A key aim of this meeting is to establish priorities for the various proposals through discussion, and then bring together the highest-priority projects as part of a coherent plan for the next wave of development at ILL – the 'ILL 2020 Vision'. The timescale we envisage involves preparing this plan for discussion and refinement with our Scientific Council in Spring 2011, and then presenting it to our Steering Committee in summer of 2011 with the aim of winning approval for funding from 2013–2017.

A number of factors must be taken into account in drawing up priorities, and these should form much of the framework of discussion at the meeting.

• How might the various projects lead to significant scientific advances, both in the areas that ILL traditionally serves and in quite new areas? We are also being asked increasingly to demonstrate that our facility has an impact on some of the 'grand challenges' in areas to which science is applied, such as health, energy, the environment and information technology and communications. Although we continue to belief fervently that we should have a strong commitment to fundamental science, we also need to have compelling reasons for support framed in terms of direct or indirect 'societal impact'.
• What is the size and strength of the user community that each new development will serve?
• What technological developments have become available or need to be developed – to enable new types of experiments?
• How do these developments relate to those at other neutron facilities – now and planned for the future. These include various national sources, which all have particular strengths, as well as a future European Spallation Source. Such a source will not come up to full operating strength and capacity before about 2025, and our large and active community will continue to need access to a facility such as ILL, complemented by many national sources at least until that point. Even when ESS is fully operational, there will be a number of important fields where a powerful reactor source will still provide significant advantages, and these should also be noted when the future needs of our community are considered.

We will argue vigorously that the most efficient use of resources would be to add more instruments to our suite and to take even more advantage of the high flux our reactor delivers; however, we may also have to balance our priorities for new instruments and infrastructure against existing equipment. To help this process ILL is organizing a review of its instrument suite, aided by external experts and aiming to assess and report towards the end of this year. However, at this meeting you may also wish to express your opinion on the priority you would give to existing facilities relative to the new ones being proposed.

Finally, the tools for data analysis, support laboratories and other 'softer' factors can make a crucial difference to the success or failure of an experiment. There are a number of key issues here, including the following. Do problems remain in analyzing data? Should there be greater integration of software within and between institutes? Should we develop new interface or support laboratories such as the Deuteration Laboratory or the Partnership for Soft Condensed Matter, both of which are now enabling users to make much better use of our neutron beams? We look forward to your views on these and all other factors that help ILL deliver the best possible science for many years to come.

1. HiQ - A high-Q diffractometer for PDF measurements

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Abstract

The local structure of many important functional materials is often different from the average structure, as revealed by diffraction, due to, e.g. doping, mixed site occupancy, or formation of time-dependent local distortions. To get information on both the average and the local structures one needs to perform a joint Rietveld and PDF analysis of the total scattering, for which we need data to Q = 30 - 35 Å with $\Delta d/d \sim 3 \times 10^{-3}$. Here, we describe how the hot-source diffractometer D4 can be adapted to achieve this capability, and outline one possible design of a dedicated high-Q diffractometer at the ILL, using the vacant inclined hot-neutron beam IH2.

Motivation

Rietveld refinement of high-resolution powder diffraction data revolutionized materials science [1]. However, this method uses just the Bragg peaks, discarding the diffuse scattering as background, and therefore gives information only on the time- and spatially-averaged structure. In recent years development of electronic materials, like high-T_C superconducting and colossal magnetoresistive materials, has made it necessary to investigate the local structure of these materials. This is because the electronic properties of these materials are sensitive to the nanoscale rather than to the average structure. The local instantaneous structure of these materials is often different from the average structure due to the formation of time-dependent local distortions, such as polarons. Such deviations from the average structure are by no means restricted to the above-mentioned materials but are typical of almost every important functional material.

One of the major reasons why nanoscale structural complexity is important to advanced functional materials is that solids which contain competing internal forces are often highly sensitive, and these forces result in a complex structure. If two or more forces are competing, then a small external force can sometimes destroy the balance causing the system to respond with a very large effect. An example of this is the colossal magnetoresistance effect (CMR) produced by a relatively small external magnetic field in materials where the internal competing forces are caused by the spin, charge, orbital and lattice degrees of freedom. The CMR materials are located right at the metal-to-insulator (MI) transition in the phase diagram, and an applied magnetic field greatly reduces the resistivity by inducing a MI transition. In order to investigate the nanoscale local structure of these materials, we need to use the total scattering data, including both the Bragg reflections and the diffuse background.

Egami and coworkers have recently developed the pair distribution function (PDF) analysis of the total scattering data [2], a method well known to the scientific community investigating liquids and amorphous materials.

