Session III - Neutron scattering, Tuesday, June 21

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OPPORTUNITIES AND PERSPECTIVES AT THE INSTITUT LAUE LANGEVIN: THE ENDURANCE UPGRADE PROGRAMME

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The Endurance upgrade programme covers the period 2016 – 2023 with a budget of 60 M€. About 30 projects have been delivered or are nearing completion. They include neutron guide systems, new and upgraded instruments, sample environment and data and software services. The upgrade programme as a whole ensures that research capability at the ILL will continue to be world leading for the next decade, offering new opportunities and perspectives for excellent science, both for academia and industry. The Endurance programme will be presented, including specific examples and initial results, and set in the context of future reactor operation, given the recent agreement by the ILL Associates to fund the Institute for the period 2024 – 2033.

L13

NEUTRON DIFFRACTION TO STUDY THE STRUCTURE OF MATERIALS

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For the inspection of processes involving condensed matter, *in situ* neutron powder diffraction proves itself to be a versatile tool, giving insight into processes of technological pertinence. Only a few high-intensity powder diffractometers at intense neutron sources allow for this. D20 at Institut Laue-Langevin provides the highest available intensity in constant wavelength neutron powder diffraction. A stationary, curved linear position sensitive detector allows for in-situ diffraction studies down to a second and encourages the use of complex sample environments with inherently small sample sizes. D20 adapts to various levels of crystallographic complexity and rapidity of an observed phenomenon.

The portable electronics market, as well as non-polluting ground transportation, need portable energy storage solutions with improved characteristics. Li-ion batteries with solid electrolytes overcome issues of liquid electrolytes in battery safety and high-voltage operation. Neutron diffraction determines the Li diffusion pathway in solid-state Li-ion conductors. Development of better electrode materials in terms of gravimetric and volumetric energy density, temperature operation range and cycling stability needs understanding of lithium (de)intercalation phenomena. Operando diffraction techniques are well suited here. Electrochemical cells based on a neutron-transparent (Ti,Zr) alloy combine good electrochemical properties and the ability to collect neutron diffraction patterns with reasonable statistics and no other Bragg peaks than those of the electrode material. This allows detailed structural determination of electrode materials by Rietveld refinement during operation.

Solid-oxide fuel cells convert chemical energy into electricity at higher efficiency than conventional methods, with less pollution. The anode (fuel electrode) must not alter at high temperature (thermal stability), not form nonconductive phases at interfaces (chemical stability) and not degrade upon reduction and oxidation cycles (redox stability). The state-of-the-art "cermet" of Ni and yttria-stabilized zirconia ceramic loses performance upon usage as its porosity is reduced by Ni agglomeration and as oxidation of Ni causes redox instability. Cermet deactivates through carbon coking and sulfur poisoning, making it unsuited for hydrocarbon fuels. Single-phase mixed ionic and electronic conductors provide microstructural stability and increase the electrode fraction accessible to oxide ions. Many of those oxides have been investigated successfully in operando at high temperature under oxidizing and reducing gas flow by neutron diffraction, following the crystal chemistry of oxide ions during the process.

Classical *in situ* work (thermo-diffractometry) has been done on the photovoltaic materials, $MaPbI_3$ and derivates, and neutron diffraction turned out to be a perfect tool to screen the crystal chemistry of light organic atoms beside the heavy metal atoms over a wide range of temperatures.

Hydrogen is an attractive energy carrier for renewable energy sources due to its high energy density. Solid-state hydrogen storage provides higher storage capacities than compressed or liquefied hydrogen. Complex metal hydrides have high hydrogen storage capacities but suffer from poor kinetic and thermodynamic properties. Tuning the thermodynamics for dehydrogenation, to reduce the temperature at which hydrogen is evolved is achieved through the addition of a second phase, which will lead to the formation of a more stable product upon decomposition and thereby reducing the enthalpy for dehydrogenation. Neutron powder diffraction screens the crystal chemistry of the different phases *in situ*.

Finally, the work on the structure and the formation and decomposition of gas hydrates and related ice phases will be presented, as well as the prospects of work at very high pressures up to 25 GPa at low temperatures down to 1.6 K.

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SOFT MATTER SEEN BY SMALL-ANGLE NEUTRON SCATTERING, NEUTRON REFLECTOMETRY, AND COMPLEMENTARY TECHNIQUES

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Soft. Condensed. Matter. Soft matter systems are defined as those which are structurally altered when external force of the magnitude of thermal fluctuation is applied. This definition, despite being scientifically accurate, does not do justice to the complexity and diversity of soft matter mattery systems.

Soft. Condensed. Matter. It includes biomaterials, polymers, nanoparticles, emulsions, surfactants, and many other building blocks. Understanding and controlling soft matter systems, is key for technological progress and for the transition to a sustainable society: detergents, food additives, lubricants, foams, coatings, are examples of soft matter systems.

Soft. Condensed. Matter. The low energy required to trigger structural, and thereby functional changes in soft matter systems makes them the most suited ingredients for many responsive systems. These systems are characterized by a complex energetic landscape, and often by ill-defined structures.

In this contribution, through a series of examples, the use and potential of neutron scattering, and reflectometry is illustrated. The examples aim at covering the broad domain of soft matter science probed at the Institut Laue-Langevin.

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INELASTIC NEUTRON SCATTERING - FROM STRUCTURE TO DYNAMICS OF FUNCTIONAL MATERIALS

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The first part of this presentation will give an overview about the capabilities of the ILL to perform inelastic neutron scattering measurements. Depending on the use case (energy range, resolution, type of sample etc.), different classes of instruments are available: time-of-flight, triple axis, and more specialized techniques (spin-echo, backscattering). Most of the instruments at the ILL have undergone significant up-grade in the recent years. Thanks to these recent developments, long-standing questions in materials such as unconventional superconductors can now be addressed, as well as, for instance, the study of new quantum magnetic effects. The current state of the experimental possibilities, together with typical applications, will be discussed.

A particularly powerful technique for the study of magnetism are polarized neutrons. This technique allows separating different types of nuclear and magnetic processes from each other precisely; however, intensity issues sometimes limit its application in inelastic neutron scattering, which is why in only few places worldwide such experiments can be performed. We will present an example of inelastic scattering from the skyrmion phase of manganese silicide, a model system for complex magnetic order and its potential applications (spintronics etc.). The excitation spectrum of this particular magnetic order is extremely complex and has recently been measured in unprecedented detail thanks to the use of polarization analysis. In excellent agreement with theory, these works provide a comprehensive understanding of fundamental magnetic excitations of the magnetic skyrmion phase.