

Bhabha Atomic Research Centre
Mumbai, INDIA



National Facility for Neutron Beam Research

Editorial

National Facility for Neutron Beam Research (NFNBR) provides a great variety of instruments for the National Scientific Community. This facility is operated by Solid State Physics Division (SSPD), Bhabha Atomic Research Centre. Scientists from BARC, other DAE units, universities and national laboratories are welcome to use this facility through collaborative research projects with SSPD scientists. Many of these collaborations are being supported by UGC-DAE Consortium for Scientific Research, Board of Research in Nuclear Sciences (BRNS) and other agencies.

We sincerely thank everyone who contributed to this report.

Editors

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National Facility for Neutron Beam Research

Neutron scattering at Trombay started with the facility at Apsara reactor (1 MW) in 1956, and then continued with CIRUS (40 MW), which became available in 1960 and then with the present reactor Dhruva. Dhruva is a 100 MW natural uranium reactor with peak thermal neutron flux of 1.8×10^{14} neutrons $\text{cm}^{-2} \text{s}^{-1}$, tailor-made for neutron scattering experiments with tangential beam holes, through-tube, provision for separate moderators for cold and hot neutrons, guide-tube, etc. Advanced instruments, fully automatic in instrument control and data acquisition modes have been installed on various beam ports. State of the art technology was used to design and fabricate the spectrometers. 1-D and 2-D

position sensitive detectors (PSD), and associated electronics have also been developed indigenously.

National Facility for Neutron Beam Research (NFNBR) has been created as a part of the Solid State Physics Division (SSPD) during early nineties to cater to the needs of the Indian scientific community in the field of neutron beam research. Scientists from BARC, other DAE units, universities and national laboratories are welcome to use this facility through collaborative research projects with SSPD scientists. Many of these collaborations are being supported by UGC-DAE Consortium for Scientific Research, Board of Research in Nuclear Sciences (BRNS) and other agencies.

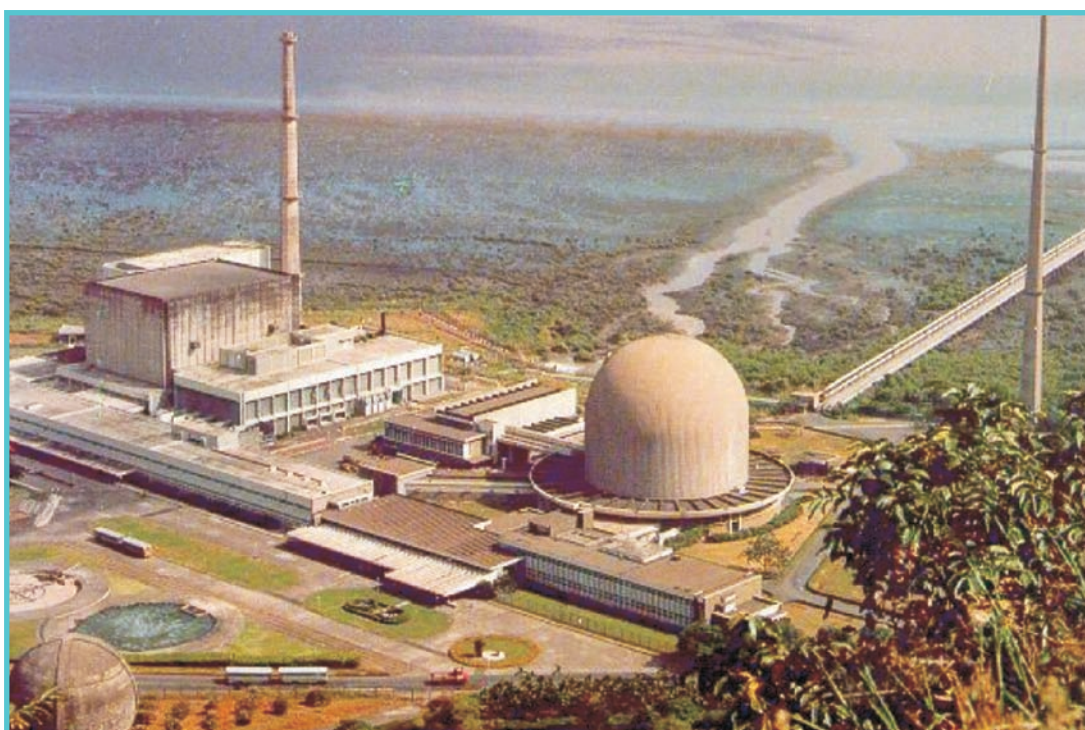


Fig. 1. A panoramic view of CIRUS and Dhruva reactors at BARC

International collaboration between neutron beam research at BARC and other countries is over five decades old. The first such agreement was the “Indian-Philippines-IAEA Agreement” signed during sixties, under which BARC-built neutron instrument was installed at Philippines, and their scientists were trained to use it. Another example is the installation of a neutron spectrometer at Bangladesh through IAEA in nineties. Scientists from Philippines, Korea, Indonesia, Bangladesh, Vietnam, Malaysia and Egypt have visited BARC to work on the neutron instruments. A neutron instrument was installed at the spallation neutron source at Rutherford Appleton Laboratory in UK. Indian Scientists avail advanced sources at UK, USA, Germany, France, Switzerland, Japan and other countries to carry out front line research, and keep themselves up to date in this field. Since 2011, India has joined Institut Laue-Langevin, Grenoble, France as a scientific member, which enables access to this international mega-facility.

General layout in the reactor hall and the guide-tube laboratory is shown in Fig. 2. There are four spectrometers at the tangential beam lines, three at the ends of the through tube, two at the beam lines looking at the hot source, and four instruments in the guide laboratory.

The present-day facilities include, single-crystal and powder diffractometers, polarization analysis spectrometer, High-Q diffractometer, triple-axis & filter-detector spectrometers and quasi-elastic scattering spectrometer, all installed in the reactor hall, and two small-angle scattering instruments and a reflectometer in the guide-tube laboratory.

