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ENDIX1: the first European Neutron Diffraction Single-Xstal Workshop

The Cosener's House, Abingdon
24th-26th April, 2017

SC Capelli, S Hull

September 2019

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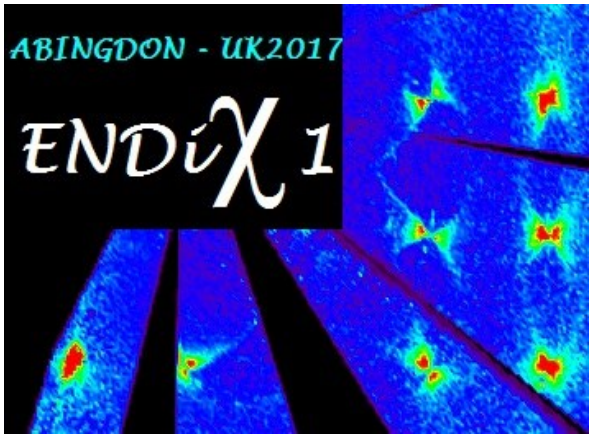
The first European Neutron

Diffraction single-χstal workshop



S.C. Capelli, S. Hull

Instrumentation at large-scale facilities such as ISIS are designed to offer the best possible environment for performing top quality scientific experiments, covering a broad range of science that is not possible at university-based laboratories. This is particularly true in the case of neutron diffraction, for which no laboratory scale source is available.

In the "niche" area of neutron diffraction experiments, single-crystal diffraction represents an even smaller "niche". However, many myths regarding the need for "big samples" and "slowness" of the experiments still surround this type of measurement, even though significant progresses has been made in recent years. To discuss and share ideas on the present capabilities and future development of single-crystal neutron diffraction, this workshop was organized by the ISIS Crystallography Group. It is especially timely, given the changing European landscape, with the new European Spallation Source under construction in Lund and whilst some older reactor-based facilities are scheduled for closure (like LLB in Orsay and HZB in Berlin).

Aims of the Workshop.

Instrument scientists and staff from the main world-wide neutron facilities, together with selected expert members of the research community, were invited to the Cosener's House in Abingdon, Oxfordshire, for a two-day workshop held on 24th-26th April 2017. The program aimed at covering both scientific and technical developments, offering the possibility of open and constructive exchanges concerning issues such as the performance of presently available instruments; the current limitations within the single-crystal neutron diffraction technique; the challenges that the size and complexity of new samples bring about and the direction of future single-crystal instrumentation to meet the changing needs of its user community (whilst simultaneously expanding into new areas). The focus of the workshop was predominantly on instruments with area detectors, facing the

challenge of determining the structures of chemical and biological compounds with ever larger unit cells using smaller and smaller single-crystal samples. The main neutron facilities in the world were represented at the workshop: SNS, J-Park, ANSTO, ESS, PSI, HZB, ILL and ISIS, but also the Diamond Light Source and the European X-FEL, for a total of 38 participants from 8 different countries.

Summary of the Presentations.

The meeting started with a welcome address to the participants by Robert McGreevy, Director of the ISIS Facility, who reminded the audience that large scale facilities in general address only about 10% of the scientific population. Therefore, to be able to survive as a "niche within a niche", single-crystal diffraction must emphasise its unique benefits, whilst being very aware of the size of its user community - and their importance in developing new instrumentation and science.

The opening scientific talks set the scene, with two expert neutron users providing their views. Amber Thompson (University of Oxford, UK) stressed that a gap currently exists between the capabilities offered by neutron diffraction and the requirements of the chemistry community. Specific issues include the general low level of knowledge regarding neutron experiments; the problems with sample size and noisy data; complex sample environment and comparisons of the final statistical parameters with the corresponding X-rays ones. Peter Moody (University of Leicester, UK) presented a snapshot comparison of protein crystallography with neutrons and X-rays, to emphasise how neutron diffraction has not taken enough advantage of the big developments in the corresponding X-rays technique (for example in the automation in mounting, centring, evaluating a good crystal for experiment or in the efficiency of data collection using "strategy" programs). Further talks from Christina Hoffmann and Leighton Coates (both SNS, USA), and Chick Wilson (Bath University, UK) focussed on the challenge of single-crystal neutron diffraction experiments on smaller and smaller samples, both in chemical and biological crystallography, while Romain Sibille (PSI, Switzerland) showed a corresponding example within the field of physical crystallography.

