Some contributions to neutron scattering in India and Asia-Oceania Region: 1958–2012*

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National, regional and international cooperation is well known nowadays when it comes to building and using major scientific facilities like nuclear reactors, particle accelerators, space exploration, etc. It was not so when I started my research career in 1958 at Atomic Energy Establishment Trombay (AEET), now renamed Bhabha Atomic Research Centre (BARC). Asia-Oceania Neutron Scattering Association (AONSA) was established some years ago in recognition of this need in the region specified in its name. In the present article I shall deal with some aspects of my contributions to the growth of neutron scattering techniques and science, and highlight how cooperation among various bodies has helped in the growth of science based on neutron scattering.

Keywords: Asia-Oceania, growth, neutron-scattering.

INDIA became independent on 15 August 1947, a backward and impoverished nation without a manufacturing base worth its name for such a large country, but with a substantial legacy of intellectual pursuit of several millennia. Homi Bhabha, with great confidence and audacity, convinced the then Prime Minister Jawaharlal Nehru of the need for a broad-based atomic energy programme amidst considerable criticism and opposition. However, Nehru with his developmental vision for the country backed him to the hilt. The first reactor, Apsara, also the first in Asia–Oceania, was built indigenously with a small group of scientists and engineers. It became critical on 4 August 1956 (Figure 1). The United Kingdom supplied the highly enriched uranium core in a great spirit of scientific cooperation. This was a swimming pool reactor with a flux of $> 10^{11}$ n/cm^2/s at 100–250 kW, the power at which it operated most of the time.

Initiation at Trombay (1958–)

P. K. Iyengar initiated the Indian programme on neutron scattering at Apsara reactor after his return from Canada in March 1958, where he had worked for some time with B. N. Brockhouse (Nobel Prize, 1994). Following our founder Bhabha, it was generally accepted at BARC that if one wished to establish a large-scale and sustainable research programme, it would be necessary to develop the needed techniques and instruments ourselves. First, this would generate the required expertise to innovate and carry out long-term research and secondly, building equipment locally would cost substantially less compared to importing by paying in foreign currency, of which there was a severe shortage.

N. S. Satyamurthy and I joined Iyengar about four months after his return from Canada. Our first task was to build an automatic powder diffractometer for neutrons. Its basic design was similar to the Canadian machine: all the mechanical parts as well as electronics and automation, and the detector were built within the Establishment. Figure 2 shows a photograph of this instrument. Figure 3 shows the first set of data on $FeSn_2$ and its proposed magnetic structure. It required several days to record these data. The observation of the super lattice (100) peak at 300 K vanishing at 400 K, clearly established the antiferromagnetic nature of the material. This was reported at the International Conference on Magnetism in Japan in 1961 and published the following year[1].

In parallel, a commercial diffractometer from the UK was converted to an inelastic scattering spectrometer (Figure 4) and some phonons in Fe were reported at the Conference on Inelastic Scattering of Neutrons in Solids at Vienna in 1961 (ref. 2).

To Chalk River, Canada (1961–)

After three years in Trombay, I was deputed to Chalk River, Canada to work with Brockhouse under a Colombo Plan fellowship in August 1961. During the next 16 months, the major experiment that I would be doing was on liquid argon, a canonical classical liquid, at the high-flux

*This is a modified version of the acceptance talk of the 'AONSA-2013 Prize' of the Asia-Oceania Neutron Scattering Association delivered at the International Conference on Neutron Scattering (ICNS) 2013 at Edinburgh, UK during 8–12 July 2013. The original version can be found on the website: neutronsources.org.

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NRU reactor, apart from experiments on temperature dependence of phonons in Ge. The well-known constant-**Q** technique introduced by Brockhouse was established by this time and we collected such data on a triple-axis spectrometer. Data could not be collected on the triple-axis spectrometer for small wave-vector transfers as it was beyond its range. Hence, time-of-flight data were collected on a rotating crystal spectrometer at several closely spaced scattering angles. It was converted to constant-Q information. As late as 2006, R. A. Cowley from Oxford re-emphasized the importance of constant-Q data for certain sensitive experiments[3], since time-of-flight technique can introduce a peak in the spectrum. Incidentally, this was also a period when there was considerable debate about peaks in time-of-flight data, at a fixed scattering angle, being mistakenly seen as evidence of well-defined phonons in liquids. Combining these two constant-Q datasets, and removing the effects of resolution at the level of intermediate scattering function, we derived the van-Hove time-dependent self- and pair-correlation functions (Figures 5 and 6)[4]. While on the subject of simple liquids, let me add that much later, in 1974, when I was on a sabbatical at Kernforschungsanlage, Juelich with Springer, we[5] observed Rayleigh and Brillouin peaks in constant-Q experiments in normal phase of ^{4}He at 4.2 K at small Q values between 0.06 and 0.2 A^{-1} (Figure 7), and examined the limits of classical hydrodynamics. Distinct Brillouin peaks could be observed only below $Q = 0.15$ A^{-1}.

Figure 1. Apsara reactor: neutron diffractometer in the forefront.

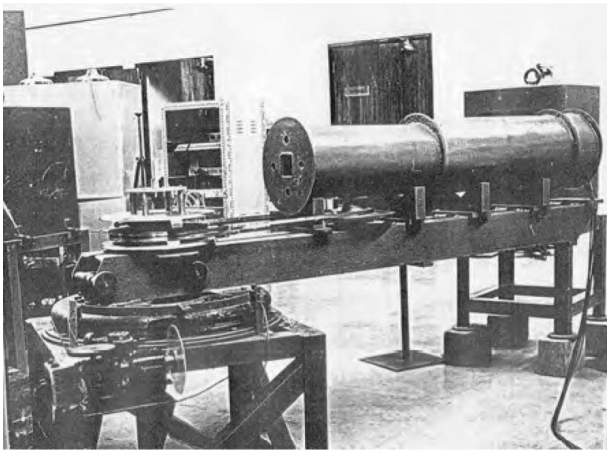

Figure 2. First automatic diffractometer (~1958–59).

Back to Trombay – Cirus (1963–)

I returned to India in January 1963. Even before I had left for Canada, the second reactor, Canada India Reactor (CIR) to be renamed Cirus, had become critical. Cirus was a medium flux reactor delivering a flux of about 10^{13} n/cm^2/s, much better than Apsara, but an order of magnitude lower flux compared to some of the other existing reactors. A major neutron scattering programme was initiated at Cirus by P. K. Iyengar. By the end of 1961, three more diffractometers – a powder machine, a triple-axis spectrometer and a filter detector spectrometer – were set up and the instruments at Apsara were shifted to Cirus. G. Venkataraman and K. Usha built a rotating crystal spectrometer. Inelastic scattering measurements on phonons in Mg and librational modes in ammonium halides were reported at the 1962 Conference of the International Atomic Energy Agency (IAEA), Vienna, held in Chalk River, Canada. IAEA thereafter decided to hold the next meeting on the subject in India in December 1964 on invitation from our country. The ideas of window filter spectrometer – with Be filter and BeO back reflector – and multi-arm spectrometer were introduced and implemented by Iyengar and his team. Window filter improved the resolution of the analyser vis-à-vis the Be filter, both in energy and momentum[6]. This led to measurements of (a) anharmonicity of the rotational potential in NH_4Cl and (b) phonons in Mg. All this was during my absence from Trombay.

