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.