Insights on technical advances in detectors for time-of-flight neutron diffraction were provided in the talks from Dorothea Pfeiffer (ESS, Lund, Sweden) and Jeff Sykora (ISIS, UK). The former described the Gd-GEM detectors currently under development at the ESS, while the latter illustrated preliminary results obtained with new 2D wavelength shifting fibre detectors (WLSF) being

developed at ISIS. Stuart Ansell (ESS, Lund, Sweden) and Goran Skoro (ISIS, UK) contributed their expertise in designing neutron moderators, including bespoke features to optimise their performance for diffraction studies of small single crystals, whilst Phil Bentley (ESS, Lund, Sweden) updated the audience on recent developments in focussing neutron optics. Peter Willendrup (DTU, Denmark) completed the instrument design session with a talk on simulating a single crystal neutron instrument using the McStas software.

A number of contributions dealt with the design or upgrades of specific instruments: Oksana Zaharko presented ZeBRA at PSI (Switzerland), Allison Edwards showed results from KOALA at ANSTO (Australia), Takashi Ohhara reported the construction of SENJU at J-Parc (Japan), Esko Oksanen illustrated the scope for NMX at ESS (Lund), Michael Torvar showed FALCON at HZB (Berlin), Trevor Forsyth presented results from D19 at ILL (Grenoble), Matthias Guttmann gave an update on SXD (ISIS, UK) and Silvia Capelli presented a possible design for LMX at ISIS (UK). Several presentations were also devoted to data processing: from control and analysis of big data at the European XFEL (Sandor Brockhauser) to updates on single crystal algorithms in MANTID (Vickie Lynch, SNS), whilst software for single crystal neutron diffraction work was discussed at length in a focus group after the presentations of Laurent Chapon (Diamond Light Source, UK) about the NSXTool project (ILL-Grenoble and FRM-II-Münich), and Gwyndaf Evans (Diamond Light Source, UK) about the DIALS software.

Summary of the Discussion Sessions.

The workshop programme included slots dedicated to discussion of specific topics - (*i*) science and samples, (*ii*) instrumentation and (*iii*) software. All were characterised by informative contributions from members of the audience and several prioritises for future developments were identified.

Inevitably, the subject of identifying future directions of science is a difficult one. However, it is clear that structural measurements using single crystal diffraction methods will remain the best technique to characterise the crystal structures of complex materials and underpin structure-properties and structure-function relationships across a variety of research fields. Examples include characterising polymorphism within pharmaceutical compounds, recognising the mechanism of action of active sites in proteins for drug design, establishing the mechanism of gas absorption in molecular framework materials used in gas sensor and heterogeneous catalysis, understanding the interplay between the structural and magnetic properties of functional multiferroic ceramics and

probing the nature of phase transitions and bonding character within materials relevant to earth and planetary sciences (e.g. molecular ices). This workshop was focussed primarily on the chemical and biological fields and, over the past decade or so, there has been a clear trend towards the study of more complex crystal structures (larger unit cells), using ever smaller single crystals. Given the inherent flux limitations of the neutron technique, this is a major challenge. Nevertheless, and despite advances in X-ray diffraction and computational methods, single crystal neutron diffraction will continue to be only technique that can reliably determine the positions of the all-important hydrogen atoms. Other topics discussed in this session included the need for facilities and expertise in single crystal growth in order to provide samples of suitable size for neutron diffraction studies and the difficulties of preparing deuterated samples (meaning that measurements must be performed on protonated materials with their higher neutron background).

The discussion session devoted to instrumentation covered a very wide range of topics, including instrument design; the instrument life-cycle; funding constraints; any overlap/complementarity with existing instruments; competition with other instruments/techniques; limited access to moderators (due to a finite number of available beam ports); access modes and the question of what is a "good" number of instruments (and the related question of whether to build diffractometers to meet a wide science case or more specialised instrumentation). Key points included the importance of the science case in determining top level design requirements; the different approaches that can be taken to meet these requirements (e.g. instrument length, moderator choice, detector technology, neutron optics); the availability of very good tools for ray tracing (McStas, Vitess, etc.); the need for timely upgrades of instruments to ensure that they remain competitive; the key role of the business case (especially the cost/benefit analysis for various options) and the need for appropriate sample environment and user support facilities. The importance of development projects in areas such as moderator design, supermirror guides and 2D detectors with improved efficiency was also stressed.

