributed inside the cave, (ii) ventilation (conventional).The location of racks was agreed with the instrument team and ESS stakeholders for CEP, CUP, vacuum and PSS.

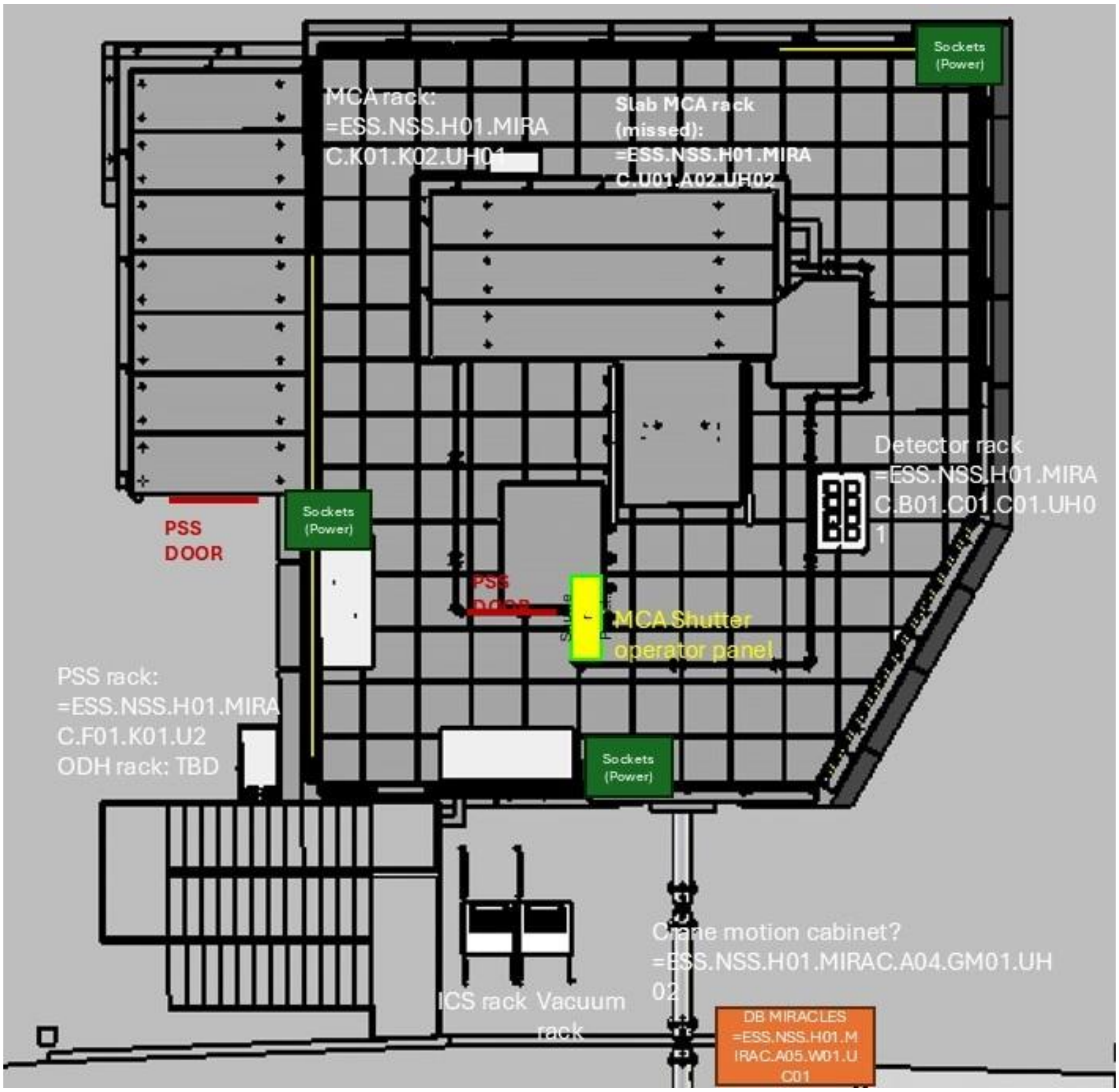

Figure 15 Utilities distribution.

