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High-Resolution Neutron Diffraction Monochromators
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Cylindrically bent perfect crystals (BPC) as neutron mono-chromators/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.
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Keywords: neutron diffractometry, monochromators, focusing

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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

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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

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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

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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

structures determination and for application of the Rietveld method in quantitative phase analysis. The utilization of this instrument is open for the brazilian and latin-american scientific and technological communities.

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Keywords: neutron diffractometer, PSD detector, focusing monochromator

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The new Single Crystal Diffractometer HEiDi at the FRM-II and its Applications

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HEiDi, one of the new single crystal diffractometers of the research neutron source FRM-II, was designed to cover a wide area of scientific applications in crystal structure analysis. It uses the high flux of fast neutrons with short wavelengths from the hot source of the FRM-II. The enlargement of the visible reciprocal space (=Q-space) allows very accurate determinations of nuclear positions in single crystals as well as more detailed quantitative informations about mean square displacements and vacancies which is of interest in reference to static or dynamic disorder effects and phase transitions. The Q-dependences of the magnetic and the nuclear cross sections of neutrons are quite different. This can be used to determine the magnetic and the nuclear order in a crystal separately. Other advantages of shorter neutron wavelengths (1.4 Å down to 0.3 Å) are the significant reduction of absorption effects in compounds with highly absorbing elements (e.g. Sm, Gd) and the reduction of extinction effects.

During the nuclear commissioning of the FRM-II in 2004 started the adjustment and characterization of HEiDi with neutron radiation. First experimental results are quite promising, e.g. an excellent resolution function (<0.1° at min.) or a perfect alignment between the calculated and the measured gain factor of 2.5 of the monochromator focussing unit. Further experimental results from the instrument and typical applications like structural phase transitions, local disorder (H bonds in RDP) or magnetism will be presented on the conference.

Keywords: neutron and X-ray diffractometry, single crystal structure analysis, neutron instrumentation

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The Italian Neutron Experimental Station (INES) at ISIS: Status and Development

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The INES project concerns the realization of a multipurpose experimental station, built by CNR at the ISIS pulsed neutron source (Rutherford Appleton Laboratory, UK). This instrument is mainly intended to operate as test and training facility for the Italian neutron-scattering community. The experimental station is equipped with a multipurpose time-of-flight neutron diffractometer, presently under commissioning. This is located downstream a water moderator of the neutron source, with an excellent time-resolution. In the present configuration the INES diffractometer contains a highly-efficient large detector area covering a range of about 170^{o} on the horizontal plane. Moreover it offers a large sample volume (about 0.25 m^3), allowing the study of almost any kind of object, including bulky archaeological artifacts. The possibility to separately analyze each single detector makes texture analysis also possible. The opportunity to operate experiments in particular thermodynamic conditions (i.e. high pressure, high and low temperatures) is also under investigation.

Keywords: neutron istrumentation, texture analysis, archaeometry

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Design of a High Resolution Macromolecular Neutron Diffractometer (MaNDi) for Structural Biology Research at the SNS

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With the advent of third-generation synchrotron X-ray sources, it was envisioned that ultra-high resolution macromolecular crystallography (UHRXMC) at resolutions of 0.5 Å to 1.0 Å would provide detailed information on the positions of critical hydrogen atoms within the active sites of enzymes. To date, in about 82 structures in the PDB in this resolution range, significant numbers of hydrogen atoms including those in the active sites could not be identified. Furthermore, only about 0.5% of all macromolecular structures in the PDB are amenable to UHRXMC and hence other complementary techniques are needed for the identification of critical hydrogen atoms involved in the catalytic mechanisms in a majority of enzyme systems.

Neutron Macromolecular Crystallography (NMC) has been shown to provide accurate proton positions, protonation states and hydration states, as well as hydrogen/deuterium exchange, in macromolecular crystals even at moderate 2 Å to 2.5 Å resolution. One major bottleneck that severely constrains the productivity of NMC is the limited flux at the current sources and the requirement of large crystals. The advent of the Spallation Neutron Source (SNS), with over an order of magnitude increase in neutron flux, the advances in neutron optics and detectors, as well as advances in structure genomics and deuteration. provide an exciting opportunity to push the NMC field to new horizons. Hence we propose to develop a dedicated world-class high resolution time-of-flight single crystal macromolecular neutron diffractometer (MaNDi) for structural biology research at the SNS. MaNDi has been designed to be able to collect a full hemisphere of Bragg data with a resolution of 1.5 to 2 Å on a crystal with a lattice constant up to 150 Å in 1 to 7 days. The higher throughput and resolution are accomplished by the use of a wide wavelength bandwidth of cold neutrons (1.8 Å < λ < 4.5 Å) sorted into a large number of high resolution wavelength channels by time-of-flight and by an array of high resolution position-sensitive area detectors covering a large solid angle. We envision that the unprecedented high data rates and resolution with MaNDi will open up new avenues and greatly advance the field of structural biology, enzymology and protein dynamics.

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Keywords: neutron macromolecular crystallography, time-of-flight single crystal diffractometer, structural biology

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Advances in Neutron Single Crystal Diffraction towards a Smaller Sample Sizes

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Single crystal diffraction has been used as a tool for structure analysis since the discovery of neutron scattering. Complementary to X-ray radiation neutron radiation is especially useful to locate 'light' elements like hydrogen next to 'heavy' elements like metals. Furthermore, neutrons are much "gentler" to organic crystals. A major obstacle for neutron diffraction is the moderate flux and therefore the significantly larger single crystal sizes and longer data collection times needed for a decent data set.