Perhaps the liveliest discussion was devoted to the topic of software, with the participants reviewing the software available for processing single crystal data at neutron facilities around the world and concluding that there is a need for a common platform with robust functionalities in order to treat the increasingly large quantities of data and increasingly challenging crystallographic problems. For example, the MANTID project, jointly developed by ISIS and SNS to treat neutron scattering data, lacks some important functionality, including the treatment of irregularly shaped, twinned and incommensurate crystals, the corrections for absorption and extinction to raw data and the

automation of the processing flow for routine measurements. The software package DIALS, developed at the Diamond Light Source (DLS) for macromolecular X-ray crystallography, already includes most of these functionalities. This example clearly demonstrates the advantages of closer collaboration between those developing software for single crystal diffraction, both within the neutron and X-ray communities. Indeed, it was generally agreed that the lack of suitable software was probably the most significant challenge currently facing the technique.

Conclusions.

Whilst the workshop took a wide view of the topic of single crystal diffraction using neutrons, it is important to consider how the various recommendations can be implemented at ISIS. At present, ISIS has only one dedicated single crystal diffractometer, SXD. The WISH diffractometer predominantly studies polycrystalline samples, but also has single crystal capability, though over a more limited range of reciprocal space than SXD. A new single crystal diffractometer for studies of large molecule systems, LMX, was proposed in the past as part of the suite of instruments for the ISIS Second Target Station, but was not approved.

The key recommendations for ISIS are :

- Whilst SXD has strengths in some areas, such as scanning diffuse scattering over large volumes of reciprocal space, it is no longer able to address the majority of structural problems facing research in the chemical crystallography field. As a result, an upgrade project should be considered so that SXD can study significantly smaller crystals. Possibilities include the installation of a neutron guide and replacing the current 2D detector modules with more efficient ones exploiting Wavelength Shifting Fibre (WSF) technology.

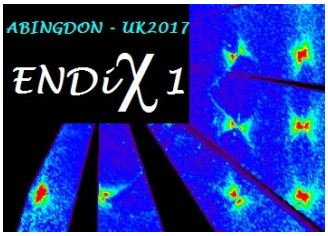
- As a complementary facility to SXD, ISIS should progress the case for an LMX instrument to focus on structural studies of more complex structural problems in large molecule crystallography, with the possibility of also investigating small protein systems. Suggestions here include performing tests on SXD, WISH and other instruments (i.e. at the ILL) using a “standard” sample, to estimate possible count rates on a future LMX. It is also recommended to revisit the original design of LMX to exploit, for example, developments in moderators and neutron optics.

• ISIS should prioritise the development of software for single crystal diffraction. In particular, routines to correct for the effects of wavelength-dependent absorption and extinction are essential if the quality of the structural information obtained at a pulsed source such as ISIS are to compete with those from a reactor-based (monochromatic) facility. Collaboration with other facilities (e.g. Diamond) is strongly encouraged.

Photograph of (most of) the participants of the Workshop.

Standing (from the left): S. Hull, T. Sorensen, E. Oksanen, P. Moody, F. Orlandi, T. Ohhara, L. Coates, T. Forsyth, P. Bentley, S. Jackson, D. Visser, S. Brockhauser, V. Lynch, J. Breternitz, S. Capelli, M. Gutmann, J. Sykora.

Sitting (from left): P. Willendrup, O. Zaharko, A. Edwards, P. Manuel, S. Ansell, R. Sibille, C. Hoffmann, D. Keen, D. Nye, P. Henry, N. Rhodes.



