Proposal Writing

Peter Fouquet

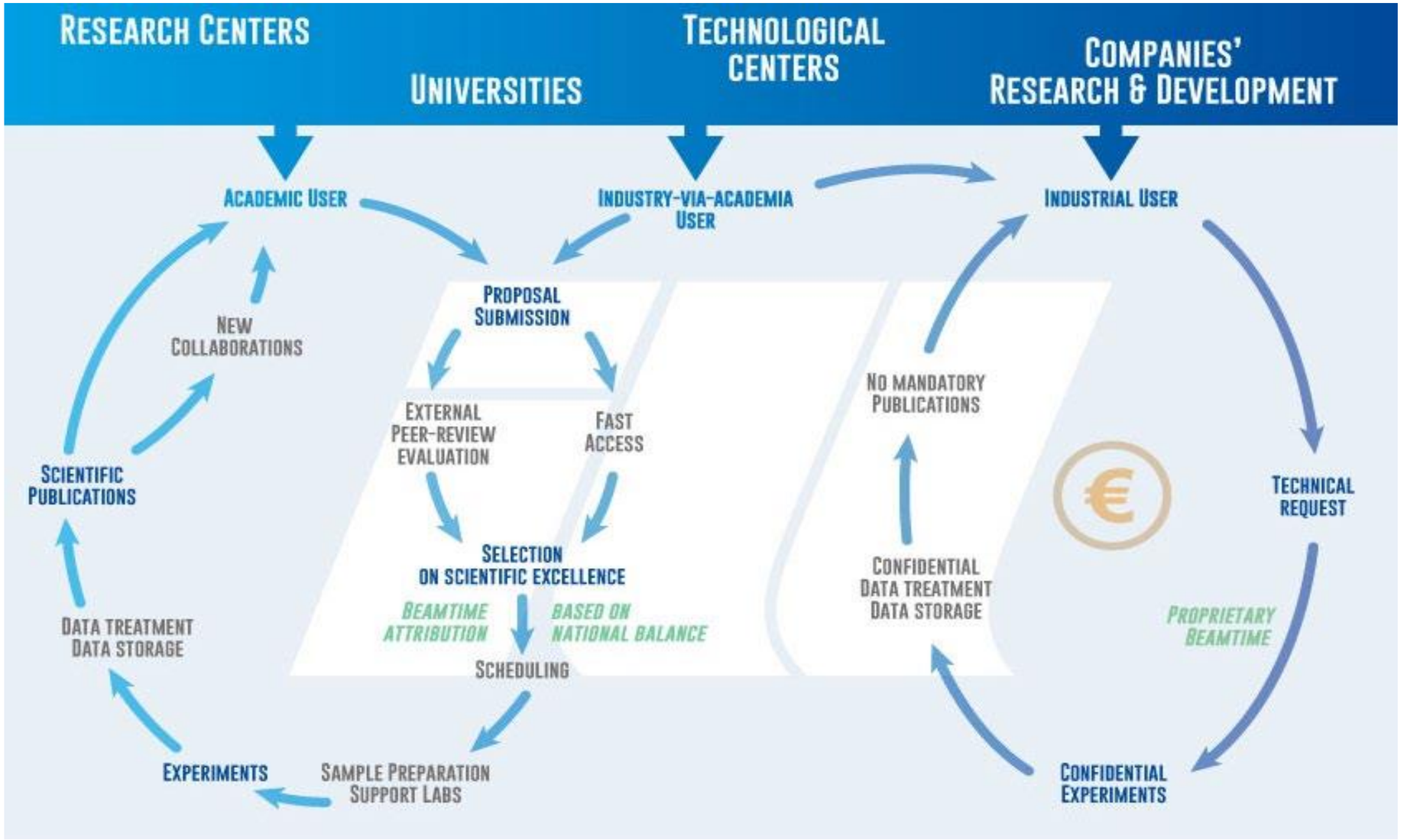
Special mention:
Giovanna Cicognani

1st School on Neutron Scattering in Björkliden 2012
2nd Winterschool on Neutron Scattering for Soft Matter in Gothenburg/Saclay 2013

... organised by Uppsala University with Chalmers and Röntgen/Ångström Cluster

NEUTRONS FOR SOCIETY

How to request beamtime at the ILL (typical for large scale facilities)



Review criteria

- Scientific *excellence*: Novelty, significance, and potential impact
- *Feasibility*: *Experimental* design, required resources, and preparatory work
- Neutron/X-ray *suitability*: Appropriateness of neutron or X-ray methods for the research question
- Potential *Outcomes*: Clear hypothesis and potential for high-quality publications
- Team *qualifications* and previous *track record*

Proposal management

Create new proposals

Electronic Proposal Submission

New Proposal

Easy Proposal Submission

New EASY Proposal

CRG Proposal Submission

D23

IN12

IN22

TEST submission

New TEST proposal

Handle existing proposals

Current proposals

Show and edit proposals

Resubmit proposal

Proposal search

Search for proposals

User Office access

Proposal integration

Proposals to transfer

NEUTRONS FOR SOCIETY

Giovanna CICOGNANI | Sign out | Switch to user: | Switch | Visitors' club

The ILL User Club

USER CLUB

Proposals | Review processes | Experiments | Instrument | Personal data/Training | Experimental report | ILL User Club administration