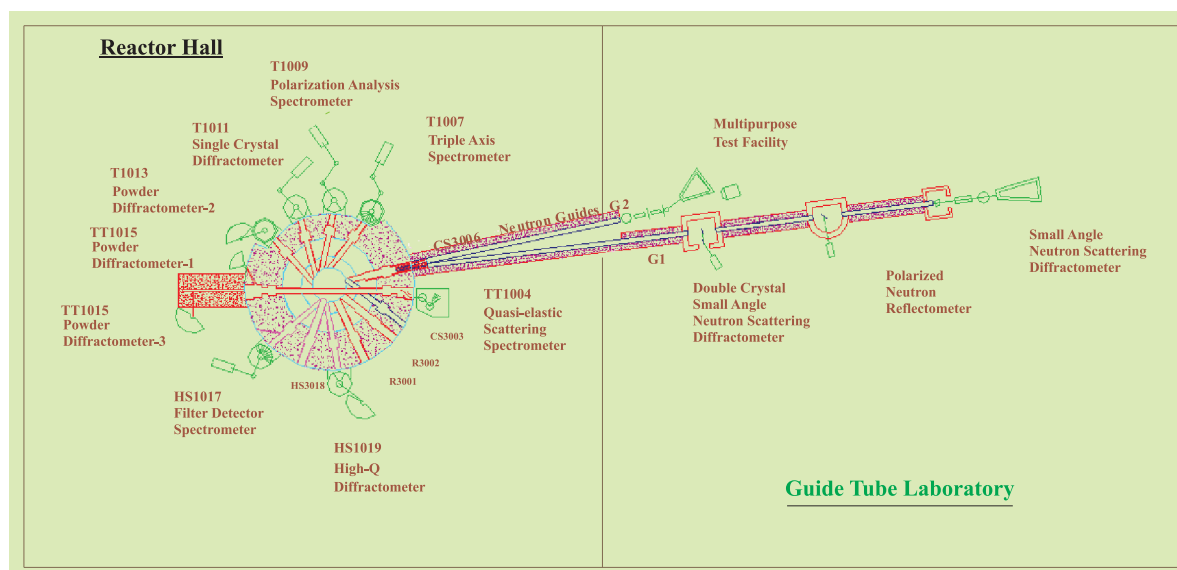


Fig. 2. A layout of the neutron scattering instruments at Dhruva reactor



Fig. 3. A view of neutron scattering facilities inside the Dhruva reactor hall

Neutrons for Condensed Matter Research

The existence of a neutral particle similar to the mass of a proton, was hypothesized by Rutherford in 1920 and this was proved by the discovery of neutron by J. Chadwick, a student of Rutherford, in 1932. Since its discovery, neutrons are having been used as a great probe for the research in condensed matter.

Due to its various special properties, neutrons provide an insight about the microscopic structures and dynamics in a wide class of materials. When get scattered by the materials, neutrons can not only tell about the position of an atom in that material but also atomic movement with time.

Neutron's properties which make all these possible

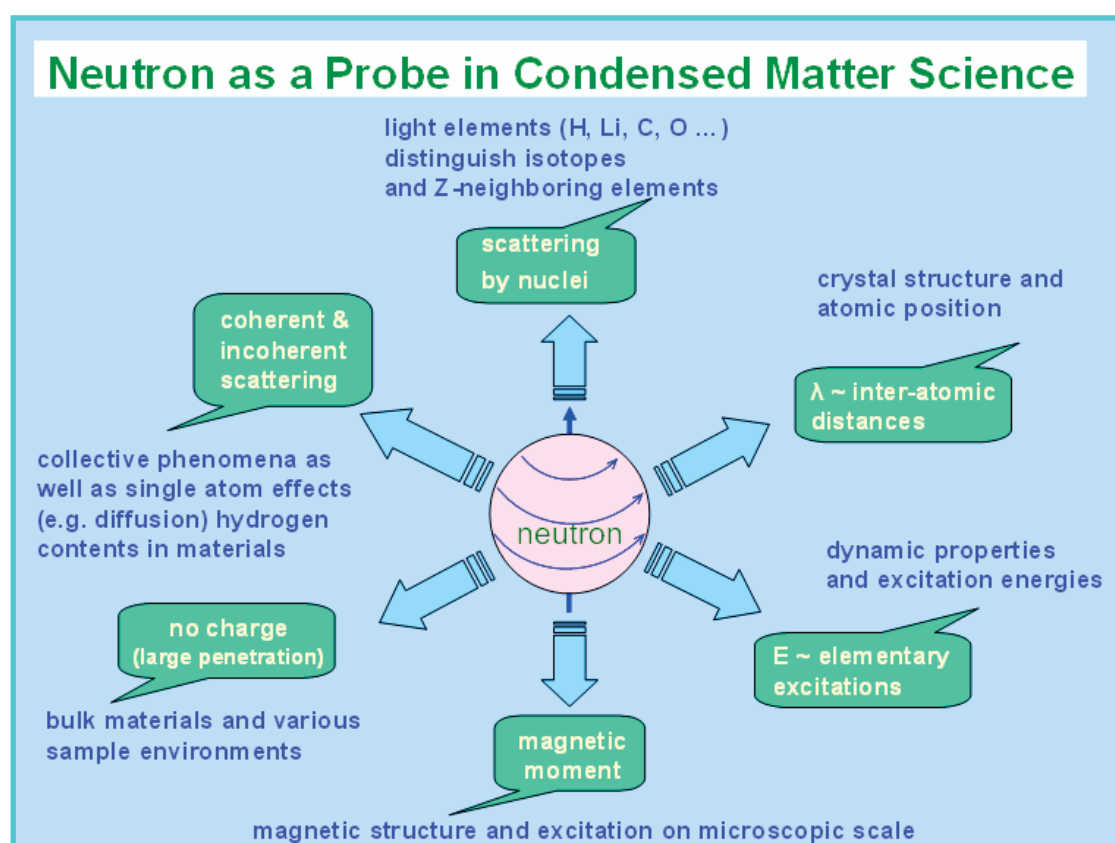
- **Wave-particle duality**
- **Compatible wavelength** with the inter-atomic distances for the thermal neutrons
- **Compatible energy** with the atomic excitation energy
- **Deep penetration** due to the charge neutrality
- **Scattering contrasts** between neighbouring elements in the periodic table
- **Isotope specific** scattering and absorption
- **Magnetic moment** and thus can interact with magnetic materials
- **Simple interaction** with nuclei (isotropic s-wave scattering). No angular dependence of scattering amplitude for nuclear scattering unlike in the case of x-ray.

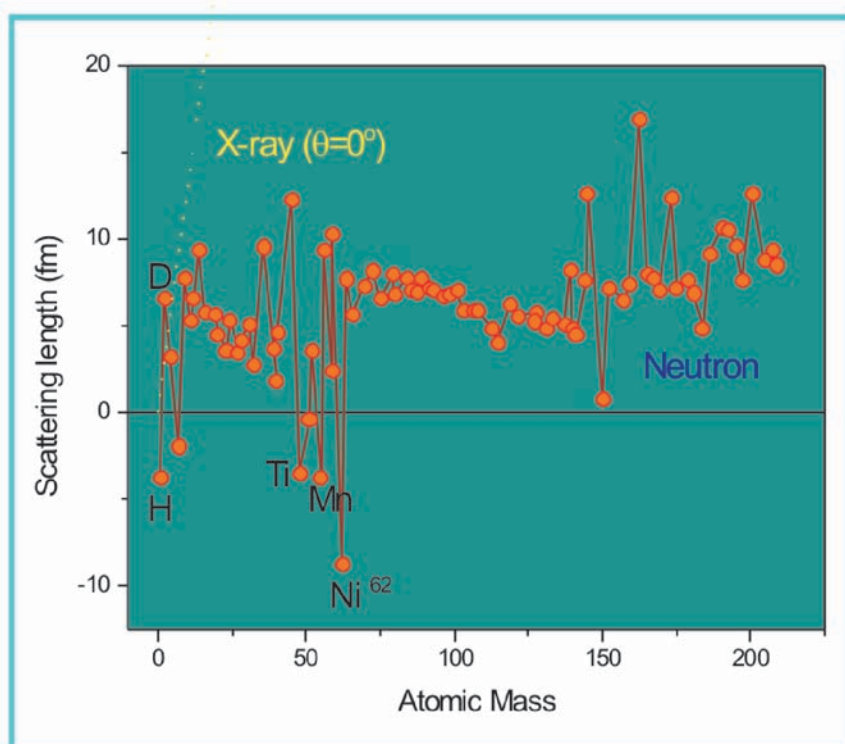
Particle Nature

- Mass = 1.67×10^{-27} Kg
- Spin = $\frac{1}{2}$, acts as a tiny magnet
- Magnetic moment = $-1.913 \mu_N$
- Velocity = 2200 m/s for thermal neutrons of energy 25 meV