I realized on returning from Canada that with a reactor like Cirus, we are always going to be struggling for intensity and therefore thought of concentrating on hydrogenous materials where intensity would be less of a constraint, since neutron scattering cross-section of hydrogen is comparatively high. After looking at the canonical liquid argon in Chalk River, CH_4, a spherical top molecule, seemed a natural choice. Rotational states of methane are separated by 1.3 meV. Rotating crystal spectrometer with a good resolution of 0.36 meV (reducible to 0.2 meV), was an ideal instrument for observing rotational lines with such a separation. Initial experiments were reported at the 1964 IAEA Conference held in Bombay (now

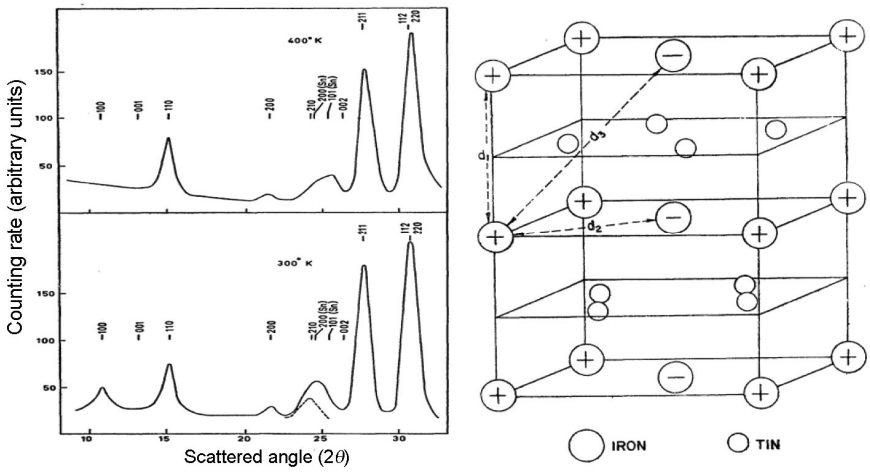

Figure 3. Neutron diffraction pattern and magnetic structure of $FeSn_2$.

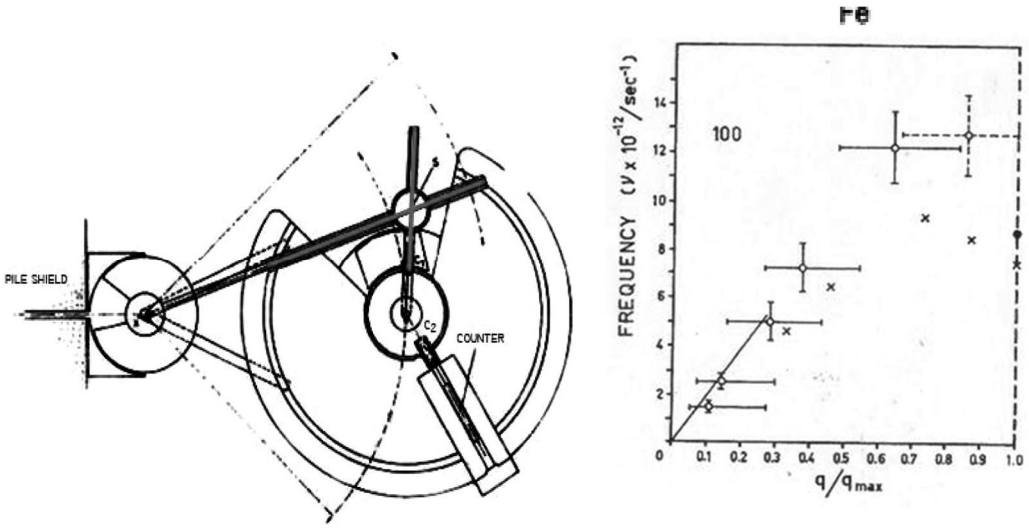

Figure 4. Diffractometer converted for inelastic studies (left) and some phonons in iron (right). Thick dark lines show two rails on which the second axis was mounted converting a two-axis diffractometer to a three-axis spectrometer.

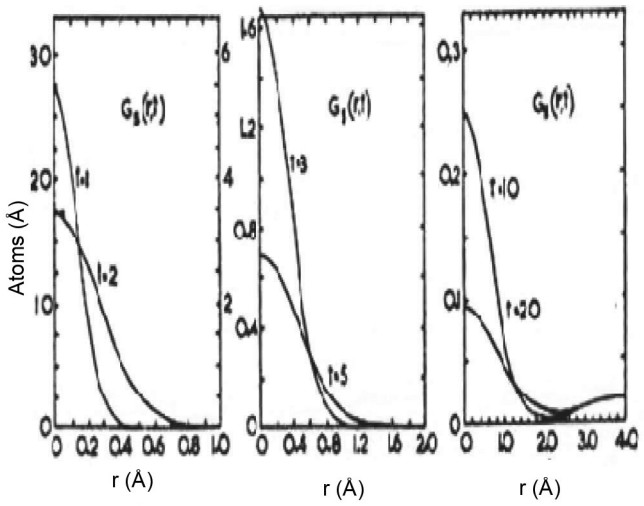

Figure 5. Self-correlation function of liquid argon as a function of time.

Mumbai)[7]. Our conclusion was that methane molecules do not rotate freely in the liquid state (Figure 8). This was contrary to some existing neutron results[8], but in agreement with infrared absorption and Raman scattering experiments. We also treated the entire quasi-elastic and inelastic spectrum in a single framework, not common then[7,9] (Figure 8). These experiments were followed by those on liquids CD_4 (ref. 10) and NH_3 (ref. 11). Sears[12] showed how to quantitatively integrate neutron and optical data into a single framework using our data on liquid methane. He utilized first- and second-order rotational correlation functions measured using infrared absorption and Raman scattering experiments to describe the neutron data. We extended the analysis to include higher-order correlations up to four[10]. As our data suffered from multiple scattering, we also examined them in detail[13]; Figure 9 gives the final comparison with our data.

A similar analysis was done for liquid CD_4 (ref. 10), though it was not necessary to apply multiple scattering correction there. However, effect of coherent scattering was accounted for using a simple model which would take care of second moment and give proper de Gennes narrowing.

