P.01.08.2
Acta Cryst. (2005). A**61**, C143

High-Resolution Neutron Diffraction Monochromators

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Cylindrically bent perfect crystals (BPC) as neutron monochromators/analyzers have been proved as an excellent alternative of conventional mosaic crystals providing a way how to increase luminosity and angular/energy resolution of some dedicated scattering devices installed at steady state sources [1-3]. In our contribution we present the recent results of test experiments with dispersive monochromators based on a double-reflection process realized either in one cylindrically bent perfect crystals (often called as Renninger or *Umweganregung* effect) or by means of a sandwich using two bent perfect crystal slabs of a different cut. Depending on the bending radius of the crystal slab (or the sandwich of two slabs) the resolution $\Delta\lambda/\lambda$and the $\Delta\alpha$ collimation of the monochromatized beam can be continuously adjusted in the range of $5x10^{-5}$ - $1x10^{-3}$. Of course, that the dispersive bent perfect crystal elements can be used also for the high-resolution analysis of the scattered beam as well as for a high precision λ-calibration of the TOF neutron scattering devices.

Neutron diffraction investigations are in this field partially supported by the projects AV0Z10480505, GACR. 202/03/0891 and MSM2672244501

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Keywords: neutron diffractometry, monochromators, focusing

P.01.08.3
Acta Cryst. (2005). A**61**, C143

Isotopic Substitution Neutron Diffraction for Enhanced Structural Information from Crystalline Powder Materials

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Why bother determining the structure of a material?

The usual answer is that structure is key in determining the properties of the material. Powder diffraction techniques allow rapid assessment of readily available polycrystalline materials. Small differences in structural features, such as the level and distribution of dopants, changes in bond lengths/angles as a function of temperature and thermal displacements of atoms, all influence properties. Therefore, to fully understand a material, extraction of the highest quality structural information is crucial.

Using isotopically substituted samples and combined data-set analysis it is possible to extract structural information of unprecedented quality from polycrystalline materials. Uses of isotopic substitution to overcome absorption effects (*e.g.* ^{7}Li, ^{11}B, ^{154}Sm and ^{160}Gd) and incoherent scattering problems (*e.g.* ^{2}H) are well established, however, using the contrast in the scattering lengths of isotopes of an element to obtain enhanced structural information has been almost exclusively restricted to local structure investigations of non-crystalline materials and liquids. For over half of stable elements there exist, at reasonable cost (between $1 and $5 per mg), two or more isotopes with strongly contrasting scattering lengths.

Several published examples of the usefulness of the technique are presented with a brief introduction.

Keywords: neutron diffraction techniques, accuracy, precision

P.01.08.4
Acta Cryst. (2005). A**61**, C143

The New Quasi-Laue Diffractometer at the Australian OPAL Research Reactor

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The new single-crystal diffractometer for the Replacement Research Reactor in Australia will be a quasi-Laue diffractometer, similar to VIVALDI at ILL, France. It will be competitive with the best instruments currently available. Data collection times for a normal structure determination will be less than a day, a considerable improvement on current data collection times, typically a few weeks at HIFAR. Also, the crystal size needed for an experiment can as small as about 0.1 mm^3, opening up new research areas where it has proved difficult to grow crystals sufficiently big (several mm^3) which are currently needed. An area of research opening up will be multiple temperature and/or pressure measurements.

More detailed information on the instrument will be presented.

Keywords: neutron diffraction, instrumentation, single-crystal structure analysis

P.01.08.5
Acta Cryst. (2005). A**61**, C143

Design of a Neutron Diffractometer at SINQ Using Monte Carlo Simulations

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Monte Carlo simulations have become an essential tool for the investigation and improvement of the performance of neutron scattering instruments. For the cold neutron powder diffractometer DMC at the Swiss spallation neutron source SINQ, the Monte Carlo program McStas [1] was chosen to investigate a detector upgrade. The simulations included all components from neutron source to the position sensitive detector, including neutron guide, monochromator, beam reduction and sample. By means of these simulations the ideal detector geometry was determined.

Monte Carlo ray-tracing simulations have been proven that the optimization of a neutron scattering instrument or the describing of the performance of such an instrument can be done in a reliable and effective way. But such simulations have a much larger potential. Another field of application is to use Monte Carlo simulations to analyze data during and after an experiment. Such a 'virtual experiment' is a full simulation of a real measurement. By means of the cold neutron powder diffractometer DMC we show that the Monte Carlo packages are in a state where virtual experiments can easily be performed.

[1] http://neutron.risoe.dk/

Keywords: neutron instrumentation, Monte Carlo simulation, neutron diffraction

P.01.08.6
Acta Cryst. (2005). A**61**, C143-C144

The IPEN-CNEN/SP PSD Neutron Diffractometer

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A new IPEN-CNEN/SP neutron powder diffractometer was constructed and installed at the 4.2 MW thermal IEA-R1m research reactor. It is an extensive upgrading of the old IPEN-CNEN/SP multipurpose neutron diffractometer. The old diffractometer was a single-detector instrument with a boron trifluoride (BF_3) detector and a flat copper mosaic single crystal monochromator. The main modification introduced in the old instrument was the installation of a position sensitive detector (PSD). The PSD is formed by eleven ^{3}He linear detector elements clamped together at each end to form a rigid plane. Placed at a distance of 1,6 m from sample, the PSD spans an angular range of 20º of a diffraction pattern, with a quite good resolution. In order to increase the neutron beam flux at the sample position, a focusing Si perfect single crystal monochromator was installed in the instrument. With a take-off angle of 84°, the monochromator can be positioned to produce 4 different wavelengths, namely 1.111, 1.399, 1.667 and 2.191 Å. In comparison to the former instrument, the new diffractometer has a better resolution and is *ca.* 600 times faster in data acquisition. The IPEN-CNEN/SP PSD neutron diffractometer has been designed mainly for crystalline and magnetic