MEETING REPORT

Conference on neutron scattering*

The conference on neutron scattering held at the Bhabha Atomic Research Centre (BARC), Mumbai against the backdrop of the celebrations of the Golden Jubilee of setting up of the Department of Atomic Energy (DAE) in India served as a useful stocktaking exercise of the evolution and performance of research in condensed matter physics using neutrons. The conference brought together about 160 professionals and students pursuing neutron beam research (NBR), to review much of the work that has happened over the past 40 years emphasizing recent research contributions using advanced instrumental facilities at ARC and elsewhere. About 15 experts from various overseas neutron scattering centres, namely ISIS (UK), San Sebastian (Spain), Atominstitut at Vienna, Paul Scherer Institute (Switzerland), LLB–Saclay (France), ILL (Grenoble), Tokyo University of Science (Japan), Hahn Meitner Institute–Berlin (Germany) and Korea Atomic Energy Research Institute–Daejun (Korea) participated in the conference.

Neutron scattering activity in India dates back to about 50 years, when on a rather modest scale, the first neutron diffractometer began operation at India's first indigenous research reactor, *Apsara* offering a maximum flux of 10^{12} neutrons/cm^2/s. The programme relied heavily on indigenous instrumentation, which evolved from comparatively simple systems when compared to the currently available spectrometers and other ancillary facilities at *Dhruva* reactor (maximum flux ~ 2×10^{14} neutrons/cm^2/s) at BARC. Beginning from electromechanical on-line control and data acquisition systems (DAS), the current DAS are on-line and PC-based, which provide state-of-the-art power for on-line control, data acquisition, data analysis and presentation in various formats. The talk on 'National facility for neutron beam research' by K. R. Rao and the evening talk 'reminiscing on earlier neutron scattering days' by P. K. Iyengar dwelt at length on the evolution of neutron scattering in India.

Earlier conferences on neutron scattering in India were held in 1964 and 1991. So, coming after nearly 12 years, this conference presented an opportunity for the current generation of researchers, especially the younger ones, to present and discuss studies of a variety of new materials and new phenomena through about 30 invited papers and nearly 80 contributed poster presentations.

Nuclear magnetic resonance and X-ray diffraction techniques have complimented neutron diffraction studies of hydrogen-bonded molecules, hydrates, etc. as pointed out by R. Chidambaram in his inaugural address. The high penetrating power of the chargeless thermal neutron, its wavelength (~ 2 Å), energy (~ 50 meV) and magnetic moment have continued to make the neutron a unique probe to examine crystal structure, atomic and molecular dynamics and magnetism of a variety of materials. Application of direct methods to solve the phase problem in neutron crystallography, established by S. K. Sikka in the 1960s, has been utilized later in solving the structure of compounds like L-threonine. So also, the systematic study of amino acids and peptides helped in understanding the ubiquitous hydrogen atom stereochemistry and hydrogen bond interactions present in all biological molecules, including proteins, DNA, etc. M. Ramanadham (BARC) pointed out how this knowledge has been effectively used in analysing the X-ray structure of an antibiotic, antitumour protein, neocazinostatin, leading to 'correlation to the primary sequence of this protein at two sites. (In addition), these correlations helped in identifying the DNA-binding site on this protein which was not known earlier'.

R. R. Choudhary (BARC) presented some of the recent investigations in the triglycine family of hydrogen-bonded ferroelectrics by neutron diffraction. The aim of these studies has been to understand how by slight alterations of crystal structure of these compounds by small quantities of, say, L-alanine, the physical properties change to the extent that depoling of the crystal (specifically TGS in this case) could be prevented. The neutron structural investigations have revealed that the L-alanine molecule which is larger than glycine, leads to an internal strain within the TGS crystal. The studies involved correct interpretation of site occupancy of L-alanine as against what is believed otherwise.

As I. Tanaka (JAERI, Japan) pointed out, 'in the neutron protein crystallography, development of neutron imaging plate (NIP) became a break-through event'. His paper clearly showed how the NIPs, coupled with elastically bent perfect silicon monochromators, have been an efficient solution to medium flux limitation at reactors. Currently there are three neutron diffractometers operating at JAERI, dedicated to the study of biological macromolecules. This has enabled high-resolution (~ 1.5 to 2 Å) structural analysis of several proteins. Currently, on an average, data on one protein structure are being obtained per month using the facilities at JAERI, an impressive record. Tanaka's talk covered also how one can realize growth of large protein crystals and the Japanese biomolecular diffraction programme at the upcoming Japanese spallation neutron source.

Soper's (ISIS, UK) talk emphasized the structure of disordered systems; this brought back to my memory some of the well-established theoretical aspects of partial structure factors in binary and ternary amorphous or liquid structures. I also remember in this connection that the Russians had studied partial phonon density of states by isotopic substitution in some copper alloys in the earlier decades, perhaps the only kind of such studies so far.