Wave Nature

- Diffraction and interference pattern
- Measurable wavelength
- Measurable scattering length

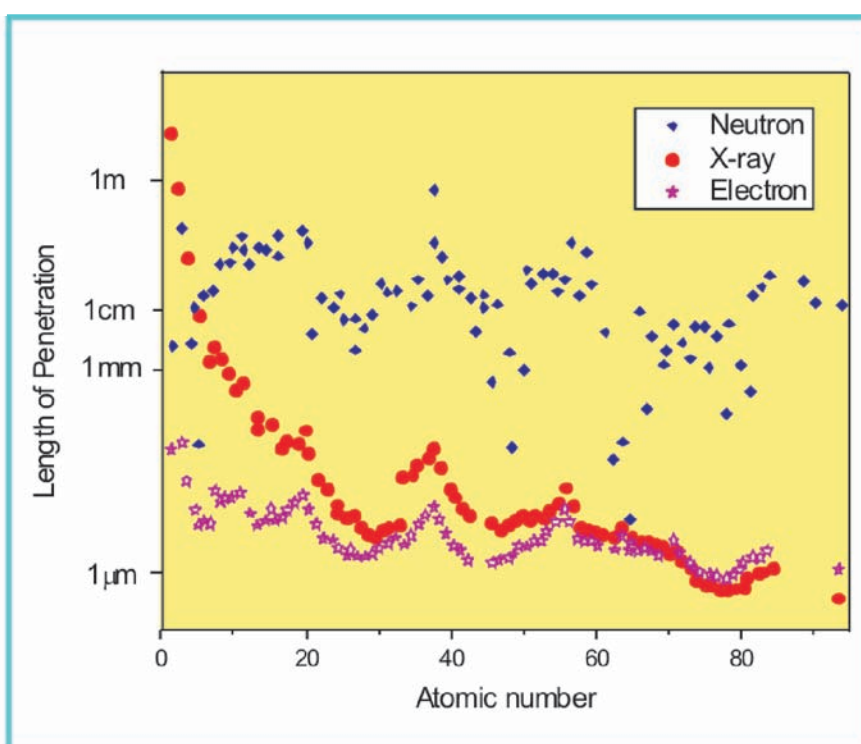




Unlike for x-rays, the neutron scattering power of elements varies in a zigzag fashion with respect to the atomic mass. Due to this special property, neutron can differentiate neighbouring elements in a material and even sees differently the different isotopes of an element. Neutrons also allow to probe light atoms that are barely visible with x-rays. The scattering length of neutron for a few isotopes of some elements are negative. Hydrogen has a negative

scattering length (-3.739 fm) while Deuterium possesses a positive scattering length (6.671 fm). Suitable combination of materials with positive and negative scattering length can be used to tune the neutron scattering contrast. Contrast matching experiments are used to obtain multi-level structures.

As the neutron does not carry any electric charge, the neutron has no electrostatic interaction with the electron cloud of an atom. For this reason, the neutron has a higher penetration power comparable to x-ray or electrons. Neutron has a spin $\frac{1}{2}$ and is sensitive to the magnetic fields created by unpaired electrons. In the magnetic materials, the order in magnetic structures and the interactions can be obtained using neutron scattering.

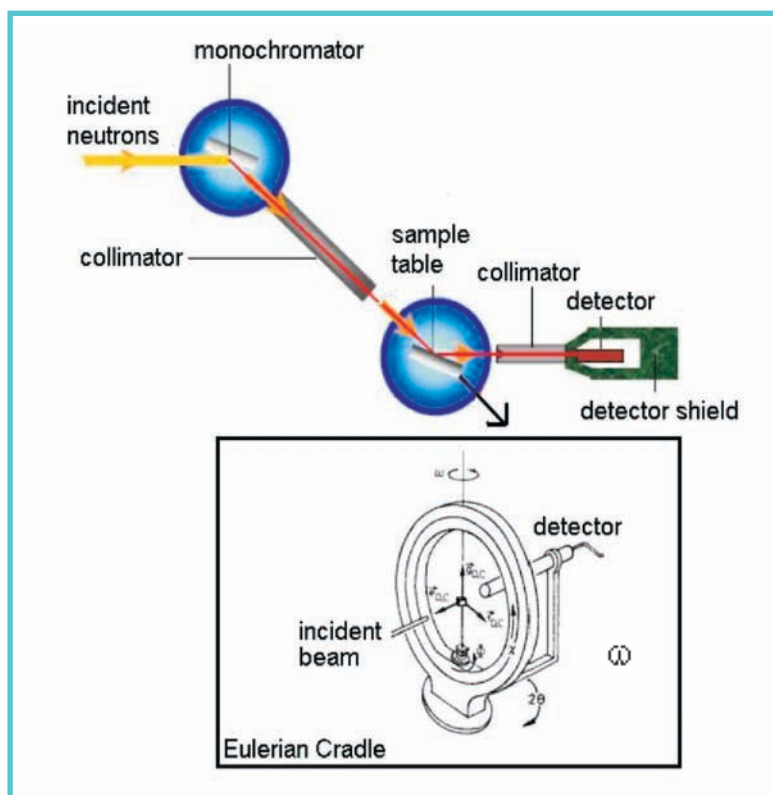


General References

1. G.E. Bacon, Neutron Diffraction (Clarendon Press, 1975)
2. P.A. Egelstaff (ed.) Thermal Neutron Scattering (Academic Press, 1965)
3. W. Marshall and S.W. Lovesey, Theory of Thermal neutron Scattering (Clarendon Press, 1971)
4. G.L. Squires, Introduction to the Theory of Thermal Neutron Scattering (Cambridge University Press, 1978)

Single Crystal Neutron Diffractometer

This Four Circle Eulerian geometry based Single Crystal Neutron Diffractometer is used for the studies on hydrogen-bonded crystal structures.



