SA-SENS2022

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The Lakes Hotel & Conference Centre

Book of Abstracts

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Author: Andrew Venter[1]

[1] *Necsa - Section Leader: Diffraction*

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Neutron techniques and applications: Neutrons - a unique analytical probe for science and innovation

Author: Mark Johnson[1]

[1] *Head of Partnerships & Communication. Institut Laue Langevin, Grenoble, France*

Neutrons are a unique and essential probe of materials, interacting with nuclei rather than electrons, except in magnetic systems. Through a range of experimental techniques and the associated instrumentation, neutrons cover about ten decades in length scale and a similar extent in time scale, affording an almost unlimited field of applications in condensed matter science and nuclear and particle physics. Neutron experiments deliver fundamental knowledge, address societal challenges and in about 15% of cases have direct or indirect relevance to industry.
In this talk, an overview will be given of neutron techniques and instrumentation, including sample preparation and environment and software. Scientific examples will be presented to illustrate the unique insight offered by neutrons covering, for example, soft matter and biology, materials for energy and quantum materials. Examples of industry applications will be given, as will longer-term socio-economic benefits, including training.

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Dr Mark Johnson joined the ILL in 1995 as an instrument scientist and then as Head of Scientific Computing from 1999. Mark became Associate Director and Head of the Science Division at ILL in October 2016. He played a leading a role in delivering a science programme of increasing quality, the ambitious 'Endurance' upgrade programme and an EU-funded PhD programme for pre-competitive research with industry partners in collaboration with the ESRF. This period as Associate Director, which included the completion of the post-Fukushima reactor response, culminated with the agreement by the ILL Associates (France, Germany and the UK) to fund the institute for another 10-year period from 2024 to 2033, a total investment of the order of 750 M€. In his current role he is responsible for Partnerships and Communication at the ILL where he is working to further expand the scientific membership of the ILL, beyond the existing 11 member countries, to deliver the additional 250 M€ of budget over 10 years that will ensure ILL is fully funded until 2033.

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Catalyses: The application of neutron scattering techniques in heterogeneous catalysis research

Author: David Lennon[1]

[1] *School of Chemistry, University of Glasgow, Glasgow, UK*

Heterogeneous catalysis plays a pivotal role in the chemical manufacturing sector. Efficient catalyst design enables reactions to be performed at large-scale and for extended periods of time. Typically, product selectivity is a primary design parameter, with waste minimisation central to the economic viability of the commercial process. Historically, the implementation of heterogeneous catalysis in large-scale chemical synthesis has tended to rely on empirical testing. However, increasingly, there is a driver to better understand fundamental physico-chemical characteristics of candidate catalytic systems. Topics of interest to the catalytic chemist include (i) the mechanism of reaction, (ii) the form of the adsorption complex, (iii) adsorption and desorption characteristics of key molecular entities, (iv) accessibility of chemical pathways under specified conditions, (v) diffusion of reagents/products within the catalyst matrix, (vi) a molecular perspective of catalyst deactivation, etc. A combination of conventional reaction testing and applied molecular spectroscopy is an established means of addressing these topics. Increasingly, neutron scattering techniques, such as inelastic neutron scattering (INS) and quasi-elastic neutron scattering (QENS), are providing useful additions to the catalytic chemist's spectroscopic toolkit [1].

The presentation will explain how INS can provide a fresh perspective to the task of catalyst characterisation, with the inspection of samples that have experienced extended periods of time-on-stream noted as being a major advantage of the methodology. The effectiveness and usefulness of a neutron spectroscopy-based approach will be illustrated by two examples of economically relevant catalytic reactions: (i) Fischer-Tropsch synthesis over iron-based catalysts [2] and (ii) the methanol to hydrocarbon reaction over a ZSM-5 zeolite catalyst [3].

References

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2. N.G. Hamilton, I.P. Silverwood, R. Warringham, J. Kapitán, L. Hecht, P.B. Webb, R.P. Tooze, S.F. Parker and D. Lennon, Angewandte Chemie International Edition, 52 (2013) 5608-5611.
3. A. Zachariou, A.P. Hawkins, Suwardiyanto, P. Collier, N. Barrow, R.F. Howe, D. Lennon and S.F. Parker, ChemCatChem, 13 (2021) 2625-2633.