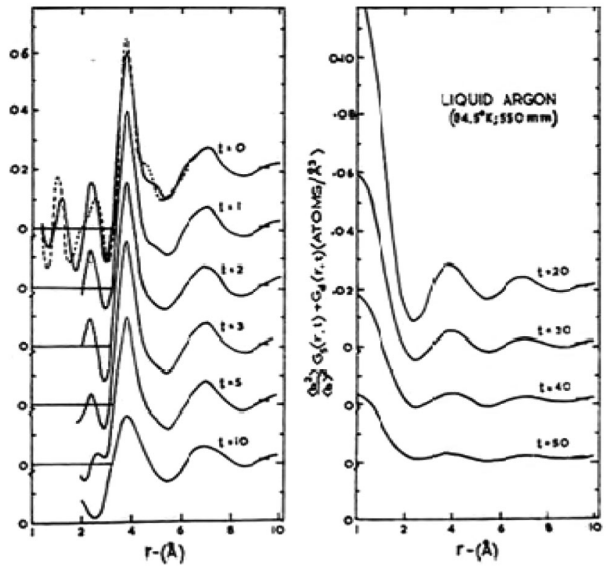

Figure 6. Pair-correlation function of liquid argon at 84.5 K.

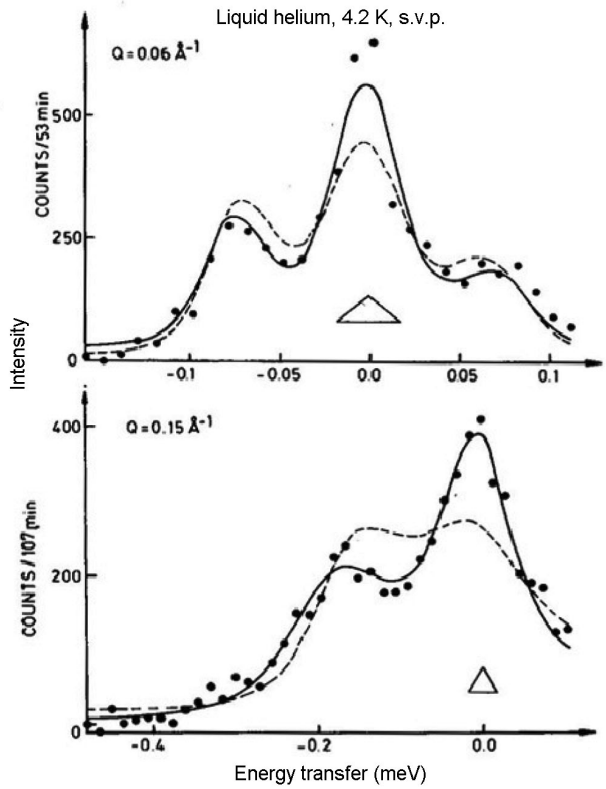

Figure 7. Rayleigh and Brillouin scattering of neutrons from liquid helium at 4.2 K.

This procedure was not feasible for liquid ammonia, as optical data were not available. So the approach of Agrawal and Yip[14], which makes a Gaussian approximation and uses only the first-order rotational correlation, was used. Thus, using our data (Figure 10), a model first-order rotational correlation function was extracted after due correction for multiple scattering.

Scattering from solids NH_3 and CH_4 was also observed to get effective phonon density-of-states, $g(\omega)$[15] in the former and to show almost identical spectra for liquid and plastic solid phases of CH_4, except for the presence

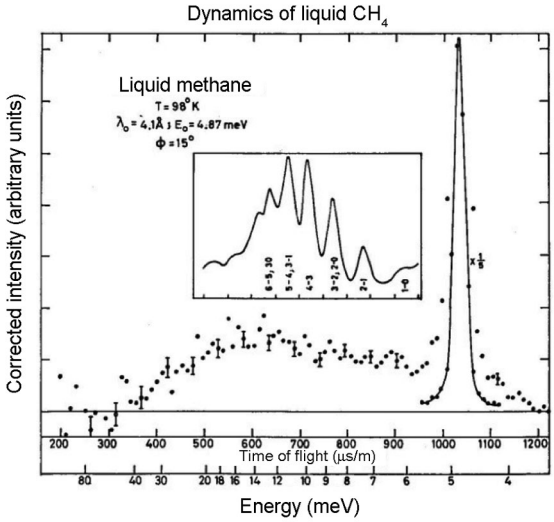

Figure 8. Neutron scattering from liquid methane at 98 K at $2\theta = 15°$. (Inset) Calculated spectrum if CH_4 molecules were rotating freely.

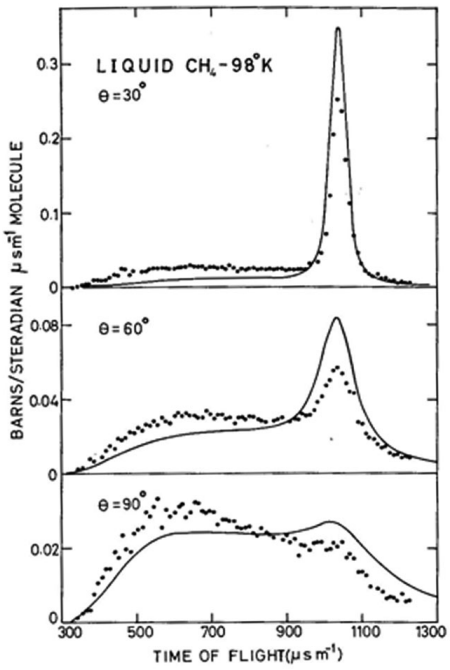

Figure 9. Neutron scattering from liquid CH_4 at 98 K compared with the calculated curves using four rotational correlation functions and allowing for multiple scattering (dashed lines).

of pure elastic peak in the solid which is absent in liquid[16]. Thus, at the freezing point, while translational diffusion changes by many orders, expectedly there is no observable change in the rotational motion as the liquid enters the solid plastic phase.

The Philippines (1966/67) regional cooperation agreement

Following the IAEA conference of 1964 held at Bombay, R. Ramanna and Iyengar proposed a Cooperative Research Project (CRP) under the regional collaboration agreement (RCA) in South East Asia under the aegis of IAEA. The goal was to train scientists from countries of the region like the Philippines, Korea, Indonesia, Thailand, Taiwan, etc. in methods of neutron scattering. BARC donated a home-built diffractometer and installed it at the Triga reactor at the Philippine Atomic Research Centre (PARC) in 1965. I visited PARC in 1966/67 for a year lecturing, building a beryllium detector spectrometer in-house and doing experiments with the diffractometer. Here again, using a small research reactor, we reported our work on neutron diffraction by liquid zinc (Figure 11)[17]. We showed that (a) the earlier X-ray data were faulty, (b) the law of corresponding states suggested by Paskin, using a hard sphere model, was not an adequate description for all monatomic liquids, and shadows of the structure of the solid are retained in the liquid near the melting point, thus permitting a quasi-crystalline model description, and (c) the use of existing pseudo potential of Animalu and Heine to calculate the resistivity gives a value almost half of the measured value; we conjectured this to be due to some basic reason. Later experiments at Trombay on phonons in another hexagonal metal, Be, proved breakdown of simple pseudopotential theory in Be. By hindsight, it seems that we could have conjectured similar breakdown in Zn. Some of the scientists who worked under RCA went on to start neutron scattering programmes in their respective countries. Some scientists who benefited from RCA and whose names come readily to my mind include M. Natera, H. Ibarra, Q. Navarro (the Philippines), Marsongkohadi (Indonesia), Therawoot and S. Chatraphorn (Thailand). G. B. Lee (South Korea), and there were several others.