User Office Quick Proposal Access

Proposal | Edit

Proposal Description

1. Characteristics
2. Proposers
3. Instruments
4. Sample
5. Safety
6. Environment
7. Abstract
8. Description

Actions

Save
Submit
Delete
Transfer

Proposal #93027 (Guidelines)

Main information

Title (8 / 140 ch.): TEST GIO

College: 1 Applied materials science, instrumentation & techniques

Category: 1-01 Metallury, metal physics

Main research area: Engineering

Keywords:

Already submitted to other facilities: ○ Yes ◉ No

Societal Indicators:
- ☐ Fundamental Science
- ☑ Earth & Environment
- ☐ Energy
- ☐ Health
- ☐ ICT*
- ☐ Other functional materials (please specify)
- ☐ Other (please specify)

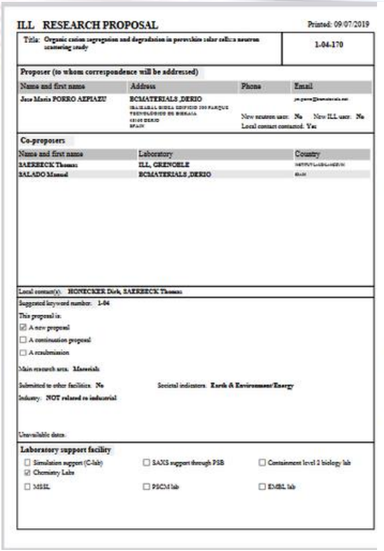
Proposal history

Type of proposal: ◉ New ○ Continuation ○ Resubmission

Laboratory support

Mechanical preparation support needed: ○ Yes ◉ No

(0 / 250 ch.)


ILL RESEARCH PROPOSAL

Printed: 09/07/2019

Title: Organic cation segregation and degradation in perovskite solar cells: a neutron scattering study

1-04-170

Proposer (to whom correspondence will be addressed)

Name and first name	Address	Phone	Email
Jose Maria PORRO ALPIAZU	ICMATERIALS_DIEXIO		

Co-proposers:

Name and first name	Laboratory	Country
SAEREECK Thomas	ILL, GRENOBLE	
SALADO Manuel	ICMATERIALS_DIEXIO	

Local contact(s): HONECKER Dirk, SAEREECK Thomas

Suggested keyword number: 1-04

This proposal is:
- ☑ A new proposal
- ☐ A continuation proposal
- ☐ A resubmission

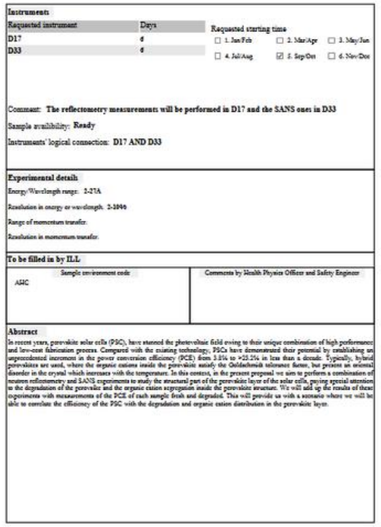
Main research area: Materials

Submitted to other facilities: No — Societal indicators: Earth & Environment/Energy

Industry: NOT related to industrial

Unavailable dates:

Laboratory support facility
- ☐ Simulation support (C-lab)
- ☑ Chemistry Labs
- ☐ MSSL
- ☐ SANS support through PSB
- ☐ PSCM lab
- ☐ Containment level 2 biology lab
- ☐ EMBL lab


Instrument

Requested instrument	Days	Requested starting time
D17	6	☐ 1. Jan/Feb ☐ 2. Mar/Apr ☐ 3. May/Jun ☐ 4. Jul/Aug ☑ 5. Sep/Oct ☐ 6. Nov/Dec
D33	6	

Comment: The reflectometry measurements will be performed in D17 and the SANS ones in D33

Sample availability: Ready

Instruments' logical connection: D17 AND D33

Experimental details

Energy/Wavelength range: 2-27Å

Resolution in energy or wavelength: 3-10%

Range of momentum transfer:

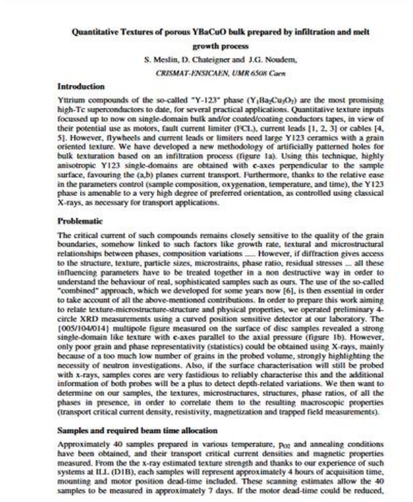
Resolution in momentum transfer:

To be filled in by ILL

Sample environment code	Comments by Health Physics Officer and Safety Engineer
ASC	

Abstract

In recent years, perovskite solar cells (PSC), have stunned the photovoltaic field owing to their unique combination of high performance and low-cost fabrication process. Compared with the existing technology, PSCs have demonstrated their potential by establishing an unprecedented increment in the power conversion efficiency (PCE) from 3.8% to >25.5% in less than a decade. Typically, hybrid perovskites are used, where the organic cations inside the perovskite satisfy the Goldschmidt tolerance factor, but present an oriental disorder in the crystal which increases with the temperature. In this context, in the present proposal we aim to perform a combination of neutron reflectometry and SANS experiments to study the structural part of the perovskite layer of the solar cells, paying special attention to the degradation of the perovskite and the organic cation segregation inside the perovskite structure. We will add up the results of these experiments with measurements of the PCE of each sample fresh and degraded. This will provide us with a scenario where we will be able to correlate the efficiency of the PSC with the degradation and organic cation distribution in the perovskite layer.


Quantitative Textures of porous YBaCuO bulk prepared by infiltration and melt growth process

S. Meslin, D. Chateigner and J.G. Noudem,

CRISMAT-ENSICAEN, UMR 6508 Caen

Introduction

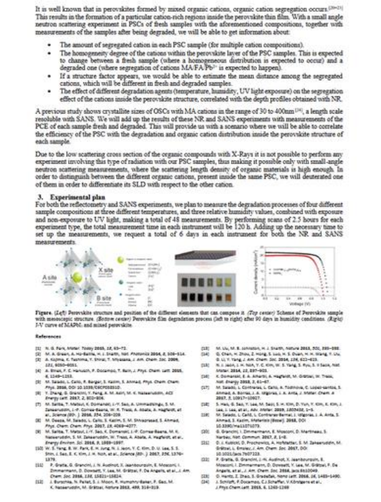
Yttrium compounds of the so-called "Y-123" phase ($Y_1Ba_2Cu_3O_7$) are the most promising high-Tc superconductors to date, for several practical applications. Quantitative texture inputs focussed up to now on single-domain bulk and/or coated/coating conductors tapes, in view of their potential use as motors, fault current limiter (FCL), current leads [1, 2, 3] or cables [4, 5]. However, flywheels and current leads or limiters need large Y123 ceramics with a grain oriented texture. We have developed a new methodology of artificially patterned holes for bulk texturation based on an infiltration process (figure 1a). Using this technique, highly anisotropic Y123 single-domains are obtained with c-axes perpendicular to the sample surface, favouring the (a,b) planes current transport. Furthermore, thanks to the relative ease in the parameters control (sample composition, oxygenation, temperature, and time), the Y123 phase is amenable to a very high degree of preferred orientation, as controlled using classical X-rays, as necessary for transport applications.

Problematic

The critical current of such compounds remains closely sensitive to the quality of the grain boundaries, somehow linked to such factors like growth rate, textural and microstructural relationships between phases, composition variations ..... However, if diffraction gives access to the structure, texture, particle sizes, microstrains, phase ratio, residual stresses ... all these influencing parameters have to be treated together in a non destructive way in order to understand the behaviour of real, sophisticated samples such as ours. The use of the so-called "combined" approach, which we developed for some years now [6], is then essential in order to take account of all the above-mentioned contributions. In order to prepare this work aiming to relate texture-microstructure-structure and physical properties, we operated preliminary 4-circle XRD measurements using a curved position sensitive detector at our laboratory. The [005/104/014] multipole figure measured on the surface of disc samples revealed a strong single-domain like texture with c-axes parallel to the axial pressure (figure 1b). However, only poor grain and phase representativity (statistics) could be obtained using X-rays, mainly because of a too much low number of grains in the probed volume, strongly highlighting the necessity of neutron investigations. Also, if the surface characterisation will still be probed with x-rays, samples cores are very fastidious to reliably characterise this and the additional information of both probes will be a plus to detect depth-related variations. We then want to determine on our samples, the textures, microstructures, structures, phase ratios, of all the phases in presence, in order to correlate them to the resulting macroscopic properties (transport critical current density, resistivity, magnetization and trapped field measurements).