Instrument Parameters

Beam hole No.	T1011
Monochromator	Cu(220)
Wavelength	0.995 Å
Scattering angle	$0^\circ < 2\theta < 90^\circ$
Flux at sample	5×10^5 n/cm ² /sec
Detector	BF ₃ Counter



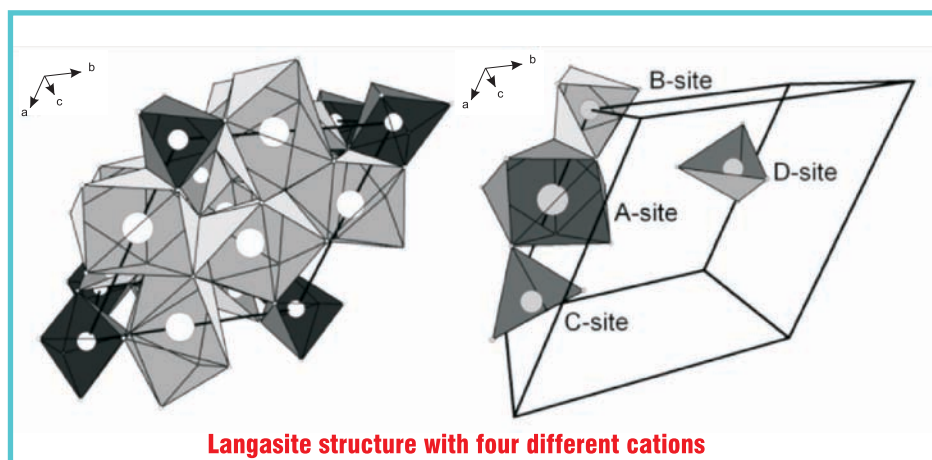
The instrument is used to study a high precision 3-dimensional structure of materials, where hydrogen plays a major role in either the stereochemistry or the physical properties of the materials. These include hydrates, biomolecules, ferro-electrics, electro-optic materials, etc.

The single crystal diffractometer is located at T1011 beam line of the Dhruva reactor. The crystal is rotated about three Eulerian axes χ , ϕ and ω , and the detector is rotated about the 2θ axis. These four axes meet at a point, which is the centre of the sample crystal. The χ circle is

mounted on the ω axis, while the ϕ circle is mounted on the χ -axis as shown in Figure. The crystal is mounted on the ϕ -axis. The geometry of axes mounting enables any reciprocal lattice point to be brought into the equatorial plane of the diffractometer.

Selected Examples

■ Structure of piezoelectric langasite family

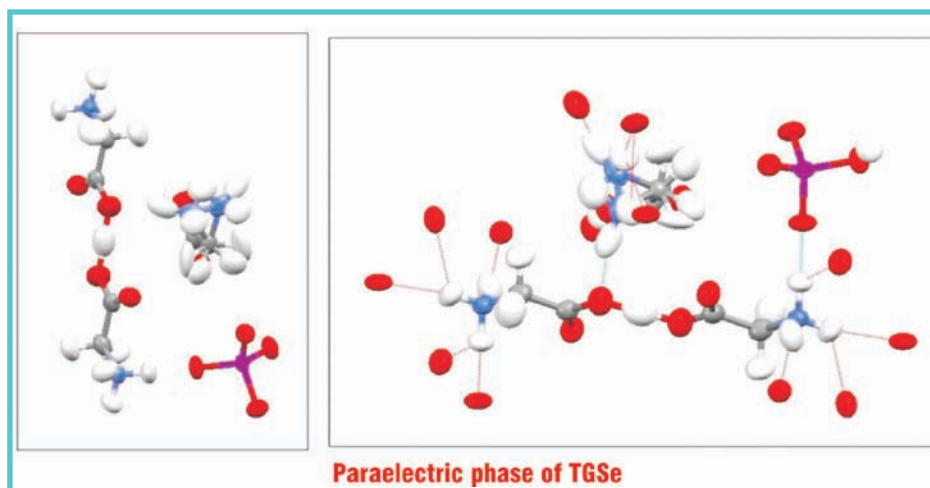


Crystals of langasite family are of interest as piezoelectric component in different devices. The properties of these classes of crystals can be modified within certain limits by isomorphous substitution. Structure of langasite contains four distinct cationic sites with the general formula of $A_3BC_3D_2O_{14}$, where A-site is the dodecahedral site,

B-site is the octahedral site, C-site is the large tetrahedral site and D-site is the small tetrahedral site (Fig. 1). The piezoelectricity of langasite is generated along the [100] direction and is found to be strongly dependent on the width of the dodecahedron (A_L) and octahedron (B_L) along the [100] direction. Single crystal neutron diffraction studies were carried out for LGT ($La_3Ga_{5.5}Ta_{0.5}O_{14}$), LGST ($La_3Ga_{5.25}Ta_{0.25}Si_{0.5}O_{14}$) and LGZrT ($La_3Ga_{5.25}Ta_{0.25}Zr_{0.5}O_{14}$) as neutron study gives a better average picture of the crystal properties over a macroscopic region of the grown crystal. The significant change in the size of D site effects the orientation of A site dodecahedra, so that its width along [100] direction changes significantly affecting the piezoelectric properties of the crystals. Hence the result of this study shows that a slight change in structure can lead to an improvement of the material properties.

■ Crystal structures of triglycine selenate/sulphate

Crystal structures of triglycine selenate (TGSe) and triglycine sulfate (TGS) were obtained from single crystal neutron diffraction. The double well single cell local potential experienced by the non-planar amino group of one of the three glycine ions (GI) of these two isostructural systems was obtained. It is suggested that the change in the nature of the ferroelectric phase



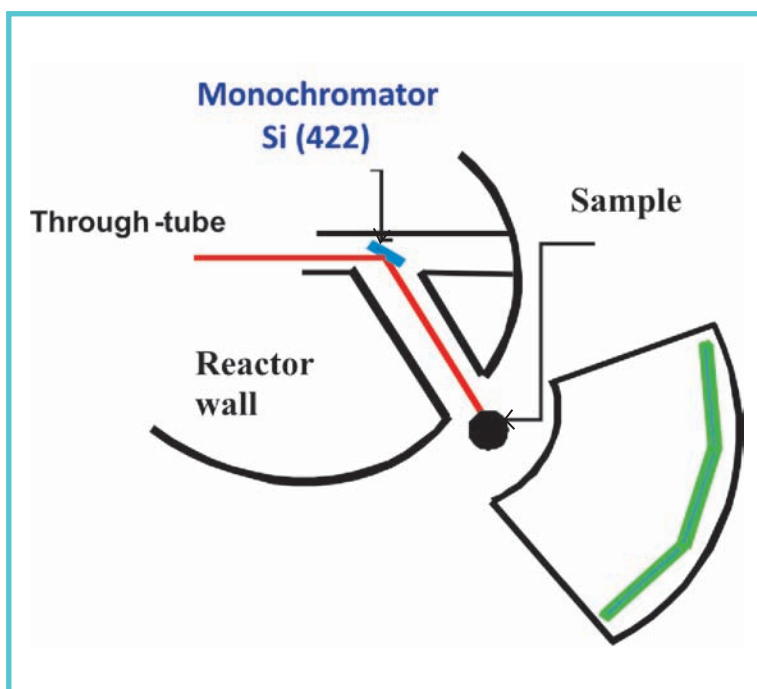
transition as one goes from TGS to TGSe is due to the increase in the zero point energy resulting due to the change in the shape and height of the double well local potential. Substitution of a selenate ion in TGSe by a sulfate ion is considered as a source of an effective chemical pressure that can be utilized to tune the ferroelectric phase boundary in these systems.