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Research in the David Lennon group involves surface chemistry and in particular applying a variety of spectroscopic techniques to probe the interaction of atoms and molecules on well-defined metal surfaces. Such substrates include supported metal catalysts as well as metal single crystals. An increased understanding of the structure and reactivity at surfaces is of fundamental importance in heterogeneous catalysis. Examples of current projects are (i) the development and optimisation of new supported metal catalysts for large scale industrial processes, (ii) spectroscopic investigations of heterogeneous catalyst systems and (iii) surface science experiments on metal single crystals. The majority of his work has industrial applications.

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Lifesciences: Neutron scattering in life science: capabilities & sample requirements

Author: Zoë Fisher[1]

[1] *Scientific Activities Division, European Spallation Source ERIC, Lund, Sweden; Biology Department, Lund University, Lund, Sweden*

Neutron scattering techniques are a powerful tool in life science research. The lack of ionizing radiation damage and the ability to use hydrogen isotope labelling & contrast make neutrons uniquely suited for the study of biological materials. With improving neutron instruments and an increasing number that are well-suited to the study of biomolecules, the expectation is that this community will only grow in the future.

In this presentation, the use of small angle neutron scattering (SANS), neutron reflectometry (NR), and neutron protein crystallography (NPX) will be introduced and specific scientific examples shown. The molecules that are of most interest include proteins, lipids, fatty acids, small organic molecules, surfactants, and even membranes. With neutrons it is possible to investigate the role of these molecules to elucidate mechanistic questions in biology.
For SANS and NR, isotope labelling (deuteration) is most commonly used to enable contrast variation, allowing scientist to selectively "match out" components of complexes. In NPX deuteration is used to boost weak signal-to-noise ratios, reduce the incoherent background due to hydrogen, improve neutron scattering length maps, and enable direct visualization of hydrogen bonds and solvent networks. As deuteration is an essential ingredient in life science research using neutrons, there are now several deuteration support labs established across the globe.

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Dr Zoë Fisher completed her undergraduate studies at the University of Stellenbosch in 2000 before moving to the USA for work and to pursue a PhD degree. After completing her doctorate at the University of Florida in 2006, she became a postdoc and later a staff scientist at Los Alamos National Laboratory in New Mexico. In 2014 she relocated to Sweden to join the European Spallation Source and today leads the deuteration & macromolecules crystallization team.

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Energy storage: Neutrons to understand improvement in battery performance upon anode modification

Author: Neelima Paul[1]

[1] *Group leader - Data evaluation group, Heinz Maier-Leibnitz Zentrum (MLZ), TU München, Garching, Germany*

Electric vehicles are on the way to replace gasoline-powered vehicles n our near future. To power such vehicles, Li-ion batteries with very high storage capacities are necessary, so that these cars travel sufficiently large distances before needing a recharge at charging stations. Moreover, these batteries should have long lifetimes so that they can be charged and discharged several times before needing a replacement. Now energy storage capabilities, rate performances and cycling stabilities of Li-ion batteries are strongly dependent on the electrode materials. As practical energy densities accessible with cathode materials are already close to their theoretical limits with the currently available electrolytes, improvements or replacement of anode materials becomes more paramount than the cathode materials. The widely used graphite anode is stable, but offers low energy density, and suffers from side reactions, which are severe at higher charging rates and low temperatures, leading to eventual capacity fading. Titanium oxide anodes offer much longer life cycles, but have even lower energy densities. Li metal anodes offer the highest possible energy density, but are prone to dendrite formation and thus not preferred for safety reasons. Si anodes offer second highest possible energy densities, but suffer from large volume changes leading to fast capacity fading. With help of several analytical methods, including neutron based methods; this contribution will show how battery performances can be enhanced by either altering the anode morphology, or by preparing composite anode mixtures, or by applying coatings to anode surfaces.

