m44.o01

Neutron diffraction facilities for structural studies of crystals and fibres

V.T. Forsyth[1,2], S.A. Mason[1], M.G. Davidson[3], J.A.K. Howard[4]

Institut Laue Langevin, 6 Rue Jules Horowitz, 38042 Grenoble Cedex 9, France, EPSAM and ISTM, Keele University, UK, Chemistry Department, Bath University, UK, Chemistry Department, Durham University, UK

In recent years there has been increasing recognition of the scope of approaches involving the combined use of both X-ray and neutron scattering. This is reflected by the priority that has been given to co-location of neutron and X-ray sources on shared sites. One of the best examples is the Grenoble campus, which accommodates the Institut Laue Langevin (ILL), European Synchrotron Radiation Facility (ESRF), and the European Molecular Biology Laboratory (EMBL) Outstation, providing a powerful scientific infrastructure for research in physics, chemistry and the biosciences.
Since neutron fluxes are typically low compared to those available at synchrotron X-ray facilities, there has been a major effort at the ILL to maximize the exploitation of the available scattering data. Much emphasis has been placed on the provision of efficient detector systems but there has also been considerable effort invested in facilities for optimal sample provision. The D19 diffractometer at the ILL is currently being upgraded to provide an efficiency gain of ~25. The new instrument will be commissioned following the restart of the ILL in June 2006. It will provide greatly improved data quality for crystallographic work in structural chemistry, physics and the biosciences, as well for fibre diffraction studies of synthetic and biological polymers. Recent results and future prospects will be discussed in the context of this development. These will demonstrate the enhanced scope that will be offered by the new instrument and will also emphasise the advantages offered through the use of selective and non-selective deuteration.

m44.o02

New opportunities for neutron diffraction in structural science

Juan Rodríguez-Carvajal

Institut Laue-Langevin, B.P. 156, 38042 Grenoble Cedex 9, France. E-mail:jrc@ill.fr

Keywords: neutron diffraction, instrumentation, data analysis

Neutron diffraction is a well developed technique with many applications in all fields of solid state sciences. It is perfectly adapted to crystallographic studies in a complementary way to X-ray diffraction. The particular properties of neutrons, compared to X-rays, make them the probe of choice to refine the position and occupation factors of light elements in crystalline materials (i.e. hydrogen in intermetallic compounds), to distinguish adjacent elements in the periodic table, to determine magnetic structures, to study all kind of phase transitions in complex environment, etc. The Institute Laue-Langevin is currently under a process of upgrading many existing instruments and constructing new ones. The Millennium Program is under strong development and diffraction instruments play an important role in it [1]. In this talk, after reviewing the most important characteristics of neutron diffraction, I will present the current situation at ILL concerning diffraction, particularly the upgrades of the high resolution powder diffractometer D2B, the high resolution mode of D20 and the single crystal diffractometers D10 and D19 as well as the new proposed diffractometer DRACULA. Some words will be also devoted to the quasi-Laue diffractometers. I will also describe the existing projects concerning the development of software for data analysis related to the high throughput of the new instruments. New materials for hydrogen storage and battery cathodes, colossal magnetoresistance, superconductors, multiferroics, etc, have been synthesized and need structural characterisation in order to properly understand and control their properties. Neutron diffraction is of paramount importance for precise structure refinements. As an illustration of the capabilities of the existing instruments I will present some neutron powder diffraction examples. In particular the use of the D20 in high resolution mode is perfectly adapted to refine crystal structures through a series of phase transitions as a function of temperature.

[1] http://www.ill.fr/pages/science/Docs/DIFF.pdf.