Selected Publications

1. R. Chitra and R.R. Choudhury, Acta Cryst. B 66 (2010) 497
2. A.P. Dudka, R.Chitra, R.R. Choudhury, Yu. V. Pisarevsky and V.I. Simonov, Cryst. Rep. 55 (2010) 1060
3. R. R.Choudhury and R Chitra, J. Phys.: Condens. Matt. 21 (2009) 335901
4. A. Jayarama , M.R. Suresh kumar, S .M.Dharmaparakash, R.Chitra and R.R. Choudhury, Pramana: J. Phys. 71 (2008) 905

Powder Diffractometer-1

This instrument is installed at the through-tube beam hole No. TT1015. This instrument is used for magnetic structural studies of powdered samples, and it has been upgraded very recently.



Instrument Parameters

Beam hole No.	TT1015
Monochromator	Si (422)
Monochromator take-off angle ($2\theta_m$)	60°
Wavelength	$1.094 \text{ \AA}$
Detector	Three linear ^3He PSD s
$(\sin \theta/\lambda)_{\text{max}}$	$0.65 \text{ \AA}^{-1}$
Flux at sample	$5 \times 10^5 \text{ n/cm}^2/\text{sec}$
Scattering angle	$5^\circ < 2\theta < 70^\circ$
Resolution ($\Delta d/d$)	1 %

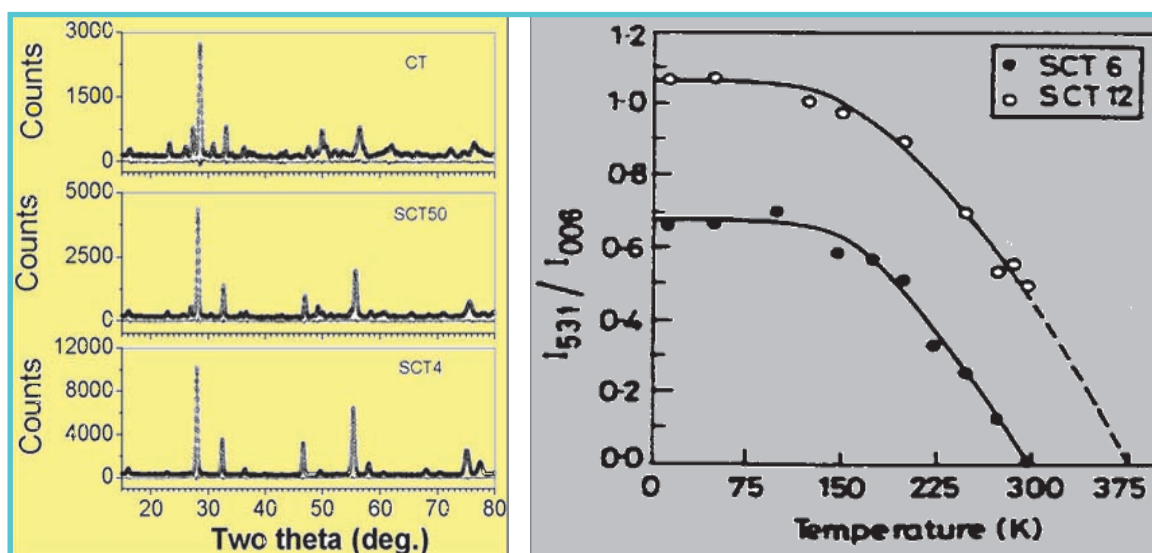


Upgraded Neutron Powder Diffractometer-I with new detector banks, radiation shielding and data acquisition system.

The diffractometer is extensively used for studying magnetic structures in a large variety of systems. These studies include titanates and zirconates showing ferro/anti-ferro-electric properties, alloys of transition metals, rare-earths and actinides (UCu_2Ge_2 , ErFe_2D_x etc.) showing exotic magnetic properties, ferrites exhibiting disordered magnetic ordering, manganites showing colossal magnetoresistance behaviour, and cobaltates showing coexistence of ferro- and antiferromagnetism, etc.

Selected Examples

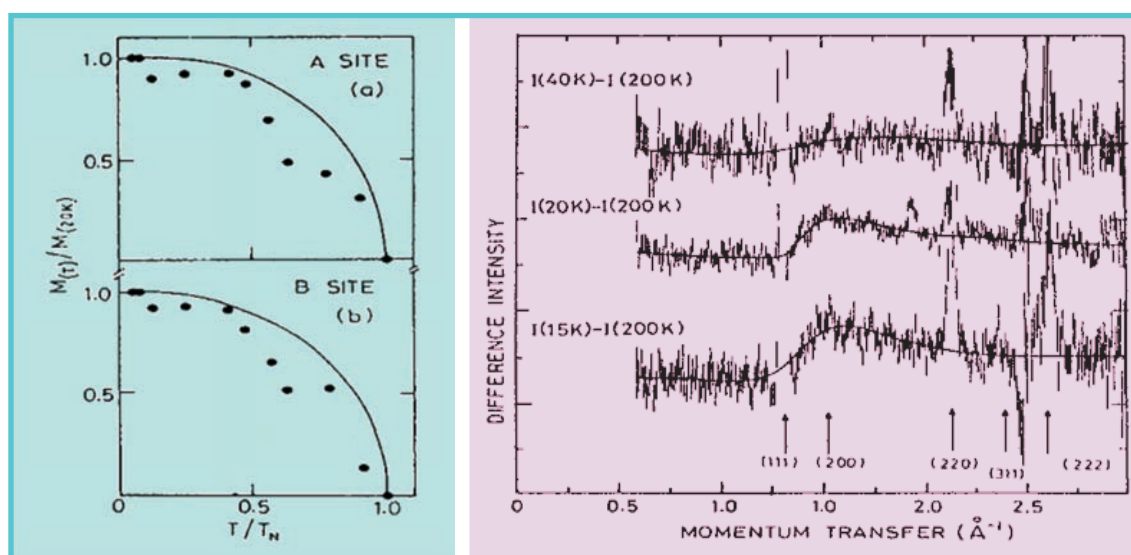
■ Structural phase transition in ferroelectric materials



Observed (O), calculated (—) and difference neutron powder diffraction patterns of CaTiO₃ (CT) and Sr_{1-x}Ca_xTiO₃ (SCT) with x = 0.04 and 0.50. For the CT and SCT (x = 0.50) samples, superlattice lines are observed.

Temperature variation of I_{531}/I_{006} for Sr_{1-x}Ca_xTiO₃ (SCT) with x = 0.06 and 0.12. The antiferrodistortive phase transition is observed around 300 K and 375 K for x = 0.06 and 0.12, respectively.

■ Mixed Ferrites: Disordered Magnetic Systems: Magnetic ordering in Zn_{0.5}Co_{0.5}FeCrO₄



The evolution of the magnetic structure factor with temperature for (a) the (220) reflection and (b) the (222) reflection for Zn_{0.5}Co_{0.5}FeCrO₄. Solid curves: The Brillouin functions.