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Dr. Neelima Paul is a physicist with background in preparation and characterization of inorganic semiconductor nanostructures and polymers using neutron, X-ray, infrared and microscopy techniques. At TUM, she focuses on Li-ion battery research and performs operando and post-mortem evaluations of electrode microstructure and morphology, and investigates Li diffusion kinetics within cells to understand the fundamental processes, so that safer Li-ion batteries with even higher energy densities and longer lifetimes can be realized

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Magnetism: Magnetic order and disorder probed by neutron scattering

Author: Martin Boehm[1]

Co-author: Thomas Saerbeck [2]

[1] *Head of the Spectroscopy Group, Institut Laue Langevin, Grenoble, France*

[2] *Instrument Scientist D17, Institut Laue Langevin, Grenoble, France*

Neutron scattering is a unique technique in magnetism and for correlated electron systems, since it measures directly the Fourier transform of the time-dependent magnetic pair correlations. We give a very brief introduction to magnetic neutron scattering and try to highlight the specificities of this technique with respect to other experimental magnetic probes, such as the unique kinematic range of cold and thermal neutrons for magnetic diffraction and excitations and the spin polarisation for the analysis of more complex magnetic structures. We give some recent examples on ordered and quantum magnetic systems, where we try to underline the complementarity between different techniques, the importance of atomistic calculations for the interpretation of the experimental data and the possibilities with new technical developments, such as the wide angle polarisation set-up PASTIS, recently commissioned on the ILL spectrometer IN20. Finally, we equally highlight examples for the analysis of magnetic thin films with the help of neutron reflectometry.

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Dr Boehm has been working on neutron scattering for more than twenty years. He was an instrument scientist at the cold Three-Axis Spectrometer IN14 at the ILL since 2004. In 2010 he became project leader of the instrument project ThALES, was interim Head of TAS group from October 2015 till June 2016 and is a scientific advisor for the MARMOT project. His scientific interests are closely related to the science case of neutron spectrometers, especially studying the dynamics in quantum magnetic and correlated electronic systems as well as application of new (machine learning) algorithms to inelastic neutron scattering with the aim of accelerating the data acquisition and interpretation.

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Magnetism & NI: Neutron imaging on magnetic materials

Author: Nikolay Kardjilov[1]

[1] *Institute of Applied Materials, Helmholtz-Zentrum Berlin for Materials and Energy, Germany*

Owing to their zero net charge neutrons are able to pass through thick layers of matter (typically several centimetres), but are sensitive to magnetic fields due to their intrinsic magnetic moment. Therefore, in addition to the conventional attenuation contrast image, the magnetic field inside and around a sample can be visualized independently by detection of polarization changes in the transmitted beam. This is based on the spatially resolved measurement of the cumulative precession angles of a collimated, polarized, monochromatic neutron beam that transmits a magnetic field.
The configuration was used for quantitative polarimetric experiments, where the polarization vector of the magnetic field associated with a sample was measured in three orthogonal directions. By applying an iterative algorithm to the measured rotation angles, it was possible to reconstruct the flux density of the 3D magnetic field that produced them. In addition a neutron beam of high spatial coherence can be used for visualization of walls between magnetic domains (Bloch walls) by means of a grating interferometer. This is known as a dark-field imaging, which was used very successfully for an investigation of the magnetic properties of high-permeability steel laminates (HPSL) which are used in the core of transformers. In the present talk examples of investigation of various magnetic materials using neutron imaging techniques will be presented.

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Dr. Nikolay Kardjilov is a researcher at the Institute of Applied Materials of the Helmholtz Centre Berlin for Materials and Energy, Germany. He was a beamline scientists at the neutron imaging instrument CONRAD-2 before the shutdown of the research reactor BER-2 in 2019. Since 2020 he is a member of the Joint Research Unit Ni-Matters supporting the construction and the operation of the new neutron imaging instrument NeXT at ILL in Grenoble, France. His research interests relate to development of new experimental techniques for investigation of the structure and property of materials the help of neutron radiation. Dr. Kardjilov has worked on the development of methods using different contrast mechanisms like phase- and diffraction-contrast imaging, visualizing of magnetic fields by polarized neutrons and high-resolution applications. These methods are implemented nowadays at different facilities worldwide and are provided to the user community for addressing a broad spectrum of scientific and industrial problems.