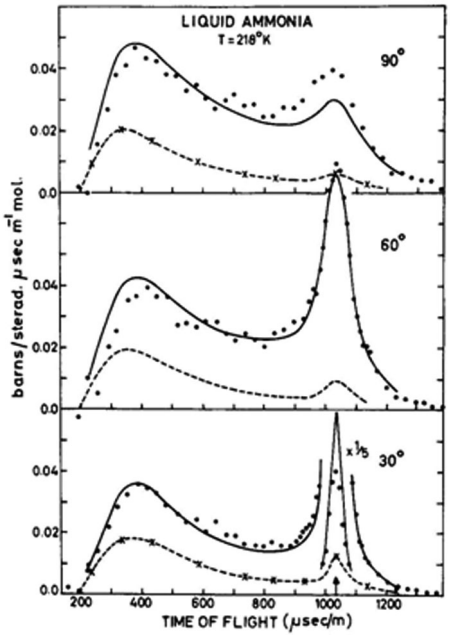

Figure 10. Neutron scattering from liquid ammonia at 218 K compared with analysis using the formulation of Agrawal and Yip[14]. Dashed line shows contribution due to multiple scattering.

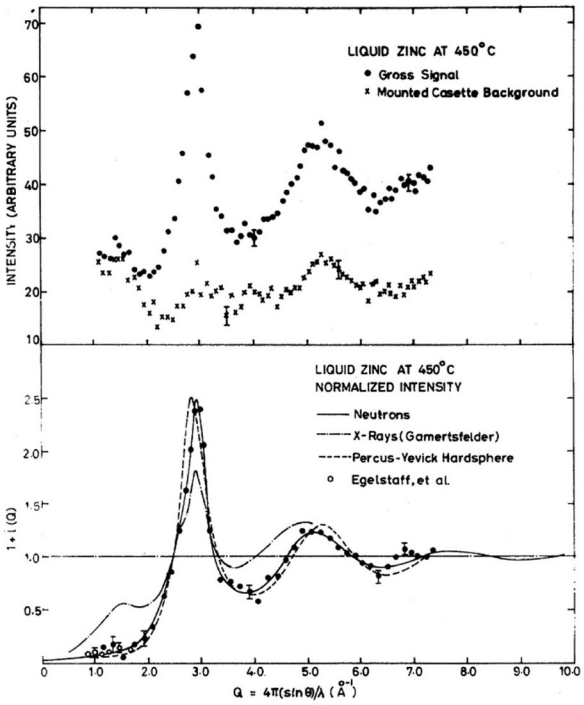

Figure 11. Diffraction from liquid zinc at 480°C.

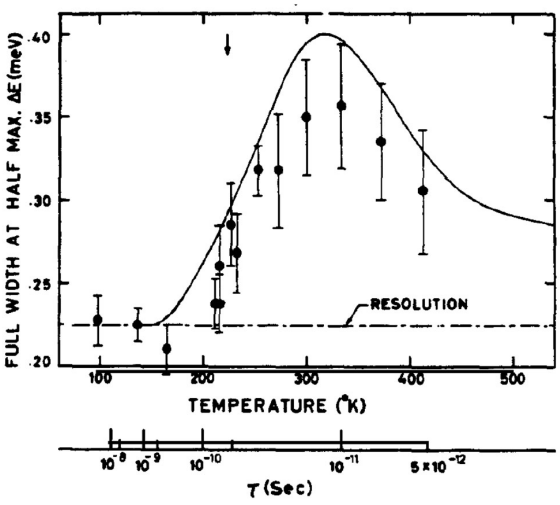

Figure 12. FWHM as a function of temperature for $(NH_4)_2SO_4$.

Cirus again: 'molecular' solids: rotational diffusion and librations (1967–)

By the time I returned from the Philippines in September 1967, scientists were beginning to appreciate that rotational diffusion of molecular groups like NH_4^+, CH_3, CH_4, etc. in solids should show a broadened peak below the elastic scattering peak. Skold[18], and Stockmeyer and Stiller[19] reported the first measurements. Vekataraman also decided to undertake such measurements on the rotating crystal spectrometer at Trombay. The first set of measurements on ammonium sulphate was done when Hun Jun Kim from South Korea was at BARC as an IAEA Fellow[20]. He would contribute to the neutron scattering programme in Korea on his return, as they built their new HANARO reactor. We looked at rotational diffusion and librations in a number of compounds with the ammonium ion in different environments: several publications ensued as a consequence[21]. I shall give only a couple of examples here.

It is now well understood that in the case of rotational stochastic motion, the scattered spectrum consists of a purely elastic peak and a quasi-elastic peak under it. Depending on the energy resolution of the instrument, the two may or may not appear as distinct parts. As the characteristic jump time changes from a small value at higher temperatures (fast motion) to a larger value on cooling, crossing the time-resolution of the instrument, the width of the composite peak first increases and then gradually falls back to its resolution. This is shown in Figure 12 for $(NH_4)_2SO_4$ (ref. 20). The other well-appreciated aspect connected with the study of stochastic rotational motion is that the intensity of the elastic part of the scattering (elastic intensity structure factor (EISF), or the ratio of elastic to quasi-elastic intensity) gives information about the geometry of the associated diffusion process. This is unique to neutron scattering. Using further quasi-elastic as well as inelastic scattering experiments on $(NH_4)_2SO_4$ and $[(NH_4)_xK_{(1-x)}]_2SO_4$, we were able to show the following[21]: (a) it is possible to get information about the two NH_4 ions separately from EISF data on pure salt alone (Figure 13), (b) the reorientation rates for NH_4(I) about its four N–H bonds are nearly same, whereas for NH_4(II) there is a distribution of characteristic reorientation times (τ) about its four N–H bonds, (c) τ_1 (10.4 ps) and τ_2 (15.8 ps) at room temperature are not very different, and (d) they do not drastically change below ferroelectric transition temperature of 223 K and continue to be nearly similar in the ferroelectric phase[21].