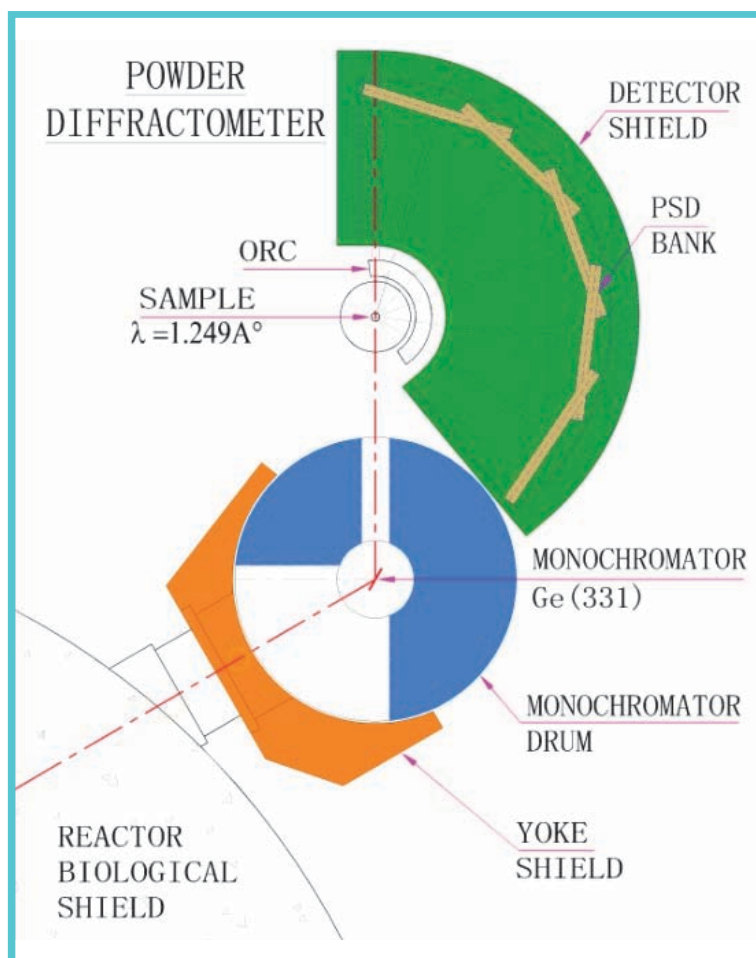
Difference neutron diffraction patterns at 40, 20, and 15 K with respect to 200 K for Zn_{0.5}Co_{0.5}FeCrO₄ showing the buildup of the diffuse hump at ~20 K around a Q-value where the (200) Bragg peak is expected.

Selected Publications

1. S.K. Paranjpe and S. M. Yusuf, Neutron News 13 (2002) 36
2. A. Das, K.R. Chakraborty, S.S. Gupta, S.K. Kulshreshtha and S.K. Paranjpe, J. Magn. Magn. Mat. 237 (2001) 41
3. S.M. Yusuf, R. Ganguly, K. Chakraborty, P.K. Mishra, S.K. Paranjpe, J.V. Yakhmi and V.C. Sahni, Phys. Rev. B 68 (2003) 104421

Powder Diffractometer-2

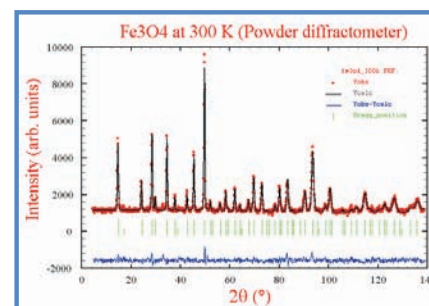
This powder diffractometer is a conventional neutron diffractometer having $Q_{\max} = 9.4 \text{ \AA}^{-1}$ with $\lambda = 1.244 \text{ \AA}$ and is used mainly to understand long range order in polycrystalline materials.



Instrument Parameters

Beam hole No.	T1013
Monochromator	Ge (331)
Wavelength	1.244 Å
Beam size	4.0 cm x 1.5 cm
Flux at sample	$8.5 \times 10^5 \text{ n/cm}^2/\text{sec}$
Scattering angle	$4^\circ < 2\theta < 140^\circ$
Q range	$0.4 - 9.4 \text{ \AA}^{-1}$
$\Delta d/d$	$\sim 0.8 \%$
Detector	5 PSDs
Sample environment	5 – 2000 K

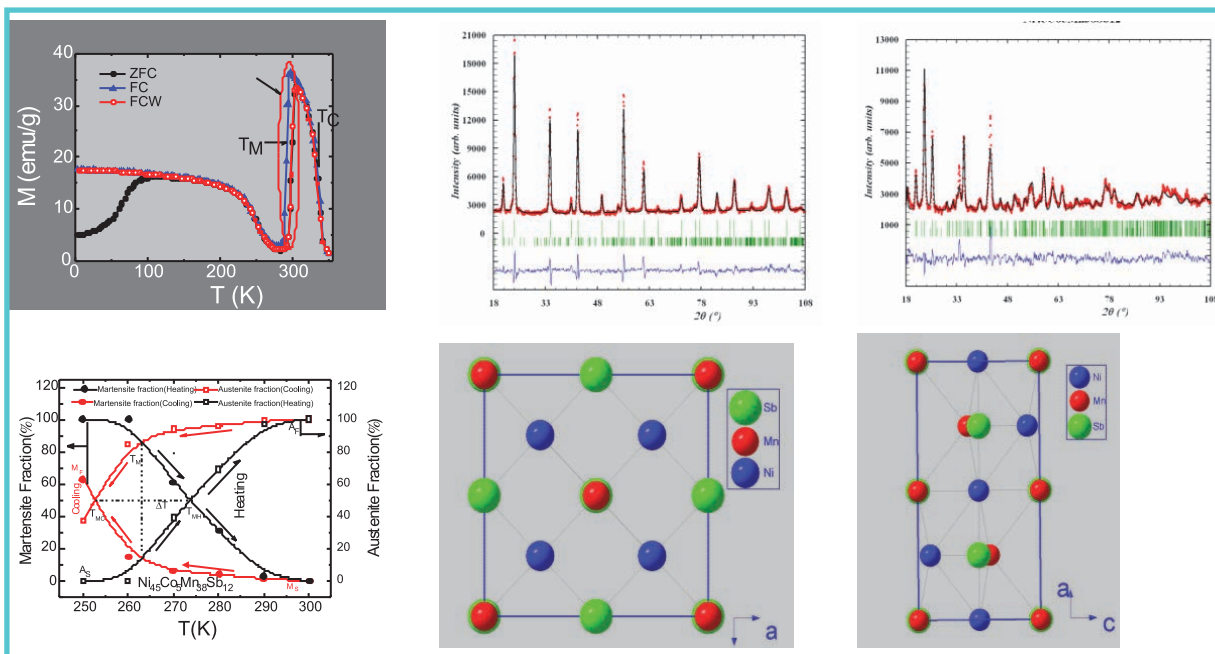
The diffractometer is extensively used for studying magnetic structures in a large variety of systems. These studies include titanates and zirconates showing ferro/anti-ferro-electric properties, alloys of transition metals, rare-earths and actinides (UCu_2Ge_2 , ErFe_2D_x etc.) showing exotic magnetic properties, ferrites exhibiting disordered magnetic ordering, manganites showing colossal magnetoresistance behaviour, and cobaltates showing coexistence of ferro- and antiferromagnetism.



