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Keywords: crystal structure prediction, organic polymorphism, computed crystal energies

MS.81.1

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Crystallography at the new Australian research reactor OPAL

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The newly commissioned 20 MW research reactor OPAL in Australia houses a number of instruments dedicated to crystallography as well instruments for neutron spectroscopy. The initial suite of instruments includes two powder diffractometers and a quasi-Laue single crystal instrument and was selected to reflect the strengths and interests of Australian Scientists. OPAL is characterised by extensive use of state-of-the-art neutron guides that deliver higher fluxes to the instruments. In this presentation I will firstly describe the technical capabilities of these instruments as well that of the closely the allied Small Angle Scattering instrument. Next I shall introduce the scientific capabilities of these instruments demonstrating how the high flux available at the instruments can be utilised either for high-speed or high resolution crystallography.

Keywords: neutron diffraction, international science, diffraction neutrons X-rays electrons

MS.81.2

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Current situation of the cold neutron research facility project at HANARO

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HANARO is the research reactor with 30 MW thermal power with 7 horizotal beam ports and has been operational since its first criticality in 1995. For last 10 years of its early phase, neutron beam instruments of high reolution powder diffractometer, four-circle diffractometer, small angle neutron spectrometer, neutron radiography facility, residual stress instrument, etc.. has been built sequentially around those beam ports using thermal beams. With rapidly increasing demand of cold neutron from continuously expanding users society of universities and industries, the project for the cold neutron research facility construction was launched in July 2003. The project consists of 4 parts; the liquid hydrogen cold moderator and its cooling system utility, the neutron guides, neutron spectrometers and the cold neutron laboratory building. There are 3 relocated neutron spectrometers with modification from the reactor hall and 3 newly developed spectrometers as day-1 instruments. In mid 2008, the cold neutron laboratory will be completed, and tight installation and commissioning schedule for all the four parts of the project is ahead from now to it expected project completion, April 2010. We report in this talk overall project status, schedule, instruments development strategy with users community, and long term prospects.

Keywords: cold neutron spurce, neutron instrumentation, neutron diffraction and scattering

MS.81.3

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SNS and HFIR: Breaking new ground

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The Spallation Neutron Source (SNS) facility became operational in the Spring of 2006, and is now well on its way to become the world-leading facility for neutron scattering. Furthermore, the SNS and the HFIR reactor facility, newly outfitted with a brilliant cold source and guide hall, were brought together within a single Neutron Sciences Directorate at ORNL providing the opportunity to develop science and instrumentation programs which take advantage of the unique characteristics of each source. SNS and HFIR will both operate as scientific user facilities. Access to these facilities is being managed under an integrated proposal system which also includes the Center for Nanophase Materials Sciences (CNMS) and the electron microscopes in the Shared Research Equipment (SHARE) program. Presently SNS has three of the eventual 25 instruments operating in the User program and seven more will begin operations in 2008.
A project to upgrade the power of the SNS accelerator to 3MW is underway and government approval is being sought for construction of a long pulse (1ms) second target station. The future is bright for neutron scattering at Oak Ridge.

Keywords: SNS, HFIR, breaking new ground

MS.81.4

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An advanced pulse neutron source and scientific challenges at J-PARC

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The J-PARC (Japan Proton Accelerator Research Complex) project, which aims at providing world best experimental facilities for condensed matter sciences, elementary particles and nuclear physics, and nuclear transmutation R&D, is now in progress toward its completion. For condensed matter science users, a MW pulsed neutron source will be realized with a number of advanced neutron instruments. The first operation for users is planned to start in December 2008. The MW neutron source with the mercury target system, the cryogenic hydrogen moderator system, and all other

critical components has been demonstrated its high performance through the stringent functional tests. Designing the challenging neutron source, various new concepts have been have been introduced and developed to maximize performances in terms of neutron pulse peak intensity, time integrated intensity and time resolution of pulse peak. For example, adopts of para-state hydrogen moderator, a high cut-off energy de-coupler, etc., would realized the high performance. Along with the neutron source, neutron instrument construction has significantly accelerated. Presently, fabrication and installation of 8 instruments e.g., the super high resolution power diffractometer, the most advanced engineering materials diffractometer, a high intensity chopper spectrometer, are to be to be available for users by the time of Day-one. This pare highlights what J-PARC provides to users with emphasis on innovation in design and engineering of the MW pulse neutron source. Along with, novel design concepts applied in so called the next generation instruments are to be discussed in light of fulfilling the key research areas based on current scientific direction and prospect with neutron.

Keywords: pulse neutron source, J-PARC, novel concept instrument

MS.81.5

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Progress for the european spallation source

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The proposal for the European Spallation Source (ESS) is still awaiting a decision to start construction. Nevertheless, there appears to be renewed interest and consensus in Europe to build a next-generation neutron source. The current understanding is that the ESS project will be based on a 5 MW linear proton beam accelerator and a long-pulse target station, feeding 22 neutron instruments. Several sites in Europe have submitted expressions of interest to host the ESS and are preparing their final bids. Furthermore, the site selection process and discussions on potential partnerships within Europe have started. Key factors for site selection include the potential for scientific environment and proximity to other European large-scale research facilities. We will present the Swedish proposal to construct ESS in Lund in more details.

Keywords: neutron sources, neutron instrumentation, neutron and X-ray scattering

MS.82.1

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Momentum density of uncompensated electron spins measured by magnetic Compton scattering

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According to quantum mechanics, the momentum density (MD) of electrons can be described by momentum-space wavefunctions which are related to real-space ones through Fourier transformation. Therefore MD directly reflects electron states in matter as well as charge density. For studies of magnetic materials, information on spin states of electrons is important. During the years since 1976 [1], it has been found that magnetic Compton scattering of circularly polarized X-rays is effective for measuring MD distribution of electron spins in ferro/ferri-magnetic materials, such as metals, alloys and compounds, all of which are composed of 3d-transition and/or 4f-rare-earth elements [2]. Following an introduction to characteristic features of magnetic Compton scattering, recent progress will be briefly reviewed by referring to notable reports. The review will include reconstructed three-dimensional MD distribution of spins from Compton profiles, that is, from twice integrated MD distributions of spins.

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Keywords: Compton scattering, electron spin, magnetic material

MS.82.2

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Inelastic X-ray scattering as a powerful probe of correlation effects in materials

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Electron correlation effects are becoming an increasing focus of attention in understanding the behavior of wide classes of novel materials. This talk discusses some of our recent work related to resonant inelastic x-ray scattering (RIXS) as well as magnetic and non-magnetic Compton scattering studies.[1-7] Specific topics include: (i) Modeling and analysis of RIXS data from electron doped cuprate Nd-Ce-Cu-O, which gives insight into the doping dependence of the Mott gap and its possible collapse with doping. (ii) Magnetic Compton scattering spectra in the double layer manganite La-Sr-Mn-O, which are shown to contain a distinct signature of the d-electrons of x^2-y^2 symmetry, allowing us to adduce significant changes in the occupancy of these orbitals as a function of temperature in the manganite. (iii) Analysis of high resolution Compton scattering spectra from La-Sr-Cu-O to delineate evolution of Fermiology and correlation effects as the system goes from the insulating to the metallic state with doping. Work supported in part by the U. S. Department of Energy.

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Keywords: magnetic X-ray scattering, inelastic X-ray scattering, *ab-initio* calculations