

## KEEPING SAMPLES UNDER CONTROL

Leading beneficiary: within INFRADEV4: ILL or ESS

Partners: see individual WU

Please do not forget evtl University partners!

Estimated budget (in person months, other direct cost) and tentative distribution per partner

To be defined

**Abstract of your innovative activity:** *(please make sure that you mention the following points)*

The vast majority of neutron beamtime at Research Infrastructures is provided on scientific merit to specific user groups. Both the evaluation system as well as the scheduling process has been well established since many years focusing on scientific excellence as well as user needs. Successful scientific use is essential for the relevance of research infrastructure in the European research environment and a driver to push their methodological possibilities forward.

With an emphasis on in-situ / in-operandi studies on 'real-world' e.g. more complex samples the need for an integrated approach combining various methods and characterisation tools increases. At the same time the specific requirements for keeping track of sample-related 'meta-data' heightens. Except for the specific shipping and handling data required for an individual experiment, no effort was made to provide a (cross-facility) overview of the meta-data related to the sample. On the other hand, only the sample-independent properties are published and available in the open literature. This information might not be sufficient in respect to the specific research project. Other aspects such as knowing the current state (prior or after conditioning), sample mount, isotope composition, activation, additional characterisation (meta-data only; it has been measured WHERE, WHEN, WHAT), safety concerns (e.g. cultural heritage samples), remote handling and associated logistics especially in respect to life science samples (and their hazards).

The here-proposed cross-facility approach should not be an administrative burden but rather a service provided for the users as well as the scientists working at the facilities.

The following work packages could be envisaged. **Work package 1** on 'open software standard for SE measurements, control data and metadata' has currently been proposed as an independent project but could actually be an essential part of this broader undertaking. **Work package 2** focuses on 'tracking samples, characterization and safety evaluation' both in respect to administrative software as well as hardware tools. **Work package 3** covers the 'radiological characterization and isotope composition' and **work package 4** the 'crystallographic characterization' in respect to the specific needs of the neutron investigation. **Work packages 5 and 6** cover the specific needs in respect to 'cultural heritage' and 'life science samples', respectively.

**Work Package 1: open software standards for SE measurements , control data and metadata**

Facility Partners        ESS, HZB, ILL, ISIS, MLZ, PSI

Estimated budget:        TBD

Details are provided in a separate document (submitted already)

### **Work Package 2: sample tracking and characterization**

Facility Partners:        potentially all neutron facilities

Estimated budget:        TBD

Each accepted proposal will have a number of associated samples, and given the number of users and proposals it is of great importance to have a way to track the history of each sample. It could be envisaged that each sample be assigned a bar code of sorts that stays with the sample throughout its existence. All aspects of the sample's journey in addition to the neutron experiment meta-data should be stored in a database, attached to this number, such as what types of characterization it underwent, e.g. x-ray, NMR, light scattering, etc. and what conditions. The types of characterization and the conditions would be recorded at each step. This will benefit the user by having a history of what methods were used. It can be critical to analysing and making sense of the data gathered at that time, and instrumental for future experiments to develop processes for a particular system. Other information such as composition is a given, but more importantly how that composition affects the safety evaluation, which information will also be attached to the unique sample number.

### **Work Package 3: radiological characterisation**

Facility Partners:        potentially all neutron facilities

University Partners

Estimated budget:        TBD

Up-to-date information on sample activation and their isotope composition is pre-requisite for safe shipping as well as for scheduling neutron experiment at different (neutron and non-neutron) facilities.

### **Work Package 4: x-ray characterisation**

Facility Partners:        potentially all neutron facilities

University Partners

Estimated budget:        TBD

X-ray characterisation of crystalline samples is an essential pre-requisite for many neutron experiments. Often characterisation is performed on 'similar' samples (either part of neutron sample, from the same badge or even only similarly produced samples) only and actually not on the same crystal. The later is relevant when keeping track of individual samples. This requires the development of (user-friendly) set-up using hard x-rays.

### **Work Package 5: security for cultural heritage**

Facility Partners:        potentially all neutron facilities

University Partners

Estimated budget:        TBD

Cultural heritage is an area that can benefit from neutron research. Items such as priceless pieces of art and archaeological finds can be investigated in a non-destructive way. In order to assure the safety of such pieces to museums and universities, a safe room is imperative. In order for the safe room to be successful a number of security measures must be in place. Not only should the room itself have strict access control, but also inside the room there is a need for

storage closets of various sizes that are further controlled. The room must have the ability to accept crated items, as well as equipment to open and reseal them.

**Work Package 6: security for life science samples**

Facility Partners: potentially all neutron facilities

University Partners

Estimated budget: TBD

Life science samples have specific needs in respect to their safe handling both prior and during the experiment. Potential risk might be mitigated with remote handling.