Samples and required beam time allocation

Approximately 40 samples prepared in various temperature, p_{O2} and annealing conditions have been obtained, and their transport critical current densities and magnetic properties measured. From the the x-ray estimated texture strength and thanks to our experience of such systems at ILL (D1B), each samples will represent approximately 4 hours of acquisition time, mounting and motor position dead-time included. These scanning estimates allow the 40 samples to be measured in approximately 7 days. If the motor dead-time could be reduced,


It is well known that in perovskites formed by mixed organic cations, organic cation segregation occurs [29-31]. This results in the formation of a particular cation-rich regions inside the perovskite thin film. With a small angle neutron scattering experiment in PSCs of fresh samples with the aforementioned compositions, together with measurements of the samples after being degraded, we will be able to get information about:

- The amount of segregated cation in each PSC sample (for multiple cation compositions).
- The homogeneity degree of the cations within the perovskite layer of the PSC samples. This is expected to change between a fresh sample (where a homogeneous distribution is expected to occur) and a degraded one (where segregation of cations MA/FA/Pb^{2+} is expected to happen).
- If a structure factor appears, we would be able to estimate the mean distance among the segregated cations, which will be different in fresh and degraded samples.
- The effect of different degradation agents (temperature, humidity, UV light exposure) on the segregation effect of the cations inside the perovskite structure, correlated with the depth profiles obtained with NR.

A previous study shown crystallite sizes of OSCs with MA cations in the range of 30 to 400nm [32], a length scale resolvable with SANS. We will add up the results of these NR and SANS experiments with measurements of the PCE of each sample fresh and degraded. This will provide us with a scenario where we will be able to correlate the efficiency of the PSC with the degradation and organic cation distribution inside the perovskite structure of each sample.

Due to the low scattering cross section of the organic compounds with X-Rays it is not possible to perform any experiment involving this type of radiation with our PSC samples, thus making it possible only with small angle neutron scattering measurements, where the scattering length density of organic materials is high enough. In order to distinguish between the different organic cations, present inside the same PSC, we will deuterated one of them in order to differentiate its SLD with respect to the other cation.

3. Experimental plan

For both the reflectometry and SANS experiments, we plan to measure the degradation processes of four different sample compositions at three different temperatures, and three relative humidity values, combined with exposure and non-exposure to UV light, making a total of 48 measurements. By performing scans of 2.5 hours for each experiment type, the total measurement time in each instrument will be 120 h. Adding up the necessary time to set up the measurements, we request a total of 6 days in each instrument for both the NR and SANS measurements.

Figure. (Left) Perovskite structure and position of the different elements that can compose it. (Top center) Scheme of Perovskite sample with monocrystic structure. (Bottom center) Perovskite film degradation process (left to right) after 90 days in humidity conditions. (Right) UV curve of MAPbI3 and mixed perovskite.