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Summary and announcements

Author: Andrew Venter[1]

[1] *Necsa - Section Leader: Diffraction*

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Author: Ama-Tabu Mozagba[1]

[1] *Necsa - MPR Project Manager*

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Opening and Announcements

Author: Tjatji Tjebane[1]

[1] *Necsa - Instrument Scientist*

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Agriculture: Water quantification measurement of therapeutic roots in soil for analyzing hydrology using neutron imaging under smart agriculture - Review and Perspective of neutron imaging for Agriculture

Author: Cheul Muu Sim[1]

[1] *Korea Atomic Energy Research Institute, 1045 Daedeokdaero Yuseong-gu, Daejeon, 303-353, Korea*

A movement of water through plants has been the focus of scientific investigation for over 250 years. Recent developments(2008-2022) of neutron imaging in the field of in vivo plant have advanced to the point of near real-time visualization of water transport both through the rhizosphere and the xylem system of plants. In this workshop, the related research will be reviewed and looked at terms of future neutron imaging tools for expanding agriculture and food production.
Neutron imaging permitted an irrigation monitoring of plant health and the detection of root pathological changes over a period of measuring root water content in situ. Monte Carlo simulation of water quantification measurement of root in soil using the thermal neutron imaging system shows that penetration rate of thermal neutron is 27% through a water content of 0.071 mL (3mm diameter and 10 mm height) ˜ 7.065 mL (30mm diameter and 10 mm height) of Al-water phantom. It was embedded in various 0˜12% humidity of soil contained with 60 mm diameter and 300 mm height of Al-pot. In practical experiments, a fitted calibration curve was constructed to quantitatively measure an amount of water of roots growing directly in Al pot. The quantification with error 5% of scattering effect of water content of 3-year-old roots in Al-pot soil of electron beam sterilization treatment with moisture of 7.7% of cultivation field was 70.0%, 55.0%, and 70.0%, respectively based on the developed calibration curve. The quantification measurement of water amount can be used for analyzing botanical hydrology of roots growing in soils in association with its seedling, breeding and culturing by neutron imaging under smart vertical farming in agriculture.

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Dr Sim received his PhD in Electronic Engineering in 1998 and has since also extensively studied the field of agricultural sciences by employing electron beam and neutron imaging techniques. He was involved with the establishment and characterization of High-Flux Advanced Neutron Application Reactor (HANARO) neutron radiography facility at KAERI. He has experience in a number of diverse fields and is involved with numerous collaborations which include development of lithium batteries, hydrogen fuels, neutron detectors, ultrasonic systems, fast neutron interrogation systems and aircraft neutron radiography inspection systems.

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Engineering: Neutrons, the perfect tool to study materials in engineering applications

Author: Ralph Gilles[1]

[1] *Head Advanced Materials, Heinz Maier-Leibnitz Zentrum (MLZ), TU München, Garching, Germany*

Due to the high penetration depth and large beam cross section of neutrons and the existence of advanced sample environments, neutron methods have received great attention as a suitable probe in the study of engineered materials, especially metals. This contribution focuses on examples of how neutrons have a great impact to solve open questions in industrial challenges. Examples as pipeline blockage, high-temperature alloy development, residual stresses in additive manufactured alloys and welded joints, needle clogging in medicine, irradiation of memory chips, electrolyte filling of batteries are presented using neutron diffraction, small-angle neutron scattering, neutron imaging, and prompt gamma activation analysis

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Dr Ralph Gilles is a physicist and heading the research group “Advanced Materials” with expertise in neutron scattering methods for studying energy materials as high-temperature alloys and batteries. At the FRM-II research reactor, he was working as an instrument scientist to design, built and brought into commission the structure powder diffractometer SPODI and the small-angle scattering instrument SANS -1 dedicated for materials science and magnetism at MLZ. In his group methods as diffraction, small-angle scattering, imaging, neutron depth profiling and neutron induced prompt gamma activation analysis are applied mainly for alloy and battery research. He has authored over 170 peer-reviewed articles (37 as first author) on topics ranging from instrumentation at large scale facilities, alloy development, thin films and ceramics over to in-situ and operando studies on batteries. Furthermore, he is the industrial coordinator for industrial use of scientific instruments at MLZ.