The number of feedthroughs and their location and the allocation of racks were agreed with the instrument team and ESS stakeholders for CEP, CUP, vacuum and PSS.

Electrical

The MIRACLES Team has resumed the discussions with NSS to join the NSS Electrical Project. A requirements document is expected, and once agreed, a formal offer will be the next step.

Sample positioning system

Neutron sources with high flux, in which measurements take less time than average, are envisioned to make use of devices that can mount more than one sample in one run. On the other hand, there is an advantage for all neutron sources in general to measure sequentially series of samples with similar beam conditions and similar environments. In this context, a prototype of a linear sample positioning system was developed and manufactured. A multiple-sample holder device has been specifically designed for cylindrical samples with a 3 cm diameter. This solution can be adapted for flat samples in the future. Moreover, this setup has an additional feature. The mounting of the cans, instead of using threaded holes, uses a bayonet-like fitting. This conveys a fast release of the sample, which can be very convenient in case of activated samples that still deliver a significant dose.

Figure 16 Multiple-sample holder device. 3 samples can be loaded in a linear sample holder.

- Loading up to 3 samples, in agreement with the Z-positioning range.
- Adaptor from treaded connection (sample stick) to bayonet connection.
- Lower ends with bayonet connection for interchangeable order, and also to make a fast release to the lead box.

MIRACLES: rescoping and impact in science

Current status and rescoping

The current MIRACLES project scope includes half scattering-detector angular coverage (i.e., the analyzer, radial collimator and ^{3}He detectors are only placed on the left side of the scattering vessel).

The completion of the instrument will include the full coverage of the scattering system: a second analyzer, another radial collimator and ^{3}He detectors on the right side. The upgrade can be done **without any disruption of the operation program**, since all the integration, installation and adjustment features were already manufactured, in anticipation to this completion exercise.

In this case, one half of this right-side analyzer will be covered with Si(111) crystals, whereas the other half will utilize Si(311) peaks, similar to other backscattering instruments (BASIS, DNA). The idea is to achieve higher Q values.[†]

There is the idea that Si(333) reflections can be exploited using the Si(111) crystals. Although some Si(333) peaks have been observed in BASIS, there is no proof that the reflections can be utilized for QENS measurements; and if so, this can only be demonstrated in MIRACLES at full power, i.e., at 5 MW. That is why we prefer to use, in the **first decade** of operation of MIRACLES, Si(311) crystals.

Strategy for rescoping

The feasibility of Si(333) reflections to carry out QENS measurements need to be demonstrated, so the completion needs to be done during hot commissioning.

Thus, the strategy for the rescoping we propose is the following:

1) To install the detector banks of the right side + preamps (the digitizer will be available with extra channels for this right-side ^{3}He tubes).
2) To install the right-side radial collimator.
3) To install the frame of the analyzer, prior to hot commissioning.
4) To install ½ of the right-side analyzer panels with Si(111) crystals (we recommend the top part).
5) To wait until Si(333) reflections are tested to decide the completion of the bottom part with either Si(111) crystals or Si(311) crystals. To determine if the Si(333) study has to be carried out only with 2 MW or at an earlier stage (is it a question of noise-statistics, or is it a question of background?).

Impact of rescoping in science

The biggest advantage of using Si333 or Si311 in neutron backscattering instruments is their ability to extend both the energy and Q-range, enabling more precise extraction of the Elastic Incoherent Structure Factor (EISF). This unique capability opens new possibilities for research and

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aims to achieve very high-count rates by collecting the full length of the ESS pulse—a critical need for life scientists working with limited biological samples.