The 1st European Neutron Diffraction Single χstal workshop

Abingdon, UK - April 24-26th, 2017

ENDiX 1

PROGRAM

Monday 24th April

13:30-13:45	Robert McGreevy - Welcome (Director of ISIS Neutron and Muon Source, UK)
13:45-14:15	Amber Thompson - Single Crystal Neutron Diffraction: What the Chemist Wants (Department of Chemistry, University of Oxford, UK)
14:15-14:45	Peter Moody - Compare and contrast the practice of X-ray and neutron crystallography. (Leicester Institute for Structural and Chemical Biology, University of Leicester, UK)
14:45-15:15	Stuart Ansell - Building a bespoke moderator -- when you can't disturb the other beamlines (European Spallation Source, Lund, Sweden)
15:15-15:30	Discussion
15:30-16:00	Tea Break
16:00-16:30	Dorothea Pfeiffer - Detectors for the NMX instrument at ESS (European Spallation Source, Lund, Sweden)
16:30-17:00	Jeffrey Sykora - Scintillator based detector options for single crystal neutron diffraction. (ISIS Neutron and Muon Source, UK)
17:00-17:30	Christina Hoffman - The smaller crystal sample challenge for neutron single crystal diffraction (Oak Ridge National Laboratory, USA)
17:30-17:45	Short break
17:45-18:30	**Focus group: science/samples**

Tuesday 25th April

9:00-9:30	Leighton Coates - Large Unit Cells and Small Crystals: Macromolecular Neutron Diffraction at SNS (Oak Ridge National Laboratory, USA)
9:30-10:00	Chick C. Wilson - Contemporary challenges in chemical sciences: how can single crystal neutron diffraction meet them? (Department of Chemistry, University of Bath, UK)

10:00-10:15	Oksana Zaharko – The new single-crystal diffractometer ZeBRa (Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, Switzerland)
10:15-10:30	Romain Sibille - Structural disorder and magnetic correlations in $Tb_2Hf_2O_7$ pyrochlore (Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, Switzerland)
10:30-11:00	Coffee break
11:00-11:30	Esko Oksanen - Key requirements for a neutron macromolecular diffractometer (European Spallation Source, Lund, Sweden)
11:30-12:00	Alison Edwards - Vivaldi down under - the KOALA experience (Australian Nuclear Science and Technology Organisation, Lucas Heights Campus, Australia)
12:00-12:30	Takashi Ohhara - Latest status of a TOF single crystal neutron diffractometer SENJU at J-PARC (J-PARC Center, Japan Atomic Energy Agency, Tokai, Japan)
12:30-13:30	Lunch
13:30-14:00	Phil Bentley - Recent developments in focussing optics (Optics Group, European Spallation Source, Lund, Sweden)
14:00-14:30	Peter Willendrup - An introduction to McStas - for single crystal diffraction (DTU Physics, Technical University of Denmark, Copenhagen, Denmark)
14:30-15:00	Trevor Forsyth - D19 - a monochromatic neutron diffractometer for high resolution crystallography (Institut Laue-Langevin, Grenoble, France)
15:00-15:15	Discussion
15:15-15:45	Tea break
15:45-16:15	Vickie Lynch - Extending Mantid to process single crystal data (Oak Ridge National Laboratory, USA)
16:15-16:45	Matthias Gutmann – SXD current status (ISIS Neutron and Muon Source, UK)
16:45-17:15	Gwyndaf Evans - DIALS – a toolkit for the development of crystallography data analysis software (Diamond Light Source, UK)
17:15-17:30	Laurent Chapon – NSXTool for processing neutron diffraction data (Diamond Light Source, UK)
17:30-17:45	Short break
17:45-18:30	**Focus group: software**
18:30-19:30	Free time
19:30	Dinner

Wednesday 26th April

9:00-9:30	Goran Skoro – How to choose a perfect moderator for your instrument (and live with this decision) (ISIS Neutron and Muon Source, UK)
9:30-10:00	Silvia C. Capelli – LMX : A second single crystal instrument at ISIS ? (ISIS Neutron and Muon Source, UK)
10:00-10:15	Michael Torvar - A neutron Laue diffractometer for fast data acquisition (Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany)
10:15-10:30	Sandor Brockhauser – Control and analysis at the European XFEL (European XFEL, Germany)
10:30-11:00	Coffee break
11:00-11:25	Christina Hoffmann: wrap-up on science and samples
11:25-11:50	Paul Henry: wrap-up on instrumentation
11:50-12:20	David Keen: wrap-up on software
12:20-12:30	S. Hull: concluding remarks
12:30-13:30	Lunch
13:30-	Departure

The 1st European Neutron Diffraction Single χstal workshop

Abingdon, UK - April 24-26th, 2017

ABSTRACTS

Compare and contrast the practice of X-ray and neutron crystallography.