Selected Examples

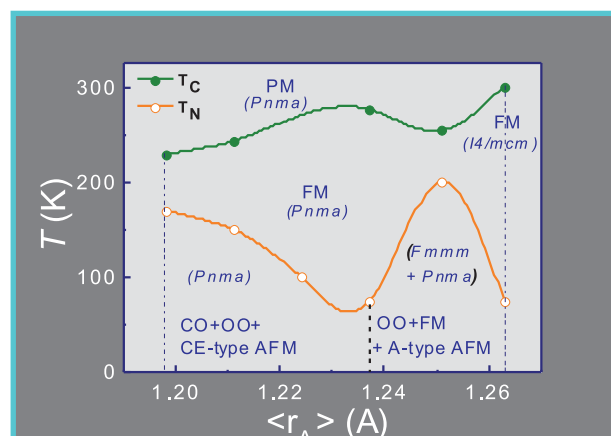
■ Magnetic and structural transition in shape memory compound $\text{Ni}_{45}\text{Co}_5\text{Mn}_{38}\text{Sb}_{12}$

Considerably sharp martensitic transition has been observed in $\text{Ni}_{50-x}\text{Co}_x\text{Mn}_{38}\text{Sb}_{12}$ system, using neutron diffraction and magnetization measurements. A comparison of the neutron diffraction data of $\text{Ni}_{45}\text{Co}_5\text{Mn}_{38}\text{Sb}_{12}$ and $\text{Ni}_{50}\text{Mn}_{38}\text{Sb}_{12}$ alloys shows that Co substitution leads to an increase in the site moments. At 300K the compound exhibits cubic L_{21} phase with excess Mn occupying the Sb site. The spins are ferromagnetically aligned with moment 1.15 and $0.85\mu_B$ at 4(a) and 4(b) site, respectively. The martensitic phase is analyzed in the $Pnma$ space group. In the martensitic phase at 6K the ferromagnetic moment obtained at site 2(a) and 2(f) is 1.8 and $1.7\mu_B$, respectively.



■ Evolution of magnetic structures in charge ordered manganites

A complex interplay of charge, spin, and orbital ordering describe the magnetism of half doped manganites. We have found that the CE-type of antiferromagnetic (AFM) structure, observed in $\text{La}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$ and other such compounds, is susceptible to ionic size disorder. The phase diagram shows the transformation from a charge ordered AFM state to ferromagnetic metallic state with increase in A-site average ionic radii $\langle r_A \rangle$, studied in $\text{La}_{0.5}\text{Ca}_{0.5-x}\text{Sr}_x\text{MnO}_3$. Such effects of phase separation has also been observed in other A-site doped compounds, $\text{La}_{0.5}\text{Ca}_{0.5-x}\text{Ba}_x\text{MnO}_3$, $\text{La}_{0.5-x}\text{Nd}_x\text{Ca}_{0.5}\text{MnO}_3$, and B-site doped compounds $\text{La}_{0.5}\text{Ca}_{0.5}\text{Mn}_{1-x}\text{B}_x\text{O}_3$ (B=Fe, Ru, Al, Ga). Doping with Fe and Ru is found to result in either ferromagnetic or antiferromagnetic phases, while doping with Al and Ga results in coexisting ferromagnetic and antiferromagnetic phases. Similarly, transformation from A-type to pseudo CE-type magnetic structure is observed in monovalent substituted $\text{Nd}_{1-x}\text{Na}_x\text{MnO}_3$ ($x < 0.20$).



Selected Publications

1. I. Dhiman, A Das and AK Nigam, J. Phys. Cond. Matter 21 (2009) 386002
2. I. Dhiman, A. Das,, P.K. Mishra, N.P. Lalla and A. Kumar, J. Magn. Magn. Mater 323 (2011) 748
3. I. Dhiman, A Das, AK Nigam and U. Gasser, J. Phys. Cond. Matter 23 (2011) 246006
4. B. Samantaray, S. Ravi, A. Das and S. K. Srivastava, J. Appl. Phys. 110 (2011) 093906

Powder Diffractometer-3

This Diffractometer, with a doubly bent focusing monochromator, uses open-beam geometry for higher flux and enables use of small samples. A variety of chemical and magnetic structures of novel materials have been studied using the low temperature-high magnetic field sample environment.



Instrument Parameters

Beam hole No.	TT-1015
Monochromator	Bent Si
Wavelength	1.48 Å (standard)
Beam size	15 x 25 mm ²
Flux at sample	7x10 ⁷ n.cm ⁻² s ⁻¹
Scattering angle	6 – 123°
Q range	0.4-7.4 Å ⁻¹
Δd/d	< 0.3%
Detector	12 Linear ³ He PSDs



This powder diffractometer, developed and installed by UGC-DAE Consortium for Scientific Research, is a multi-PSD high throughput diffractometer. It employs a bent perfect crystal monochromator at a take-off angle of 90 degrees and it is designed for a highly focused neutron beam of

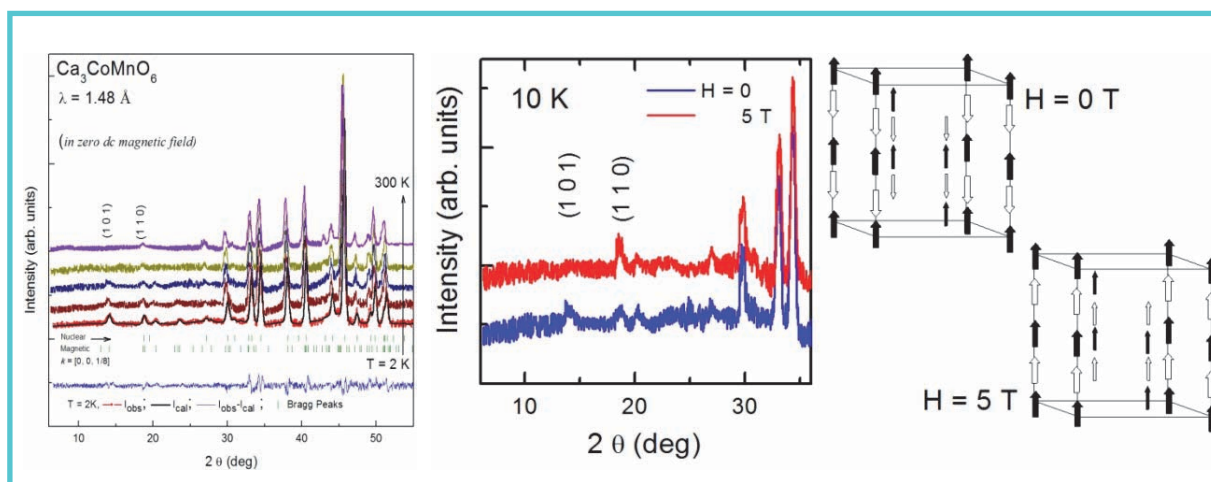
about 15 x 25 mm² in size. This enables higher flux at sample position and also use of small samples (~ 1 cc in volume). A complete diffraction pattern is obtained over four overlapping banks of three linear PSDs each, covering an angular range up to 123°. The resolution obtained ($\Delta d/d$) is < 0.3%.