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Geosciences

Author: Jens Walter[1]

[1] *Research associate at the Department of Structural Geology and Geodynamics at the Georg-August University of Göttingen*

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As a structural geologist, Dr Walter deals with (quantitative) microstructure analysis, the mechanisms and processes of rock deformation and recrystallization. In recent years Jens have been in charge of the realization of sample environments for deformation and recrystallization experiments in the neutron beam. This makes it possible to quantitatively determine deformation or recrystallization mechanisms in a time-resolved manner during the corresponding experiment. Jens also work on the archaeometric characterization of ceramics and their manufacturing processes. Since December 2013 Jens have been co-managing director and co-founder of the MASA Institute GmbH, which was spun off from the University of Goettingen

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Inorganic Chemistry: POROUS (GUEST@HOST) SYSTEMS: « sorption » vs « confinement » points of view

Author: Florence Porcher[1]

[1] *Instrument Scientist in charge of the French Contribution to the conception & construction of DREAM instrument at the European Spallation Source (ESS). Laboratoire Léon Brillouin, CEA/CNRS, Saclay, France*

Porous materials (Macro-, Meso- & Micro- porous systems) form a large family englobing as different systems as amorphous carbons, semi-ordered MCM silicas and fully crystalline Metal Organic Frameworks (MOFs). All these compounds find their attractivity as solid host media where guest species can travel through, be trapped or be converted.This give rise to their present uses as molecular sieves, catalysts, depolutant media, and maybe futur3 ones as chemical sensors, for drug delivery or as confinement media. In order to understand and improve the performance of the processes, the older microporous family (zeolites and MOFs) has been scrutinized for ~50 years by now by diffraction or modellings, taking advantage of their simple structure and long range order. This approach is also facilitated by the limited porosity of the earlier zeolites systems (typ. <10A) where the guests entities are "sorbed" as isolated or small clusters of molecules. With the increasing porosity of MOFs, the fluid-like behaviour of the adsorbed phase becomes pregnant and subverts the "atomic-scale" approach developed from the host point of view. Reversely, as the weight of the guest on the phenomena at play increases, its "confined" point of view gets preponderant, so as for mesoporous materials.
I will try to illustrate this vision on selected examples on microporous & mesoporous systems studied by neutron scattering and complementary methods.

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Dr Florence Porcher originally specialised in single crystal X-ray diffraction and completed her training in neutron powder diffraction at Laboratoire Léon Brillouin (LLB), Commissariat à l'Energie Atomique (CEA). She was delegated to National Center for Scientific Research (CNRS) as part-time researcher and came in charge of the High-resolution spectrometer 3T2 and was responsible for building the high flux, long wavelength diffractometer G6.1 as well as the high resolution cold diffractometer G4.4. During this period, she kept doing local contacting on the unpolarised single crystal diffractometer 5C2 for studies in line with her own research. As a consequence, she came in charge of the selection committee for structural studies at LLB-Orphée. During the activity of Orphée reactor, she expanded her expertise in Crystallography to the studies of metallurgy, materials for hydrogen storage, magnetic compounds, ferroelectric or multiferroic, and in terms of crystallography, from microstructural studies, to phase analysis and resolution of crystal or magnetic structures and diffuse scattering.

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Paleo & Cultural Heritage: Neutron imaging in paleontology and technical applications

Author: Burkhard Schillinger[1]

[1] *Instrument scientist for the neutron imaging facility ANTARES; Heinz Maier-Leibnitz Zentrum (MLZ), TU München, Garching, Germany*

The use of X-rays is always first choice because of easy availability and low cost - but when X-rays fail, there is a high probability that problems can be solved with neutron imaging, especially in archaeology and paleontology, where different fossilasion conditions render different contrasts for neutrons. The talk will give an overview about the examination of fossils embedded in 'red beds', iron containing rock, examination of fossilized hominid teeth, and otehr examples for neutron examination in cultural heritage.

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Dr Burkhard Schillinger currently works at the Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), Technische Universität München. He is instrument scientist for the neutron imaging facility ANTARES, the facility with the brightest and best collimated beam world-wide. Burkhard does research in Experimental Physics, Materials Science and Nuclear Physics. Current projects include 'Humidity Transport in Insulations', fossils in irion 'red beds', namely hearing capabilities in Therapsids/pre-mammals, detector design and neutron imaging facility design as advisor for many international facilities.