References

https://userclub.ill.eu/

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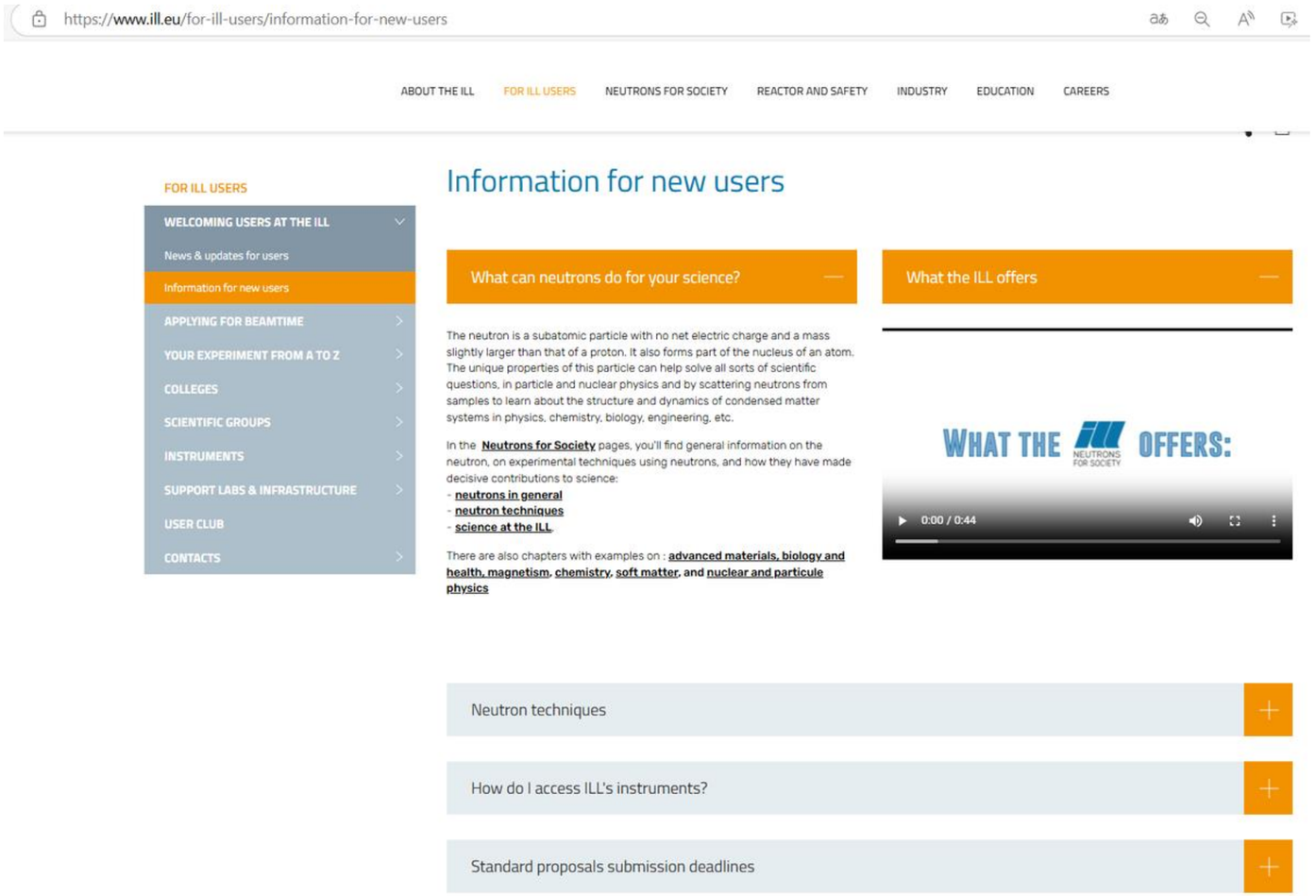
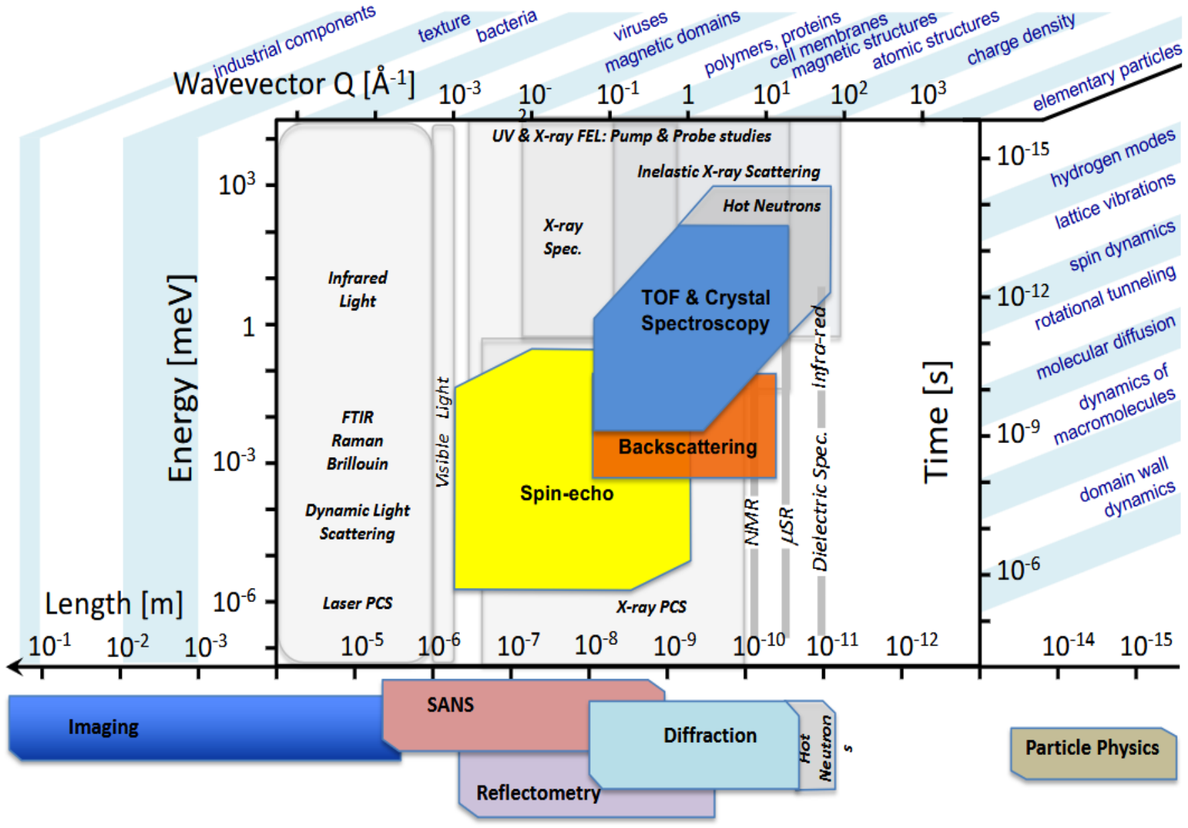
Proposal writing –plan your proposal

- What are you trying to *learn* from neutron scattering
- Which technique best *matches* your needs
- Which *instrument* do you need
- What sample *environment* do you need
- ***Discuss with instrument scientist !!!***





Instruments list

To maintain its status as leader in neutron science, the ILL has constantly upgraded its instruments and infrastructures over the last 50 years. The latest modernisation exercise - the ENDURANCE programme (2016-2023) - will continue to develop instrumentation and support services with a view to maintaining the Institute's world-leading position for another decade at least. The instruments which have been/are being upgraded within the ENDURANCE programme show its logo in their main page.