Rauch's (Atominstitut, Vienna) talk on interferometry showed once again the continuing rich and novel contributions that have been coming from his group. He drew attention to several esoteric recent experiments concerning off-diagonal geometrical phases (see *Phys. Rev.*, 2002, **A65**, 052111), confinement induced phases (see *Nature*, 2002, **417**, 630) and contextuality (see *Nature*, 2003, **425**, 46), etc. This was one of the few papers that dealt with fundamentals of physics (quantum physics) realizable by use of neutrons. A. G. Wagh's (BARC) presentation was a complimentary paper in this area. I remember my visit to Atominstitute some 25 years ago, when I was thrilled to learn about techniques like dynamical radio-

*A report on the Conference on Neutron Scattering held during 2–4 January 2004 at Bhabha Atomic Research Centre, Mumbai.

graphy, 3D polarography, high-resolution, small-angle scattering and of course, neutron interferometry, all coming from a 250 kW reactor. Flux limitation has never been the limitation to the kind of novel concepts that this centre has ushered in, time and again under the leadership of Rauch.

As I proceed further, I can make only a few random selections from the conference proceedings.

Mukul Gupta (PSI, Switzerland) discussed the apparatus for multi-optional reflectometry at the SINQ facility at PSI and some of the results therefrom. The PSI centre has progressed to an advanced stage in a matter of about a decade; some of the younger colleagues from BARC have carried out experiments using various facilities at PSI.

It was clear that neutron powder diffraction and small-angle neutron scattering have been the most popular techniques, as exemplified by about 25 papers under each of these categories. In India, P. S. Goyal, V. K. Aswal and S. Mazumder have successfully exploited this technique for the study of a variety of agglomerates formed of surfactants, ferrofluids, ceramics, cements, etc. In this conference there has been a discussion of small-angle polarized neutron scattering also, to involve the magnetic power of the neutron to study magnetic systems.

A number of invited talks covered studies of magnetic materials by a variety of polarized and unpolarized neutron scattering. S. M. Yusuf (BARC) and coworkers have studied a large number of frustrated, disordered magnetic materials, such as mixed ferrites, 3D alloys, actinide-based intermetallic compounds, etc. using macroscopic probes as well as using neutron diffraction and depolarization techniques covering a wide range of length scales. Yusuf described some of their recent results on studies of manganese-based colossal magnetoresistance (CMR) pervoskites. So also, Tapan Chatterji (ILL, Grenoble) dealt with spin dynamics and charge-orbital ordering of CMR manganites. K. Motoya (Japan) dealt with, among other aspects, the nature of two kinds of spin-wave excitations that coexist in a reentrant spin-glass material $Fe_{65}(Ni_{0.866}\ Mn_{0.134})_{35}$. He also referred to time-resolved small-angle neutron-scattering patterns from $Fe_{0.70}\ Al_{0.30}$ under various temperature and magnetic field conditions over 20 h, with a typical time window of 1 to 30 min. A newly developed technique of magnetic contrast variation by using small-angle polarized neutron-scattering technique, for analysis of weak magnetization fluctuations was the topic of the talk by A. Wiedenmann (HMI, Germany).

John Tomkinson's (ISIS, UK) talk on neutron spectroscopy was the only one that dealt with application of neutrons for industrial situations. The talk dealt with development of catalysts. I would have liked to see a few more papers relating to applications. From India, one could have had some applications related to neutron radiography or strain measurement and the like; on the other hand, I saw a large number of papers related to basic studies.

We have come a long way as far as lattice dynamical studies using inelastic neutron scattering techniques are concerned. Mala Rao (BARC) reviewed results from a study of a large variety of geologically important minerals. A question that cropped up was 'what is the importance of these studies?'. In other words, one would have liked to learn of the relation of these studies to geophysics or seismology. Lest it be construed that the relation is not forthcoming, I hasten to add that the BARC group has indeed studied comprehensively these aspects by recourse to detailed molecular dynamical calculations and computer experiments that have shed light on phase transformations of a variety of minerals as a function of temperature and pressure. Perhaps, the organizers did not plan for a talk on these aspects as these studies fall outside the scope of a neutron scattering conference.

Porosity in materials whether it be in zeolites or in cement and the like, has been the subject of studies using techniques of small-angle neutron scattering, quasielastic neutron scattering or perhaps even by neutron radiography. Molecular modelling and computer simulation have been effectively used in interpretation of the much data.

An important development of the late eighties was establishment of collaborative programmes with the students and faculty in the universities. DAE opened the doors of its major research facilities – *Dhruva* at BARC, Variable Energy Cyclotron at Kolkata and the INDUS-I synchrotron at Indore – to the university community by setting up the Inter-University Consortium for DAE Facilities (IUC-DAEF) in collaboration with the University Grants Commission. Under this joint programme, one of the (IUC-DAEF) centres was set-up at BARC. The programme involved training of research students in NBR and supporting joint research programmes. This programme has been mutually beneficial for furthering research in various materials by NBR in our country. Whereas synthesis of new and novel materials and their characterization were undertaken in the universities, their study by NBR was undertaken at BARC and the interpretation and understanding of the data was a cooperative joint endeavour. It has given scope to bring in young researchers and students, new materials and fresh ideas as well as the benefit of neutron scattering expertise. Anil Kakodkar (Chairman, AEC) announced in his inaugural presidential address that encouraged by the success achieved so far, both the UGC and the DAE have been keen to enhance the present level of interaction to cover major research programmes of mutual interest. A fresh MOU has been entered into between the UGC and the DAE to achieve this objective, effective from 10 December 2003, extending and enlarging the on-going activities.

K. R. Rao, 29/2, 11th Cross Road, Malleswaram, Bangalore 560 003, India.
e-mail: krrias@yahoo.com