Peter Moody, Institute for Structural and Chemical Biology, University of Leicester, UK.
(pcem1@leicester.ac.uk)

The processes of macromolecular neutron crystallography will be described from the perspective of a user who is used to the procedures of X-ray work. This will be illustrated by describing some of our recent experiments to trap the intermediates of the heme peroxidase reactions, a study undertaken to determine their protonation states. There will be an emphasis on the comparison of the equivalent or analogous steps used in X-ray work. The possible cross-over between the methods used will be discussed and how some of the ideas implemented at synchrotron beam lines might be applied to neutron work.

Large Unit Cells and Small Crystals: Macromolecular Neutron Diffraction at SNS

Leighton Coates, Oak Ridge National Laboratory, Oak Ridge (TN), USA. (coatesl@orln.gov)

The Macromolecular Neutron Diffractometer MaNDi at the SNS routinely studies unit cell dimensions over 100 Angstroms in length from crystals well below 1mm in volume. To make such data collections feasible we have deployed 40 SNS Anger cameras which are arranged in a sphere like arrangement around the sample. This reduces the number of crystal orientations needed for a complete dataset to between 6-10 typically. The use of fully perdeuterated samples has also allowed us to collect data from crystals 0.2mm in volume and below. However as crystal volume decreases exposure time must increase. How do we balance collecting data from smaller crystal volumes against the number of experiments per year.

A neutron Laue diffractometer for fast data acquisition

Michael Torvar, Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany
(tovar@helmholtz-berlin.de)

At Berlin neutron source BER II a Laue diffractometer was launched providing reasonable Laue data acquisition in the range of 10 s up to 2 min. Sample environment is under progress to offer in-situ measurements from 80 to 600 K. The instrumental set-up as well as worked examples will be briefly presented.

Key requirements for a neutron macromolecular diffractometer

Esko Oksanen, European Spallation Source, Lund, Sweden (esko.oksanen@esss.se)

The ESS long pulse design together with high-brilliance low-dimensional moderators is ideally suited for a macromolecular diffractometer. A system engineering approach was used for the design of the NMX Macromolecular Diffractometer. High-level requirements were first derived from the scientific drivers and motivated the instrument architecture. These requirements and other, practical considerations based on our design philosophy formed the basis of the engineering design, where I will highlight some key compromises made.

Structural disorder and magnetic correlations in $Tb_2Hf_2O_7$ pyrochlore

Romain Sibille, Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, CH. (romain.sibille@psi.ch)

Magnetic systems with competing interactions can adopt exotic ground states. Some of these phases feature quantum spin liquid states, which arise from long-range entanglement in the ground state wavefunction. In Tb2Hf2O7, single-crystal neutron diffraction experiments indicate that correlations typical of a magnetic Coulomb phase develop despite a massive amount of structural disorder around non-Kramers ions. A possible scenario is that the non-magnetic structural disorder transforms this Ising pyrochlore into a quenched random transverse field Ising magnet, inducing quantum fluctuations.

The new single-crystal diffractometer ZeBRa

Oksana Zaharko, Laboratory for Neutron Scattering and Imaging, PSI, CH.(oksana.zaharko@psi.ch)

A new single-crystal diffractometer ZEBRA optimized for small samples and extreme sample environment conditions is built at the Swiss Spallation Neutron Source SINQ at PSI. Scientifically this enables to study challenging systems available as small crystals only or systems with interesting properties emerging at extreme magnetic fields, high-pressures or low temperatures. A new optimized neutron delivery system and new nonmagnetic high-precision sample-positioning and analyser-detector units will be in operation in spring 2017, after the SINQ shutdown.