To get complete structural information one needs to perform a joint Rietveld and PDF analysis of the total scattering data to a high value of momentum transfer Q. At present the ILL has no diffractometer optimised for such investigations. The diffractometer D4 has a sufficient Q-range but its Q-resolution is not really good enough for such analysis. Despite this limitation, several very successful PDF studies have already been performed on D4 (e.g. [3]), and the number of PDF proposals now rivals the number of proposals for liquids and amorphous materials. We propose that the ILL should develop further this capability on D4, and eventually construct a dedicated high-Q powder diffractometer with optimum Q-resolution, to remain at the forefront of structural research of functional nanomaterials.

One argument often presented against building a high-Q diffractometer at the ILL is that excellent high-Q diffractometers already exist at the spallation neutron sources, and therefore the ILL should not build something which cannot compete with them in performance. This is simply not true! A high–Q diffractometer at a spallation source uses polychromatic neutrons which sometimes creates difficulties in the inelasticity (Platczek) and absorption corrections necessary to generate reliable PDF's. Resonance effects for certain elements also pose difficulties. A high-Q diffractometer at the ILL can use monochromatic neutrons and therefore the inelasticity and absorption corrections can be much better done, and possible resonance problems can generally be avoided. In short, a high-Q diffractometer at the ILL can generate cleaner data and hence more reliable PDFs.

Description of instrument/infrastructure

a) Improvements to D4 for PDF measurements

In the short term we will continue to improve the suitability of D4 for PDF measurements, in aspects which do not compromise D4's present excellent capability for liquids and amorphous materials. Possible changes include:

- optional tighter α_1 collimation (before the monochromator)
- extension of the range of take-off angle
- addition of a larger-radius small-angle detector
- development of algorithms for deconvolution of the resolution function

b) Design of a dedicated high-Q diffractometer

At the same time we will develop the design of a dedicated high-Q diffractometer at the ILL. A possible location is on the inclined hot beam tube IH2 which makes an angle of 35º to the horizontal, and is not used at the moment (Fig. 1). We want to collect data to Q = 30 - 35 $Å^{-1}$, with $\Delta d/d \sim 3 \times 10^{-3}$. While we do not exclude consideration of a time-of-flight diffractometer, despite the disadvantages stated earlier, we will concentrate initially on the optimisation of a monochromatic diffractometer. The challenge is to obtain the Q–resolution.

The desired neutron wavelength is in the range 0.35-0.5 Å. In order to get good resolution we must also use a large monochromator take-off angle $2\theta_m$.

For the 773 reflection from a Cu monochromator $2\theta_m$ = 60.40/91.89º for λ= 0.35/0.50Å. Let us calculate the intensity losses when using Cu (773) instead of the Cu(331) presently used on D4 for λ = 0.50/0.35Å. The structure factor of Cu is F = $4b_{CU}$ for all reflections, where b_{CU} is the scattering length of Cu, so we lose intensity due to the Lorentz and Debye-Waller factors only. The losses are 5.0 and 6.2, respectively, to give a total loss of 31, which is considerable. However we can increase the intensity of all reflections by cooling the monochromator, for which the gain factor is expected to be about 3 if there is no extinction problem. By sacrificing intensity by about a factor 10 we can thus gain the required resolution. This is an acceptable sacrifice since the scattering from these crystalline materials is usually quite strong.

For best resolution the diffractometer will operate in the vertical plane (Fig. 2), but with present-day technology that should cause few difficulties for the detector support and sample environment. The likely detector configuration is a monolithic multi-wire 2D D19-type detector, with an oscillating radial collimator to minimise the background, both well-established technologies.

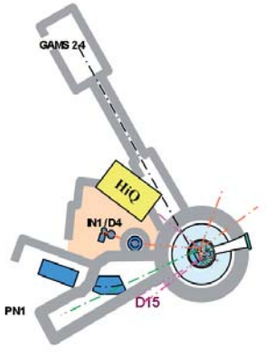

Figure 1: *Schematic view of the region around the IH2 beam with the possible location of the diffractometer HiQ indicated.*

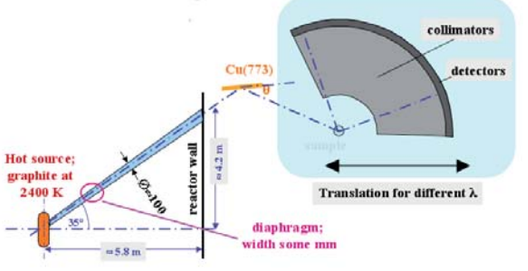

Figure 2*: Side view of IH2 and HiQ.*

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