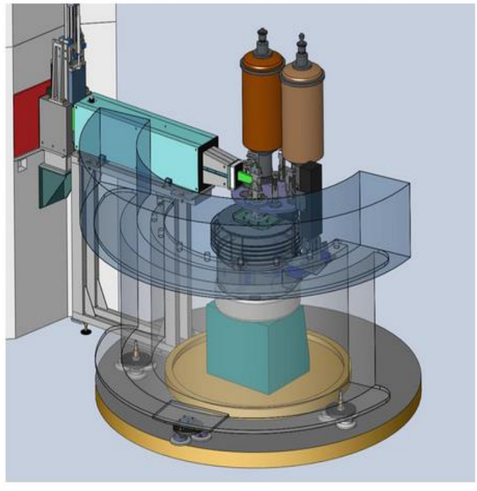
Select your instrument

INSTRUMENT OVERVIEW

D2B

High-resolution two-axis diffractometer

D2B



D2B - HIGH-RESOLUTION TWO-AXIS DIFFRACTOMETER

D2B is very high-resolution powder diffractometer designed to achieve the ultimate resolution, limited only by powder particle size ($\Delta d/d$ 5x10^{-4}), but is was built so that an alternative high flux option, with resolution comparable to that of D1A, but much higher intensity, could be chosen at the touch of a button.

Applications

- The structural chemistry of non-rigid molecules
- Ab-initio structure solution from powders
- Crystal and magnetic structure determination of powder compounds (even small samples)
- Dependance in temperature/pressure/magnetic field structural (or magnetic) studies for powders

Instrument layout

D2B seen from behind the detector, i.e. from the opposite of the normal access to the experimental area.

Proposal writing –structure and content

- Clear objective

  Clear, concise summary of the project Brief mention of the scientific aims and expected outcomes

- Scientific rationale

  Highlight the novelty of the proposed work

  Why is this experiment important ? What

  gap in knowledge does it fill ?

- Methodology

  Detailed description of the experimental setup Specify the neutrons scattering technique to be used Explain how the technique address your research question

- Expected results and impact

  What outcomes are anticipated from the experiment?

  How will these results contribute to the field ?

- Timeline and Beam Time Request

  Estimate the required number of days for the experiment

  Suggest a feasible timeline for completing the work

- Preliminary data and background

  Include relevant previous work and literature Provide any initial data or pilot studies to strengthen your case -> *Add Graphs !*

- References

  Cite literature that supports the experimental approach

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Tips for writing successful proposals

- Start early

  Proposals require careful planning and preparation. Give yourself time to gather necessary data and refine your ideas
- Know your audience

  Reviewers may not always be experts in your specific field, so make sure the proposal is accessible to a broad scientific community
- Be concise

  Stick to the point and avoid excessive jargon
- Provide supporting data

  Include any preliminary results that shows the experiment is feasible
- **Contact the experts!**

  Engage with facility staff or experienced users to refine your proposal and increase its strength

Common mistakes to avoid

- Unclear objectives

  Vague or poorly defined scientific aims
- Overly ambitious

  Be realistic about what can be achieved
- Lack of feasibility

  Failing to clearly explain how the experiment can be performed at the facility
- Weak background

  Insufficient background or literature support can undermine the proposal's impact

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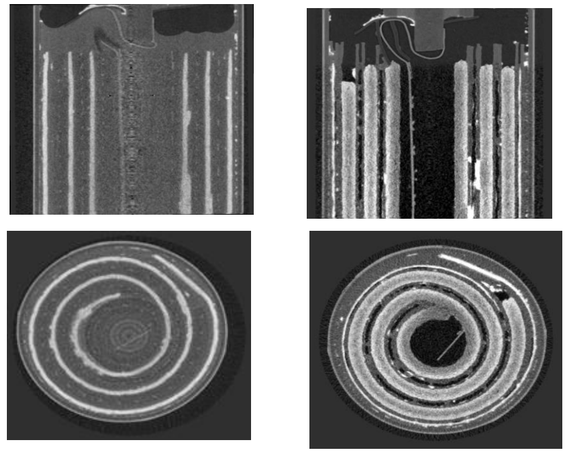
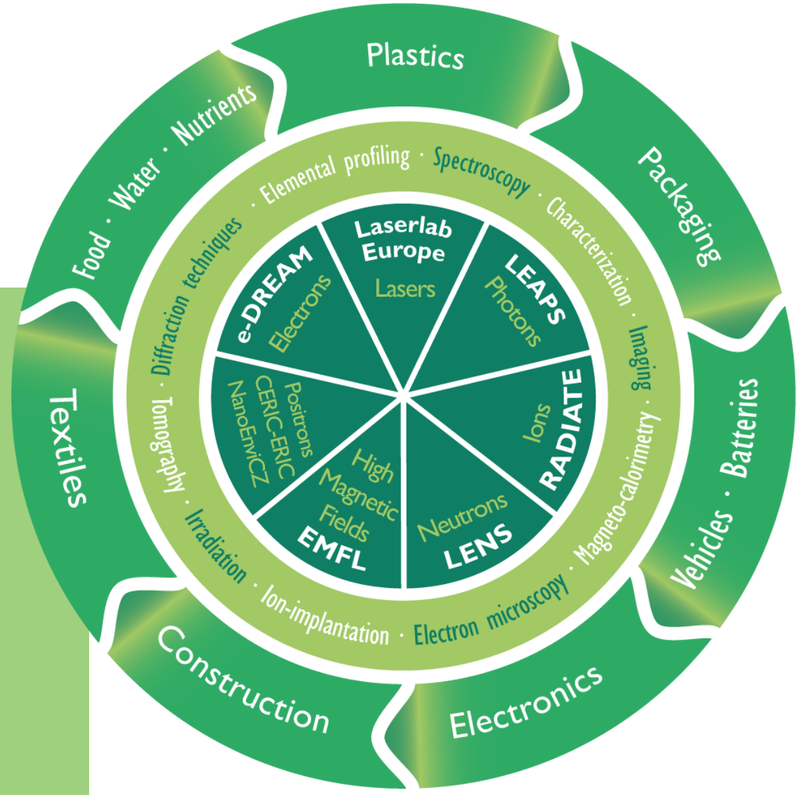
The hub for battery research