Latest status of a TOF single crystal neutron diffractometer SENJU at J-PARC

Takashi Ohhara, J-PARC Center, Japan Atomic Energy Agency, Shirakata 2-4, Tokai, Ibaraki 319-1195, Japan. (takashi.ohhara@j-parc.jp)

Single-crystal neutron diffraction technique has been used in various scientific fields, including physics, chemistry, molecular biology, materials science, and energy science, and has the potential to be an irreplaceable analytical tool for the development of new functional materials. However, the number of single-crystal neutron diffractometers in the world remains insufficient, and consequently, the number of experiments is limited. Thus, construction of a high-performance single-crystal diffractometer is required to

alleviate this limitation and enable the measurement of many important materials. The author and collaborators constructed a TOF-Laue single crystal neutron diffractometer, SENJU, at the BL18 of J-PARC Materials and Life Science Experimental Facility (MLF) [1]. SENJU has a vacuum sample chamber for low-background measurements of small single crystal (< 0.1 mm3). In addition, various types of sample environment devices such as a 4 K cryostat, a furnace and a superconducting magnet are available. In this presentation, the author will show the latest status of SENJU, challenges to measure a small single crystal.

[1] T. Ohhara, R. Kiyanagi, K. Oikawa, et al., J. Appl. Cryst., 49, 120-127 (2016).

Recent developments in focussing optics

Phil Bentley, European Spallation Source, Lund, Sweden (phillip.bentley@esss.se)

I will present an overview of some of the recent, and not so recent(!) developments in optics for the kind of extreme focussing conditions that are being approached with modern instrumentation. In particular, the challenge of achieving a smooth phase space whilst compressing the beam into a sub-mm spot are well understood for photons, but remain at the technical limit for neutrons.

The smaller crystal sample challenge for neutron single crystal diffraction

Christina Hoffmann, Oak Ridge National Laboratory, Oak Ridge (TN), USA. (choffmann@ornl.gov)

Single crystal neutron diffraction is continuously evolving by exploring ever more challenging scientific questions. However, a long-standing goal is to reach smaller single crystal sample sizes by increasing efficiency of data collection. Using the same sample for X-ray and neutron diffraction would simplify combined data analysis and direct co-refinement of complimentary data. A further complication is that the science questions to be answered are growing in complexity as well.

Extending Mantid to process single crystal data

Vickie E Lynch, Oak Ridge National Laboratory, Oak Ridge (TN), USA. (lynchve@ornl.gov)

Many algorithms have been added to Mantid to reduce single crystal data. These include algorithms for calibrating detectors, finding peaks, finding UB matrices, choosing the symmetry of the unit cell, indexing peaks, integrating peaks, and viewing peaks. The history of planning each of these capabilities will be presented along with a comparison of results from algorithms in detector space and reciprocal space. These algorithms have been used in an SCD Event Data Reduction Interface as well as a python script for parallel reduction of orientations with an input configuration file for users. Also, an algorithm for normalizing data collected at different orientations has greatly benefitted viewing both Bragg peaks and diffuse scattering results. Future work planned includes experiment planning of goniometer settings using Mantid algorithms, improved peak integration using 3D fits of the strong peaks and machine learning for selecting 3D fits for the weak peaks, and a live data viewer that does live reduction.

SXD current status

Matthias Gutmann, ISIS Neutron and Muon Source, UK (matthias.gutmann@stfc.ac.uk)

A 3D profile function suitable to integrate Bragg reflections in time-of-flight experiments will be presented. This function can be used for a number of other tasks and these will be discussed. The accuracy, long-term stability and reproducibility of the SXD instrument will be discussed as well along with a few science highlights.

DIALS – a toolkit for the development of crystallography data analysis software

Gwyndaf Evans, Diamond Light Source, Harwell Science Campus, UK (gwyndaf.evans@diamond.ac.uk)

The DIALS (Diffraction Integration for Advanced Light Sources) project (dials.diamond.ac.uk) is a major software collaboration between several synchrotron light sources and CCP4 (Collaborative Computational Project No. 4). As well as providing a diffraction image analysis software package for end users it also provides a rich development platform for prototyping new ideas and algorithms for data analysis. The versatility of DIALS is lending itself to the analysis of electron diffraction data and its exploitation by the neutron crystallography community is being explored. The high degree of convergence between neutron and X-ray crystallography requirements, especially in light of recent pink beam synchrotron and XFEL X-ray beamlines, should allow a number of joint developments across different communities.