The MIRACLES spectrometer will offer a wide range of energy resolution, spanning from 2 to 32 µeV. Combined with its broad accessible Q-range and ability to achieve very small energy transfers, MIRACLES will facilitate the investigation of a wide variety of biological and biophysical systems. This design also addresses challenges such as small sample sizes, fixed energy resolution, and limited accessible Q and energy ranges, thereby reinforcing existing research fields and opening new avenues of study.

In particular, the dynamics of liquids confined in nanoscale geometries have greatly benefitted from Quasi-Elastic Neutron Scattering (QENS) techniques. Emerging fields now focus on confined complex fluids, such as mesomorphic phases and multicomponent systems, which are crucial for technologies like electrolyte membranes, nanochemistry, and nanofiltration. Confinement and interfacial effects introduce spatial restrictions and dynamic heterogeneities, including glassy dynamics, which broaden the relaxation time distribution. Traditional QENS methods struggle with these complexities, but the broad dynamic range provided by MIRACLES could overcomes these limitations, removing the need for multiple spectrometers. The wide Q-range also enables more accurate extraction of the EISF and better comparison with theoretical models and molecular simulations of confined molecules. This is particularly important for studying diluted systems, such as fluids in nanotubes or nanoporous membranes, where higher flux is essential. There is significant interest in the life sciences for such measurements, especially for understanding the interactions and dynamics of biological organisms, complex systems, and the fundamental role of water in these systems. MIRACLES will enable to explore these areas with its combination of short counting times, variable resolution, and extended energy range.

There are two main effects in the rescoping exercise of MIRACLES.

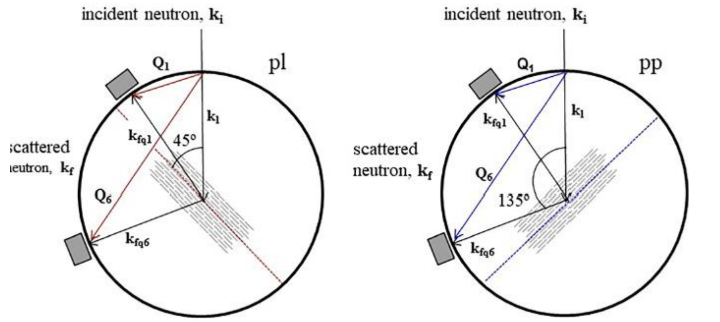
Anisotropy dynamics

On one hand, it is interesting to test the anisotropy of the dynamics of water in some materials, like oriented films.‡

- An example can be shown in hydration in layered clays.
- In neural fibers such as nerve, white matter in spinal cord, or white matter anisotropic water diffusion is sensitive to the underlying tissue microstructure and provides a unique method of assessing the orientation and integrity of these neural fibers. With the full capability from both instrument and source smaller samples can be used and systematic studies using various fibers or membrane proteins will allow for pertinent pathological models.

‡ *Applied Clay Science 201 (2021) 105928 & J-Parc new data*

- With full coverage, simultaneous measurements in the transmission mode and in the reflection mode can be carried out, with exactly the same conditions.
- With the current, scope, the only option is to rotate every time the samples, and measurements will not be done at the same time.



<u>Flux increase (and likely Q-range increase)</u>

Depending on the feasibility of the Si(333) reflections to carry out QENS measurements, the impact of full coverage in the MIRACLES science case can be:

- Assuming Si(333) can be used: Neutron flux will increase a factor of 2 (100%). This opens new windows to hidden features that require high flux on sample.
- Assuming Si(333) cannot be used, then full coverage consists of ½ Si(111) and ½ Si(311): Neutron flux will increase 50% working with Si(111) reflections. Moreover installing Si(311) analyzer will widen the Q range leading to higher Q values (see kinematic range figures on page 3), plus a wider bandwidth around the elastic (larger energy-gain side).

Expanding the Q range to Q>3 $Å^{-1}$ will allow exploration of restricted and confined diffusion effects at the atomic length scale (of the order of d < 2 Å).