The **ReMade@ARI** project provides scientists in academia and industry
with analytical tools to explore the properties of recyclable materials for batteries





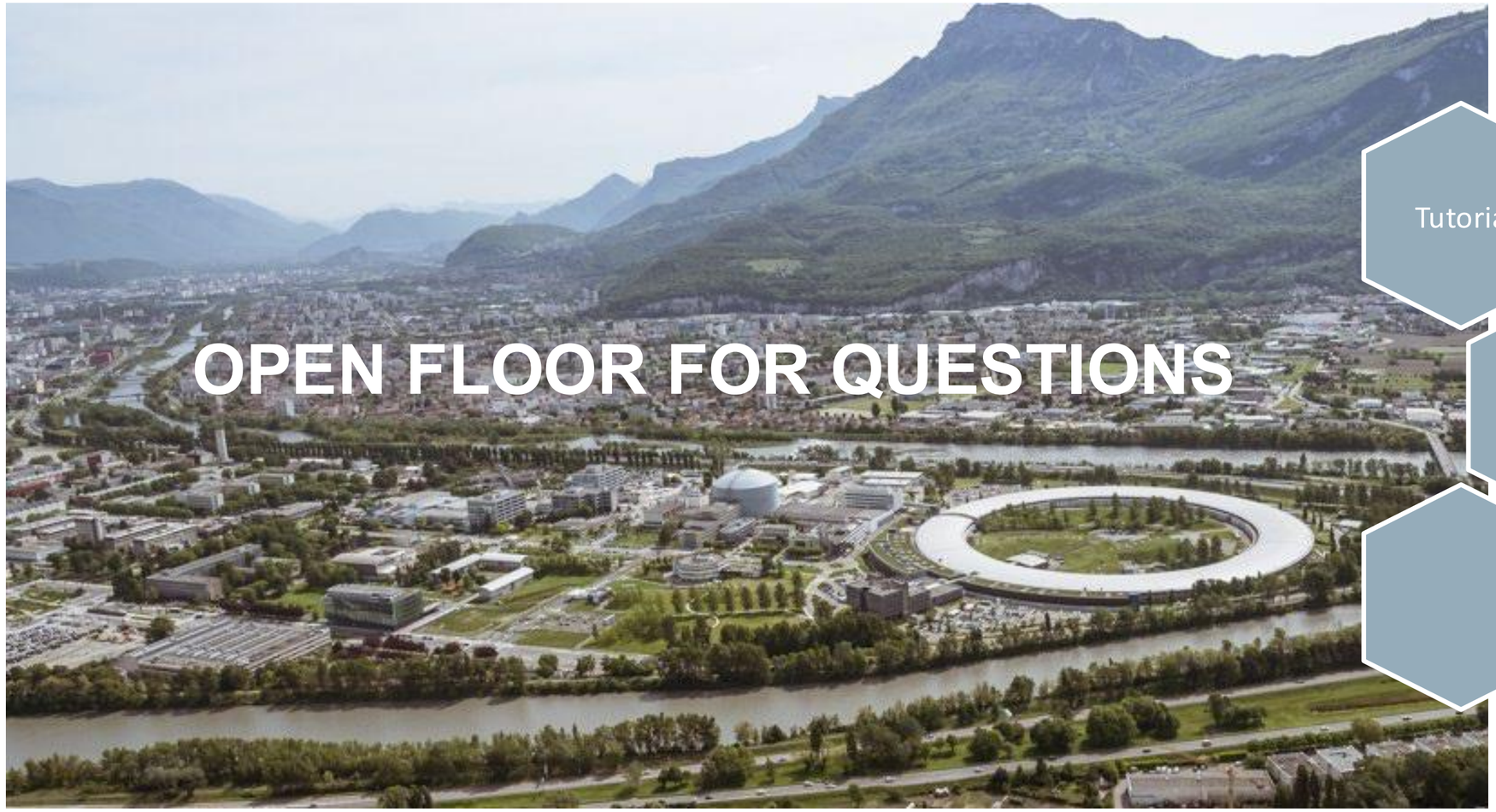
Contact us

info@remade-project.eu for general information
sciencesupport@remade-project.eu for scientific support
industry@remade-project.eu for industrial support

remade-project.eu

The consortium

More than 50 analytical research infrastructures from the ARIE network (arie-eu.org) comprising synchrotrons, neutron sources, lasers, electron microscopes, ion & positron beams, & high magnetic field facilities.