Building a bespoke moderator -- when you can't disturb be other beamlines

Stuart Ansell, European Spallation Source, Lund, Sweden (Stuart.Ansell@esss.se)

In the ideal world a new SXD instrument would have its own dedicated moderator, however that would present many problems to existing or other proposed instruments as normally moderators are shared between beamlines and have to be a compromise. Typical SXD instruments need to measure a high resolution dQ/Q over a finite dynamic wavelength range. This requirement can be mapped by selecting from a construction phase space of x,y (the position(s) of a virtual moderator(s)), L1, the primary flight path, t, the neutron [effective] emission time and E, the neutron energy. I will show three possible modifications to reflector-moderator assemblies that exploit engineering features of typical spallation and reactor sources to enhance the neutron field provided to a "standard" SXD beamline without impacting other instruments.

Detectors for the NMX instrument at ESS

Dorothea Pfeiffer, European Spallation Source, Lund, Sweden (Dorothea.Pfeiffer@esss.se)

European Spallation Source instruments like the macromolecular diffractometer (NMX) require an excellent neutron detection efficiency, high-rate capabilities, time resolution, and an excellent spatial resolution in the order of a few hundred micrometers over a wide angular range of the incoming neutrons. GEM detectors with Gd converter in combination with the VMM3 ASIC are a promising option for this instrument class.

Scintillator based detector options for single crystal neutron diffraction

Jeff Sykora, ISIS Neutron and Muon Source, UK (jeff.sykora@stfc.ac.uk)

ISIS has provided scintillation based detector solutions for many of the diffraction instruments at ISIS. Most of these have been based on ZnS:Ag/6LiF scintillator read out with coded arrays of clear fibres and single anode hotomultiplier tubes. More recently, ISIS has been developing scintillator detectors based on coded arrays of WLS fibres and multi anode photomultiplier, which offer higher position resolution and are significantly easier to manufacture. This presentation will discuss the primary challenges for detector technology in next generation single crystal diffractometers. Some detector developments achieved at ISIS to date and potential solutions for a 2D position sensitive detector for future single crystal applications will be discussed.

An introduction to McStas - for single crystal diffraction

Peter Willendrup, DTU Physics, Technical University of Denmark, Copenhagen, DK. (pkwi@fysik.dtu.dk)

The talk will introduce the Monte Carlo Ray-tracing package McStas which is widely used for instrument design, optimisation and virtual experiments. Further, relevant capabilities for simulating single crystal diffraction at steady-state and ToF sources will be outlined. Finally, a "Rietveld-like" refinement approach from powder diffaction will exemplify where capabilities may move in the future.

How to choose a perfect moderator for your instrument (and live with this decision)

Goran Skoro, ISIS Neutron and Muon Source, UK (goran.skoro@stfc.ac.uk)

The importance of the choice of a "perfect" moderator for particular type of experiments (such as single crystal neutron diffraction, for example) will be discussed. This will be illustrated with description of the water moderator which serves ISIS SXD instrument. In addition, the details about full neutronics model of ISIS Target station 1, simulation and experimental results related to TS-1 water moderator(s) and a short and eventful history of their operational issues will be presented.

Contemporary challenges in chemical sciences: how can single crystal neutron diffraction meet them?

Chick C Wilson, Department of Chemistry, University of Bath, UK; (C.C.Wilson@bath.ac.uk)

A range of current areas of structural interest in chemistry and related sciences will be outlined, with a particular focus on the challenges presented to the chemist and of the potential value of single crystal neutron diffraction (SXND) in meeting these. The evolving nature of the materials of contemporary interest in chemistry (and of the challenges raised for SXND) will be outlined, governed both by intrinsic fundamental curiosity and by the drive towards creating and understanding functional materials, targeted at application. Examples will also be given in the domain of process chemistry, focusing on pharmaceuticals, where the characterisation needs focus not only on molecular structure but on particle properties and also identify requirements for in process experimentation. Opportunities and challenges for SXND in this area will also be discussed.

LMX : A second single crystal instrument at ISIS ?

Silvia Capelli, ISIS Neutron and Muon Source, UK. (silvia.capelli@stfc.ac.uk)

Plans for LMX, a dedicated single crystal macromolecular beamline on TS-II, have been discussed for well over ten years. However, despite strong support from the user community, the instrument has not been built, largely due to cost concerns. Considering the uncertain future of single crystal instruments at reactor sources, and taking into account the progresses in developing and building new ones at spallation sources, it seems now the right time to revive the LMX project in the contest of a larger project aimed at extending the overall single crystal capabilities of the ISIS facility.