In another detailed set of experiments, we examined stochastic and librational dynamics of NH_4 ion in pure NH_4I and its mixed salts $(NH_4)_{0.16}K_{0.84}I/Br$, where all the phase transitions of the pure salt are quenched and NH_4 ion continues in its octahedral first neighbour environment down to low temperatures. 'Localized' translational mode, a broad librational spectrum and quasi-elastic spectra were observed; an attempt was made to explain diffraction, quasi-elastic and inelastic scattering observations in a symbiotic fashion using a model proposed by us[21].

On a slightly different note, I think we were the earliest to examine the polarization dependence of incoherent scattering, through the $\mathbf{Q} \cdot \boldsymbol{\alpha}$. term in the incoherent scattering cross-section, in single crystals of barium chlorate monohydrate and potassium oxalate monohydrate, to identify the character of water librations and measure its angular dependence[22]. Figure 14 shows how the librational spectrum changes depending on whether wave-vector transfer, **Q**, is parallel or perpendicular to the H–H

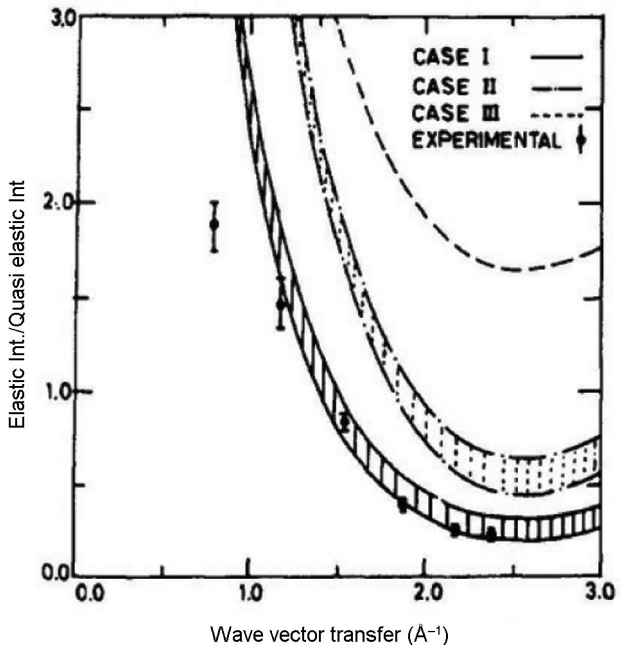

Figure 13. Ratio of elastic to quasielastic scattering intensity for $(NH_4)_2SO_4$. Data show that the reorientation rates for the two NH_4 ions are comparable (case I).

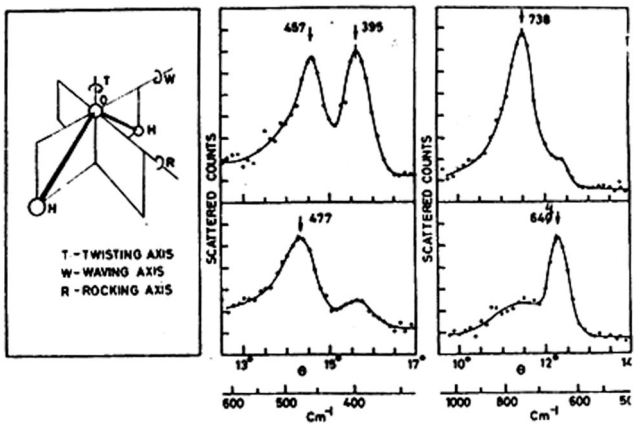

Figure 14. Polarization dependence of incoherent scattering of neutrons from librational modes of water molecule in single crystals of $K_2C_2O_4 \cdot H_2O$ and $Ba(ClO_3)_2 \cdot H_2O$.

vector, thus permitting unambiguous identification of the rocking mode. This is further ascertained by observing the cosine angular distribution of the intensity of the mode (Figure 15). While on the subject of classical stochastic reorientations, let me also mention that during my sabbatical in 1974 at Juelich, I had the opportunity to collaborate with B. Alefeld and A. Kollmar to make one of the earliest observations of quantum rotational tunnelling in 4-methyl pyridine[23]; this was a precursor of a great many experiments on quantum tunnelling of molecular groups.

Filter detector for phonons (1966–)

Filter detector spectrometer (FDS) is not an instrument of choice for measuring dispersion curves of phonons as the wave-vector of the scattered neutron is not well defined. However, when one is working with a FDS, the available intensities of incoming neutrons, especially for large energy transfers is substantial. With Cirus reactor, it was prohibitively difficult to observe phonons higher than about 13 THz (>54 meV) in Be using a triple-axis spectrometer. So we decided to examine the feasibility of FDS for such measurements. We demonstrated quantitatively, through line-shape calculations using an asymmetric resolution function, that the FDS can indeed be used

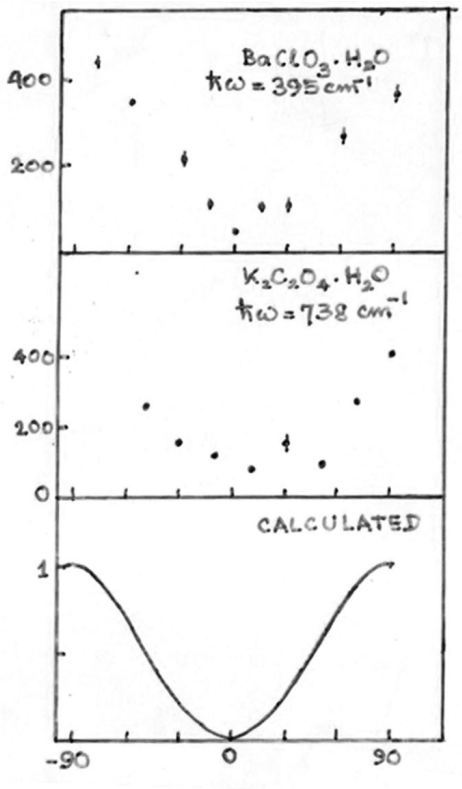

Figure 15. Angular dependence of librational modes in single crystals of $K_2C_2O_4 \cdot H_2O$ and $Ba(ClO_3)_2 \cdot H_2O$: curve show the calculated behaviour.

to accurately measure even steep dispersion curves in Be[24]: we measured phonons from ~7.5 to 20 THz using the moderate flux Cirus reactor. Roy *et al*.[25] provided experimental proof of the breakdown of simple pseudo potential theory in Be (Figure 16). This opened up the possibility of measuring high-energy phonons even with a modest reactor.

Dhruva (1972–)

In 1972, BARC decided to build a reactor with a higher flux than Cirus. As a slight diversion from the main theme, let me mention here that building Dhruva was a landmark in the growth of India's atomic energy programme. Our first reactor, Apsara, was a small (1 MW), indigenously designed and built reactor with fuel from the UK. Cirus (40 MW) was designed by Canadians and built indigenously, with half of first charge of fuel from BARC, under Canadian supervision. Dhruva was the first large (100 MW) reactor, with its own novel features and advanced engineering, which was entirely designed and manufactured by Indians.