Tutorial

Facility website

RESOURCES & SUPPORT

Proposal writing hints

User Office and Instrument Scientists

CONTACT

https://www.ill.eu/for-ill-users/applying-for-beamtime/standard-access/step-by-step-standard-proposal-submission-guide/proposal-writing-hints

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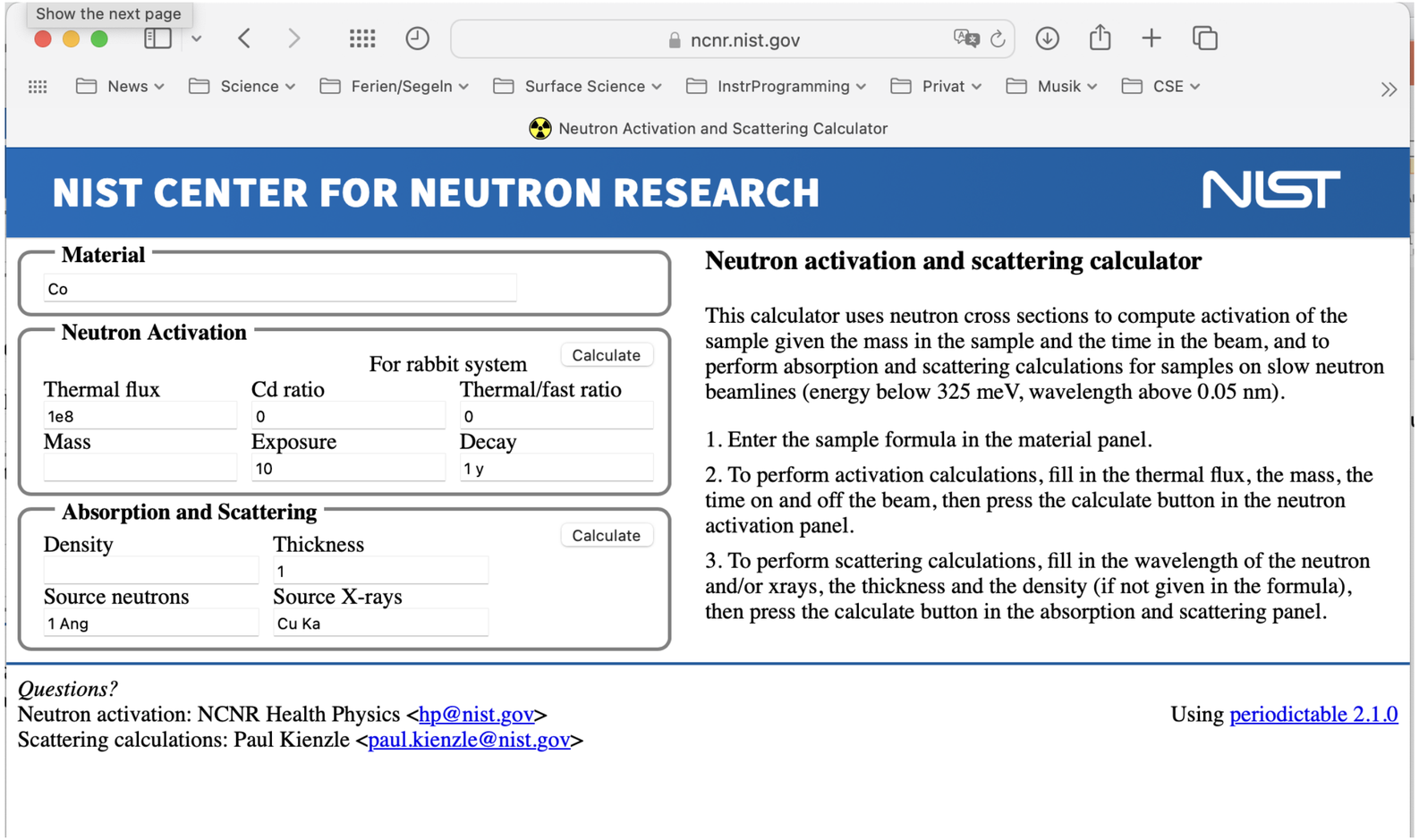
A very useful tool for the preparation of the technical details of a neutron/X-ray proposal: The NIST scattering calculator



https://www.ncnr.nist.gov/resources/activation/