neutron instrument suite will be highlighted with particular emphasis on performance parameters of the diffraction instruments. The instrument parameters of the Spallation Neutrons And Pressure (SNAP) instrument will include a discussion of planned micro-diffraction capabilities. Specifically, recent progress in micro-focused neutron beams demonstrates that neutron diffraction from sub 100 micron samples held within 'more standard' opposed gem anvil cells (e.g. DACS) might be feasible. Beams focused to 90 x 90 microns have been demonstrated to produce at least an order of magnitude increase in flux at the focal spot. This technique does not significantly increase beam divergence. Recent neutron diffraction results from single crystal micro-samples (300 microns) mounted on fibers and micro samples (200 microns) under pressure in opposed gem anvil pressure cells will be presented.

Keywords: neutron diffraction, instrumentation, high pressure

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ISIS Crystallography on TS-II: what can we do with 60 kW?

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European facilities in general and ISIS in particular are facing a major challenge from the construction of a new generation of pulsed neutron sources in the US and Japan. Although the European research community must warmly welcome these developments, it is nevertheless crucial for us to maintain a leadership role, if not in sheer flux, at least in the creative development of new neutron instruments and techniques and in the operation of a cutting edge science program.

The construction of the Target Station II at ISIS will enable us to extend pulsed neutron crystallography to cover a much wider domain of momentum transfer Q. A combination of high peak flux and state-of-the-art target, guide and instrumentation design will result in world-leading performances, in spite of the fact that the integrated power of the source is only a fraction of that at SNS and J-PARC.

The new diffractometer WISH at the ISIS TS-II will further push the envelope of low-Q crystallography. WISH is primarily designed for powder diffraction at long d-spacing on magnetic and large-unit-cell systems, with the option of enabling single-crystal and polarized beam experiments.

The conceptual design for a new single-crystal diffractometer for large molecule crystallography and structural biology will also be presented. Although the instrument design is quite different from comparable instruments at high-repetition rate sources (such as the SNS), detailed Monte Carlo simulations have shown that this machine will have excellent performances overall, and will be particularly competitive for medium-resolution crystallography on small samples.

Keywords: neutron diffraction, instrumentation, ISIS

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Hydrogen and Hydration Sensitive Structural Biology

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It is well known that neutron diffraction provides an experimental method of directly locating hydrogen atoms, but unfortunately, to date, there are relatively few examples of neutron crystallography in biology since it takes a long period of time to collect a sufficient number of Bragg reflections. The recent development of a neutron imaging plate (NIP) became a breakthrough event in neutron protein crystallography [1]. At the Japan Atomic Energy Research Institute (JAERI), we have constructed several high-resolution neutron diffractometers dedicated to biological macromolecules (called BIX-type diffractometers), which gives several interesting results regarding hydrogen positions and hydration in proteins and oligomer DNA.

However, neutron protein crystallography still remains an intensity limited technique. Recently next generation spallation neutron sources, such as J-PARC (Japanese proton accelerator research complex) and SNS (Spallation neutron source in USA), are being constructed and several protein crystallography diffractometers will be installed there. Then about two orders of magnitude gain in neutron intensity would be expected and neutrons absolutely expand the field of structural biology. In this microsymposium, the future prospect for neutron protein crystallography will be discussed.

[1] Niimura N., et al, *Nucl. Instrum. Method. Phys. Res*., 1994, **A349**, 521-525.

Keywords: neutron diffraction, hydrogen, bio-macromolecules

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Shaping the Future of Neutron Powder Diffraction

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Neutron powder diffraction is recognized as a powerful technique to clarify the relationship between the crystal structure and the properties of functional materials. Its application fields have been expanding in materials science, and prominant results obtained across a large number of diverse disciplines. New neutron powder diffractometers (NPD's), in various stages of construction at new facilities in Europe, Australia, the US and Asia, will exceed the present limits of application, and stimulate the existing 60 NPD's in the world. Some of these new diffractometer projects including the ones in Japan will be presented and the prospects for new scientific impact will be discussed.

Keywords: neutron powder diffraction, materials science, structure-properties relationship

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Neutron Protein Crystallography (nPX) Development: reaching yet higher Molecular Weight Capability

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The unique property of the neutron scattering interaction with deuterium being as strong as C, N, O means that medium resolution crystal structure studies can discern the hydrogenation and hydration of a protein structure. We have used the Institut Laue Langevin (ILL) LAue DIffractometer 'LADI' to compare with Ultra-high resolution X-ray PX to define such details of the lectin concanavalin A [1] and performed a 15K nPX analysis of concanavalin A structures, then a 15K to 293K comparison [2]. This latter study [2] also brings time-resolved freeze trapping nPX studies as a potential for the future. New nPX instruments at LANSCE-USA, the ILL, ISIS 2 UK (proposed), SNS-USA (under construction) and SNS-Japan (under construction) will further expand the capabilities including into yet higher molecular weight protein complexes and protein DNA complexes. We will review our contribution to the nPX developments [3] and also we offer new simulations addressing the category of non-crystallographic symmetry cases where we show that even higher molecular weight can be examined in nPX studies of deuterium atom placement.

[1] Habash J., Raftery J., Nuttall R., Price H.J., Wilkinson C., Kalb (Gilboa) A.J., Helliwell J.R., *Acta Cryst*., 2000, **D56**, 541. [2] Blakeley M.P., Kalb (Gilboa) A.J., Helliwell J.R., Myles D.A.A., *PNAS USA*, 2004, **101**, 16405. [3] Blakeley M.P., Cianci M., Helliwell J.R., Rizkallah P.J., *Chem. Soc. Reviews*, 2004, 548.

Keywords: neutron protein crystallography, synchrotron radiation, hydrogens and hydration in proteins