This offered new opportunities to develop better instruments for neutron scattering and also design more efficient neutron beam delivery devices. To start with, I was given the task of proposing a set of beam tubes required for neutron scattering experiments. Figure 17 shows the layout of the beam channels. Besides several conventional radial beam tubes in the pile block, there are four tangential beam tubes, two through tubes and beam tubes to install cold and hot neutron sources. The design also incorporates built-in recessed cavities and cutaways in the biological shielding to enable closer access to the high-flux region. Two guide tubes beginning at the reactor vessel go outside the reactor hall into the adjacent guide tube laboratory. Thus, the design permits improved availability of neutrons and better signal-to-noise ratio, providing major advantages for neutron scattering experiments.

The plan of the neutron scattering programme was drawn up by the group under the leadership of N. S. Satyamurthy. It was decided to have a suite of instruments which can be divided into three groups[26]: (a) Classical four-circle diffractometer, triple-axis spectrometer (TAS), polarized neutron TAS and filter detector spectrometer; (b) instruments based on position sensitive detectors for quasi-elastic scattering, high-Q diffraction and powder diffraction, and (c) instruments (like SANS, USANS, polarized neutron reflectometer and spin-echo spectrometer) installed on the two tubes leading outside the reactor hall. On the unfortunate and sudden passing away of N. S. Satyamurthy in 1984, K. R. Rao and I took charge. I took specific interest in the PSD-based instruments and focusing crystals as I was convinced that the future lay in their extensive utilization. The reactor became critical in 1985

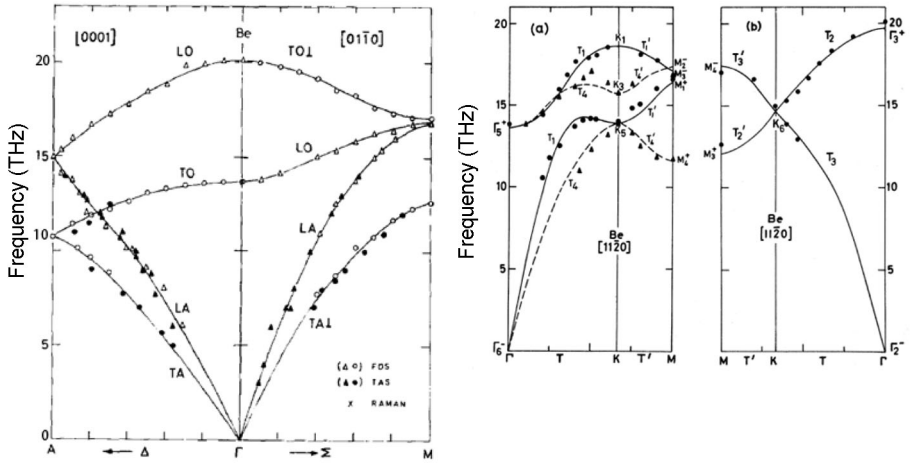

Figure 16. (Left) Phonon dispersion curves in Be at room temperature. Curves through the data are guide to eye[24]. (Right) Proof of non-local pseudo potential in Be through measurement of phonon dispersion relations[25].

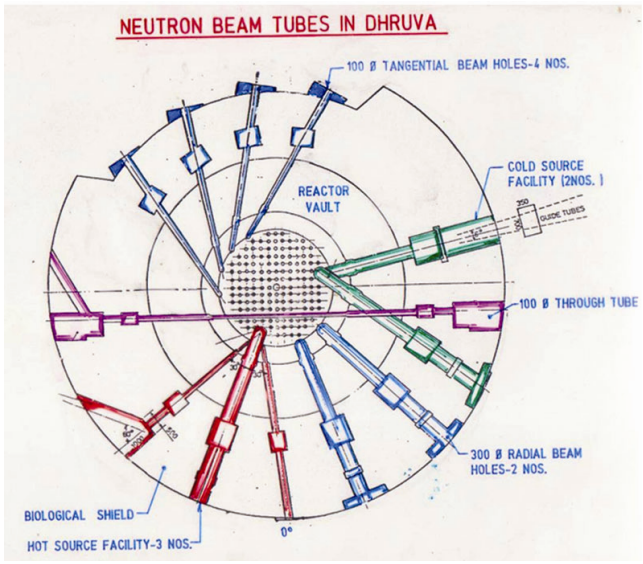

Figure 17. Beam channel layout at Dhruva.

Figure 18. Some neutron instruments at Dhruva (~2003).

and is now functioning normally. Figure 18 shows a recent photograph of some of the instruments at Dhruva reactor hall.

Dhruva national facility (1986–), IUC-DAEF (1989–)

Completion of this reactor had a major impact on increasing the use of neutrons in India. With the increased intensity as a combined result of (a) higher reactor power, (b) superior beam channel design and (c) better instrument design, it would become possible to do experiments more than one order of magnitude faster than at Cirus, and that too with better quality. Thus, the instruments would be more readily usable by scientists from universities. So Dhruva was made a National Facility. Special funding was allocated by BARC for university scientists to participate. Schools for neutron scattering started to be held, with the first one being organized by BARC in 1986 as an IAEA School at Mumbai. Inaugurating this School, I expressed my dream of creating a community of at least a couple of hundred users of these instruments in India. In 1989, an agreement was signed between University Grants Commission (UGC) and Department of Atomic Energy (DAE) to establish a new Inter University Consortium for Utilization of DAE Facilities (IUC-DAEF), wherein UGC took over the responsibility of funding users from universities and DAE of providing the use of neutron instruments (among many other facilities from VECC, Kolkata and RRCAT, Indore), free of cost. Then onwards regular neutron schools were jointly held between BARC and IUC-DAEF. The number of users increased rapidly. A recent School in this series was held in 2010 at BARC in cooperation with AONSA.

In December 1995, I moved over from BARC and took up the Directorship of IUC-DAEF to help consolidate this joint effort of the Solid State Physics Division, BARC and IUC-DAEF, Indore. I was a happy and satisfied person as a large number of participants from about 40 institutions spread all over India started using neutrons before I left IUC-DAEF in October 2002. I shall return to

another facet of IUC-DAEF (renamed UGC–DAE–CSR or University Grants Commission – Department of Atomic Energy Consortium for Scientific Research) later.

