

Neutron scattering and mesoscopic systems*

A school and conference on neutron scattering and mesoscopic systems was held in October 2009. The school entitled 'Neutrons as probe of condensed matter', held at the Bhabha Atomic Research Centre (BARC), Mumbai during 5–10 October 2009, was attended by 60 participants. The school had both theory sessions and hands-on experiments at the neutron scattering facility in *Dhruva*, covering all aspects of neutron scattering. It was the 14th in the series of workshops/schools on neutron scattering. For the first time experts from abroad delivered lectures in the school.

Following the school, the conference was held during 12–14 October 2009 in the scenic International Centre at the Talegaon Plateau, Panaji, Goa. The whole event was part of the Dr Homi J. Bhabha birth centenary year celebration. The conference comprised of 28 invited talks and 97 posters, with a total of about 150 participants. The invited speakers included experts from several international centres of repute in neutron scattering, notably Laboratoire Léon Brillouin (LLB), Saclay, France and Institut Laue-Langevin (ILL), Grenoble, France, along with Indian speakers. Among the Indian participants, it was a good mix from various universities and from the neutron scattering group at BARC. The talks were distributed over eight technical sessions in three days with two poster sessions in the afternoon during the first two days.

The first session on 12 October had two speakers from ILL. Juan Rodriguez Carvajal and R. Wagner. The other speakers were Isabelle Mirbeau (LLB) and T. Pradeep (IIT Madras, Chennai). Juan spoke about neutron diffraction studies on manganite systems with charge ordering, a subject of current interest. While discussing structural phase transitions in such systems, he explained how the pro-

gram AMPLIMODES allows symmetry mode analysis of displacive phase transitions. Mirebeau spoke about two classes of interesting samples, viz. pyrochlores and multiferroic systems with geometrical frustration. She reviewed high-resolution neutron diffraction results on such systems. Pradeep discussed dynamical studies of alkyl chains coated on Au and Ag nanoparticles in collaboration with the Quasi Elastic Neutron Scattering group at BARC. Wagner (Director, ILL), was the last speaker in the session. His talk focused on instrument renewal programme at ILL. At present modernization plans in two phases, M-0 and M-1, are in progress. Wagner acknowledged the expertise of India in neutron scattering and mentioned that ILL looks forward to India's participation in the modernization as well as in the scientific programme as a future non-European scientific partner.

The afternoon session of the day was dedicated to the most popular technique, small angle neutron scattering (SANS). M. Imai (Ochanomizu University, Japan) discussed the interaction between membranes and how they are modified due to the presence of guest molecules, viz. polymer chains and spherical colloidal particles. The geometry of the membranes was obtained from the SANS profiles. V. K. Aswal (BARC) described the kinetics of protein gelation under heating, using the SANS technique at the *Dhruva* reactor Trombay. SANS has been used to study the structural evolution and kinetics of temperature-induced gelation in bovine serum albumin protein. D. Sen (BARC) described SANS as well as small angle X-ray scattering (SAXS) to study the effect of sintering on the mesoscopic structures in cement paste, ceramics and in self-propagating, high-temperature synthesized intermetallics. The last speaker, P. A. Hassan, described SANS studies on self-assembled structures that can be used as drug-delivery systems. Block co-polymer assemblies and bile-salt surfactant mixed micelles were studied using SANS and dynamic light scattering with reference to their application in encapsulating drugs like doxorubicin and sumatriptan.

The second day opened with a talk by Dananjay Pandey (Benaras Hindu University, Varanasi) on the structure of ferroic phases in mixed perovskites, viz. lead zirconium titanium-based perovskites (PZT) and lead manganese niobium systems (PMT) that show a variety of composition-related structural phase transitions. Some changes are not discernible by X-ray diffraction but are observed using neutron diffraction, since neutrons have reasonable scattering cross-section for oxygen atoms.

Zakir Hossain (IIT Kanpur) has established several phase transitions in Yb-based heavy fermion systems using muon spin rotation and magnetic neutron diffraction. Amitabh Das (BARC) presented results on magnetic Bragg diffraction on half-doped compound $\text{La}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$ (remains same). These compounds exhibit spin, orbital and charge ordering upon doping in the ABO_3 structure.

UGC-DAE Consortium for Scientific Research (UGC-DAE-CSR) has recently installed a neutron powder diffractometer at the *Dhruva* reactor with a unique sample environment of very low temperature (1.5 K) and high magnetic field (7 T). Vasudeva Siruguri (UGC-DAE-CSR) presented some recent neutron diffraction data obtained on this instrument.

Javier Campo (Instituto de Ciencia de Materiales de Aragón, Zaragoza, Spain) presented his results on neutron diffraction study at ILL on a crystal of mesoscopic single-molecule magnets. The study was done on the D10 diffractometer at ILL.

A. Thamizhavel (Tata Institute of Fundamental Research, Mumbai) presented single-crystal neutron diffraction data from AFe_2As_2 ($A = \text{Ca, Sr, Ba, Eu}$), a class of pnictide superconductor compounds.