SANS at Cirus (1985–)

While Dhruva was under construction, some relevant developments were undertaken at Cirus. Ever since I returned from KFA, Juelich in 1975, I felt the need of a small-angle neutron scattering facility at BARC, after having seen the fine work by the Juelich group at close quarters. So at the earliest opportunity, when Erwin Desa joined us, we designed and installed a rudimentary machine at Cirus and started SANS experiments[27]. The approach was again to start with a simple design to gain experience of SANS technique. The machine was gradually refined with respect to signal-to-noise ratio and data-gathering efficiency using a position-sensitive detector under the leadership of P. S. Goyal. This was with a view to having a full-fledged PSD based machine at the new Dhruva reactor (100 MW; 1.8×10^{14} n/cm^2/s). As Dhruva and the neutron guides there took some time to come to an operational stage, the SANS experiments got well established at Cirus itself, and a number of publications on structure and interactions of ferrofluids and a variety of micellar systems ensued[28]. Along with powder diffractometers at Dhruva, it became the most sought after neutron facility. A new SANS machine has been installed since then on one of the guide tubes at Dhruva[29] and continues to be much sought after by many groups in India. The role of Goyal in making this technique popular among groups from universities needs a special mention here.

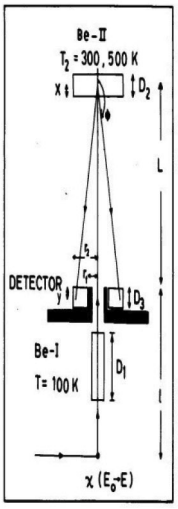

Figure 19. Schematic of a window filter.

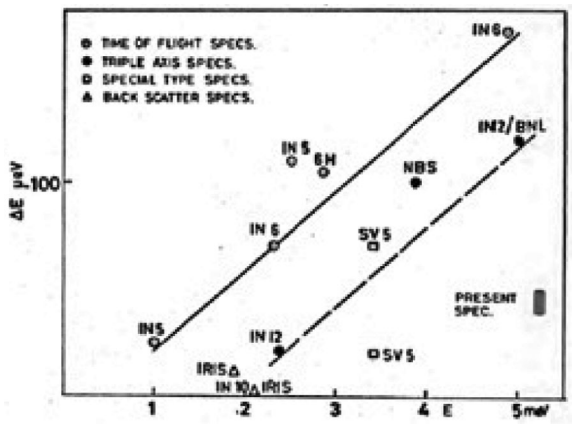

Figure 20. Typical energy resolution of various neutron spectrometers.

Spallation Neutron Source: ISIS–BARC collaboration: Δ*T*-analyser (1980/1–)

At this point, let me switch over to another parallel development which took place in the early eighties. George Manning, Director of Rutherford Appleton Laboratory (RAL), UK, was passing through BARC when Iyengar was the Director. They knew each other from their days together at Chalk River, Canada.

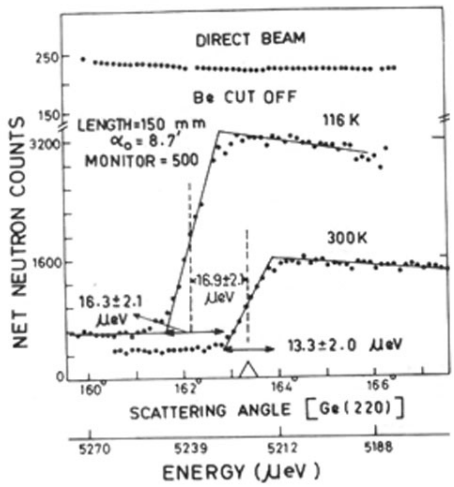

Figure 21. Measurement of width of Be cut-off and its shift with temperature.

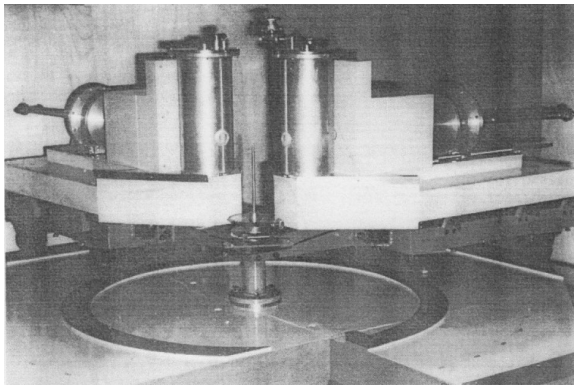

Figure 22. Photograph of a pair of Δ*T*-window analysers.

Manning mentioned to Iyengar that they were looking for international participation/collaboration for their Spallation Neutron Source (SNS) project under construction at that time. They had already decided on several instruments and were looking for collaboration if a new idea could be proposed. With an experience with different types of inelastic scattering instruments, I felt that there is room for an instrument with resolution in an energy window of tens of μeV, i.e. between a triple-axis and a backscattering spectrometer. Thus the idea of a ΔT – window analyser with an energy resolution of tens of μeV was born[30]. My colleague Goyal suggested that this could ideally match with a long incident flight path of ~60 m with regard to energy resolution at SNS[31]. We worked out various numbers and made the proposal. RAL thought it to be sufficiently different from other proposed instruments to open up a new beam with cold hydrogen moderator.

Figure 23. The IRIS user group in front of the Indian analyser.

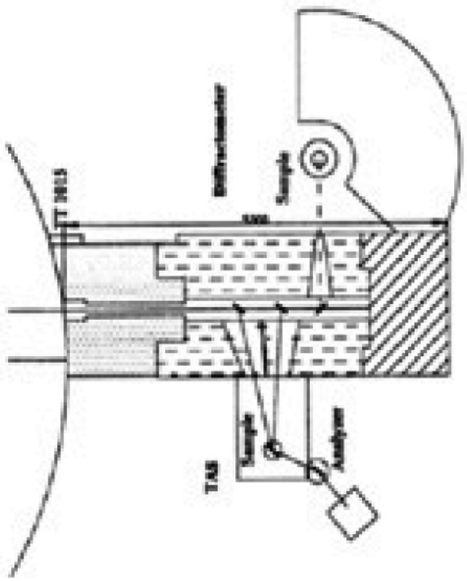

Figure 24. Conceptual layout of multiple monochromator beamline.

Let me spend a few minutes on the ΔT – window analyser. A standard window filter permits incident neutrons larger than 3.96 Å to pass through a Be filter and neutrons between 3.96 Å (Bragg cut-off of Be) and 4.7 Å (cut-off of BeO) to get nearly back-reflected and detected in an annular detector (Figure 19). This produces an energy window between ~5 and 3.7 meV, i.e. ~1.3 meV at ~4.35 meV. In a ΔT-window analyser, the Be block is cooled to liquid nitrogen temperature and BeO is replaced by a Be block at room temperature. By this simple modification one reduces width of the analyser window about 60 times to ~0.02 meV and improves the resolving power of the analyser from about 4 to 250.