The third and last day of the conference had several talks on probing dynamics of atoms and molecules using neutrons, since thermal and cold neutrons have kinetic energies well-suited to probe various dynamical phenomena in solids. Quasi-elastic neutron scattering (QENS) is a popular tool for studying diffusion. The talks in the morning session discussed the application of this technique in various systems. The first

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talk by José Teixeira (LLB) dealt with interaction of water with hydrophilic and hydrophobic surfaces. In case of biological molecules as substrate, dynamics of the water of hydration forms an interesting case for probing using QENS. Teixeira followed hydration and water dynamics in peptide forms. F. Juranyi (Paul Scherrer Institute, Switzerland) discussed diffusion of water in clays. She could quantify the effect of geometry and charge on the dynamics of water in different clay media from QENS studies and macroscopic tracer diffusion experiments. Such studies are important, since clays are a part of the barrier in radioactive waste repositories. S. Mitra (BARC) has studied rotational and translational dynamics of various hydrocarbons in zeolite cages using QENS spectrometer at *Dhruva*. He presented experiments on diffusion of various host/guest combinations, where diffusion of a guest hydrocarbon molecule is studied in a zeolite cage using QENS. Low-dimensional systems often give rise to unconventional physical properties and also provide the testing ground for simplified formalisms and theories. Stephan Rols (ILL) described a carbon nano-peapod comprising fullerenes confined inside single-walled carbon nanotubes (SWNT). This is an all-carbon structure, where the 7 Å diameter fullerene is constrained inside a nanotube of 14 Å diameter and can move along the axis of the SWNT. The low dimensionality and low roughness of the tube wall lowers orientation-related freezing of the fullerene molecules in the nano-peapod. Mala N. Rao (BARC) presented some recent results on neutron inelastic scattering carried out with a class of ternary alloys of composition $Zn_{1-x}Be_xSe$. J. A. E. Desa (University of Goa) reviewed structural studies on simple glasses of AX_2 composition and structural features of vitreous zinc chloride, germania and rare-earth phosphate glasses, using neutrons and X-rays. R. Chitra (BARC) described the various neutron-diffraction studies on the triglycine family of ferroelectric crystals carried out at the single crystal neutron diffractometer at *Dhruva*. The next two talks dealt with the application of neu-

tron reflectometry for thin film characterization. Mukul Gupta (UGC-DAE-CSR) explained about the determination of Fe and N self-diffusion in FeN films using the difference in scattering cross-section between different isotopes of Fe and N and neutron reflectometry. Surendra Singh (BARC) described the use of off-specular polarized neutron reflectometry to determine the morphology of a magnetic interface and its differences with respect to a chemical interface. R. V. Upadhyay (Charotar Institute of Science and Technology, Gujarat) described SANS work on surfactant-coated magnetic nanoparticles in determining the aggregation number and geometrical shape of the micelles. K. Guruswamy (National Chemical Laboratory, Pune) described work on phase separation of silica nanoparticles in a hexagonal lyotropic liquid crystal mesophase, using TEM and SAXS, a complementary technique of SANS. The neutron scattering facility at *Dhruva* uses neutron detectors built indigenously by a dedicated group in the Solid State Physics Division at BARC. Shradha S. Desai from this group described various detectors developed by them. These include BF_3 gas-filled neutron detectors and 3He gas-filled one-dimensional position-sensitive detectors that are being used in *Dhruva* extensively.

Apart from the invited talks, there were 97 contributed papers presented in form of posters during the first and second days of the conference. The largest number of papers were from the two most popular techniques, neutron diffraction and SANS, 39 papers in each category. There were eight papers on neutron reflectometry, five on inelastic neutron scattering, four on QENS and two on neutron instrumentation. The papers on SANS demonstrated the true interdisciplinary nature of this technique, by its application in physics, chemistry and biology. A group in BARC has developed a super-ultra small angle neutron scattering instrument nicknamed SUSANS, in collaboration with Hahn Meitner Institute, Berlin, which was described in a poster. A large number of papers presented in the diffraction section dealt with magnetic and piezoelectric samples of current

interest, viz. ferrites, substitutional perovskite compounds, multiferroic compounds, strongly correlated electronic systems and lead-bismuth titanates. One paper dealt with the effect of pressure on magnetic structure. There were a sizable number of posters on neutron diffraction work on glassy materials. The papers on neutron reflectometry dealt with multilayer thin films, which included Co/Cu multilayers, Fe/Au multilayers and ferrocene-incorporated Langmuir-Blodgett films of arachidic acid. One paper described the changes in a thin-film soft magnetic material due to ion irradiation as understood by neutron reflectometry.

Inelastic neutron scattering posters included rare earth-based RPO_4 class of compounds, II-VI group semiconductor ZnSe and a compound with negative thermal expansion, $Sc_2(MoO_4)_3$. Several papers in the category of QENS looked at the diffusion of hydrocarbons and water in various confined geometries. There was a paper on development of a stepper motor control system for neutron focusing devices at *Dhruva*, and another on development of a high-efficiency square cross-section neutron detector for single-crystal neutron diffractometer at Hanaro, Korea.

The ambience at the venue of the conference also stimulated many discussions and debates among the participants during tea and lunch breaks, besides the technical sessions.

In the concluding session, Wagner, appreciated the idea of holding the conference at Goa University. He commented that it was a good move to spread the importance of neutron scattering as a technique and wished to see the next conference also being organized in a university at another part of India. R. Carvajal (ILL) expressed his happiness in sharing the excitement of new data analysis techniques with young Indian researchers and complimented the organizers for their efforts.

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