One obtains a resolution of 0.4% at ~5 meV, which was favourably removed from any other available spectrometer (Figure 20)[32]. However, to validate this idea we still had to be sure that the natural width of cut-off of hot-pressed Be block is well below the difference in the Be cut-off at room temperature and liquid nitrogen temperature. As the best available measurement[33] was done with a resolution of 20 μeV, we had to set up a special spectrometer with a resolution of ~5 μeV to measure the width of the cut-off and also its shift between the two temperatures (Figure 21)[34]. Having validated the basics, the ΔT – window analyser was built at BARC (Figure 22) and installed at the end of a 30 m long incident flight path at the hydrogen cold source at SNS, later called ISIS, to receive day-1 neutrons. Thus, a unique beamline with energy resolution of ~30–50 μeV at ~5.0 meV and Q up to 3.0 A^{-1} was opened up at ISIS (Figure 23).

Experiments on reorientation in NH_4Br, ferroelectric to paraelectric transition in $(NH_4)_2SO_4$, tunnelling in methyl acetate by the Nottingham group of Clough and motion of H_2 in intercalated carbon $[C_{24}Cs(H_2)_{1.8}]$ by the Oxford

Figure 25. Diffractometer based on multi-monochromater layout. White monochromator shield and green detector shield are seen in the photograph at Dhruva.

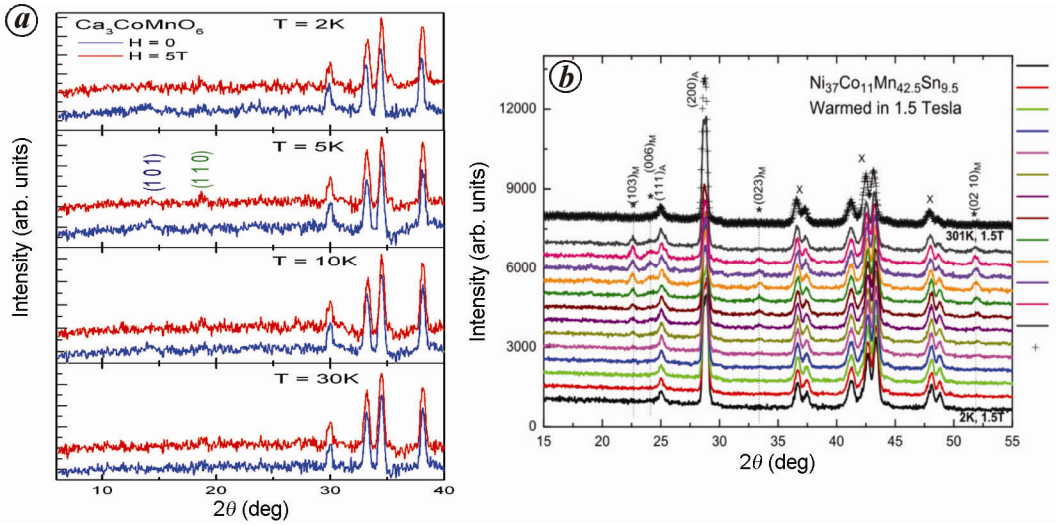

Figure 26. ***a***, Magnetoelectric coupling in Ca_3CoMnO_6. ***b***, Kinetic arrest of austenite to Martensite transition in a shape memory alloy.

group of John White were performed in 1985/86 (RAL Annual Reports 1985, 1986). The analyser was later replaced with a more versatile one using many crystals of pyrolytic graphite. This improved the throughput using many pyrolitic graphite crystals which also gave improved energy resolution, but it reduced available range in wave vector transfer Q. The most important consequence of this collaboration, from the Indian point of view, was that scientists from India were given access to all the neutron instruments at the world's best pulsed neutron source, ISIS, at that time and indeed for a long time to come. Many Indian scientists benefitted from this collaboration over nearly two decades.

IUC–DAEF (now UGC–DAE CSR) beamline at Dhruva (1994–)

With the BARC–University cooperation maturing, IUC–DAEF thought it fit to involve itself deeper in the neutron scattering programme by proposing to build instruments on a new beam line. The through-tube TT-1015 was made available to IUC-DAEF for this.

In an IAEA workshop on Research Reactor Utilization at Budapest in 1994, I had examined the possibility of using multiple instruments in tandem on a single beam line as it improves the utilization of available neutrons; it was decided to use this idea. This necessarily meant minimum use of Soller collimators and an open design without any Soller collimators was opted for (Figure 24). This was the first time we used this idea at BARC.

The needed resolution in wave-vector transfer was to be attained through the use of focusing perfect crystals[35]. Monte Carlo simulations for a powder diffractometer[36] and a triple-axis spectrometer[37] showed that in both cases one would gain in resolution as well as intensity. For the diffractometer one obtains full widths of Bragg peaks of about 0.3° over the full angular range from 10° to 125° at 1.48 A. For the triple axis-instrument with pyrolitic graphite monochromator, the energy resolution is ~0.2 meV at 4.83 meV (resolving power of ~24), whereas with Si(311) at 15.5 meV, the resolution can be ~0.1 meV (resolving power of 155), though with much reduced intensity. A single integral shield has been designed and installed for three monochromators in tandem; however, only the diffractometer has been installed. Another interesting feature of this endeavour was that groups from universities were given the responsibility of developing specific components like boronated rubber (now commercialized), toroidal monochromator and relevant Monte Carlo simulation programmes; Mumbai Centre of IUC–DAEF under Goyal was responsible for the overall project. Such a diffractometer has been installed (Figure 25) and has completely borne out the anticipated promise. It has a $\Delta d/d < 0.3\%$, with flux of 7×10^7 n/cm^2/s at the sample. Now with the addition of low temperature (from 1.5 K) and high magnetic field (7 T) sample environment[38], the Indian neutron scattering community has access to a top-of-the-line diffractometer locally. This has permitted one to address sophisticated problems on multiferroics, quasi 1D systems, kinetic arrest in magnetic glass, etc. Figure 26 shows some recent high-resolution data demonstrating the use of low temperature and high magnetic field.

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ACKNOWLEDGEMENTS. Neutron scattering experiments are necessarily implemented at facilities which involve a large number of persons to run them and they also involve many colleagues. At the outset, I would like to thank my seniors from whom I learnt the rules of the game, my contemporaries and colleagues for continued intellectual and physical cooperation over many decades and the younger scientists for their inputs and endeavours to the programme at Trombay. I regret that lack of space prevents me from mentioning each one of them by name. However, I owe a special debt of gratitude to R. Ramanna, P. K. Iyengar, G. Venkataraman and N. S. Satya Murthy who, in their different ways, were responsible for moulding me. I particularly thank K. R. Rao with whom I had a long collaboration and P. S. Goyal who took his initial steps in neutron scattering working with me and became a dear colleague. I also thank V. Siruguri and P. D. Babu for assistance in preparing the original text and power point presentation. This talk is dedicated to my father, Dr Balebail Dasannacharya, whose influence was responsible for my interest in and dedication to science.

Received and accepted 9 February 2016

doi: 10.18520/cs/v110/i11/2067-2078