The monochromator can be rotated or flipped to give a range of wavelengths from 1.1 Å to 2.3 Å. The sample environment consists of a 4K CCR for standard measurements and a cryogen-free 7 Tesla magnet cryostat with VTI for in-field measurements down to 1.6 K. An oscillating radial collimator installed before the detectors suppresses the extraneous contributions from the magnet and CCR shrouds. The data acquisition system has an input for up to 16 PSDs and the software enables recording various sequences of measurements with respect to incident neutron flux and sample temperature and magnetic field.

A.V. Pimpale, B.A. Dasannacharya, V. Siruguri, P.D. Babu, and P.S. Goyal, Nucl. Instrum. Meth. A481 (2002) 615

Selected Examples

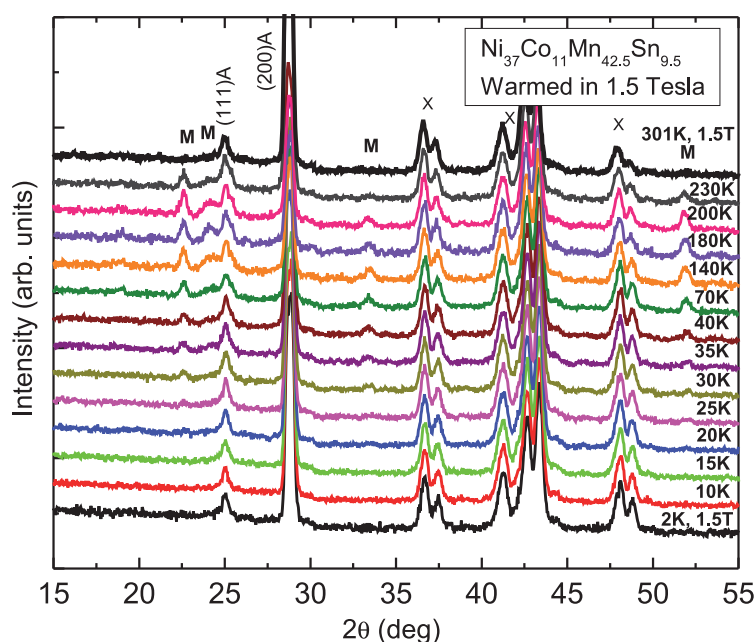
■ Understanding magnetic structure of Quasi 1D compound $\text{Ca}_3\text{CoMnO}_6$



Magnetic structure of multiferroic, quasi 1D compound $\text{Ca}_3\text{CoMnO}_6$ has been studied as a function of temperature by in-field neutron diffraction. The evolution of magnetic peak (101) is indicative of the onset of long-range magnetic ordering. At 10 K, in the zero field magnetic structure, Mn (black arrows) and Co (white arrows) are coupled antiferromagnetically, as shown in the schematics above. Application of a field of 5 T reduces the intensity of the AFM order, resulting in a net FM state, which is evident from the in-field ND pattern as well as FM coupling between Mn and Co spins as shown in the schematics.

■ Kinetic arrest of the austenite to martensite transition in $\text{Ni}_{37}\text{Co}_{11}\text{Mn}_{42.5}\text{Sn}_{9.5}$

Neutron diffraction measurements, performed in presence of an external magnetic field, have been used to show structural evidence for the kinetic arrest of the first-order phase transition from the high temperature austenite to the low temperature martensite phase in the magnetic shape memory alloy $\text{Ni}_{37}\text{Co}_{11}\text{Mn}_{42.5}\text{Sn}_{9.5}$ and the formation of a glass-like arrested state (GLAS). The CHUF (cooling and heating under unequal fields) protocol has been used to establish phase coexistence of metastable and equilibrium states of GLAS in the neutron diffraction patterns. Figure shows the sample cooled in a field of 7 T and warmed in 1.5 T. Austenite phase is seen to be kinetically arrested up to 25K after which devitrification to martensite takes place, followed by a reentrant transition to the austenite above 230 K.

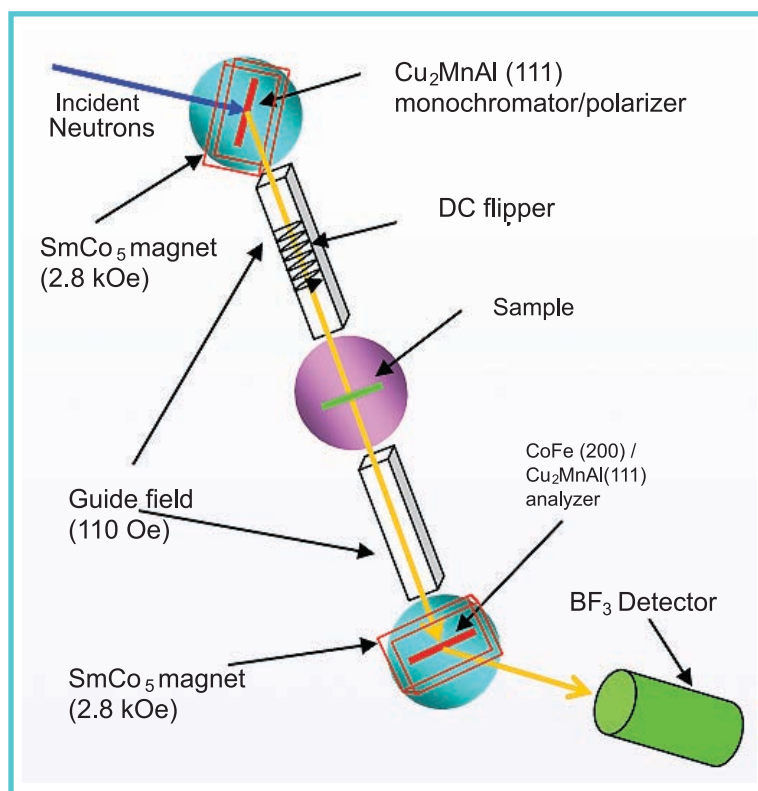
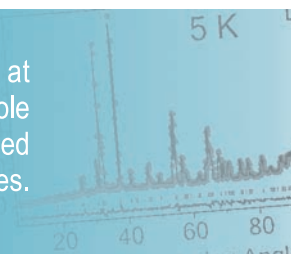


Selected Publications

1. A. K. Singh, S. Patnaik, S.D. Kaushik and V. Siruguri, Phys. Rev. B 81 (2010) 184406
2. S. D. Kaushik, S. Rayaprol, J. Saha, N. Mohapatra, V. Siruguri, P.D. Babu, S. Patnaik and E.V. Sampathkumaran, J. Appl. Phys. 108 (2010) 084106
3. V. Siruguri, S.D. Kaushik, P.D. Babu, A. Biswas, S.K. Sarkar, K. Madangopal and P. Chaddah, arXiv:1211.0238

Polarized Neutron Spectrometer

This instrument is installed at The end of the tangential beam hole No.T1009.The spectrometer is used for magnetic correlation studies.



Instrument Parameters

Beam hole No.	T1009
Wavelength	1.201 Å
Beam Polarization	98.83%
Flipper	DC flipper
Flux at sample	3.6×10^5 n/cm ² /sec
Scattering angle	$0^\circ < 2\theta < 120^\circ$
Analyzer efficiency	97.36 % / 99.89 %
Detector	BF ₃ counter
Available <i>T</i> range	1.5 – 300 K
Available <i>H</i>	1.2 kOe

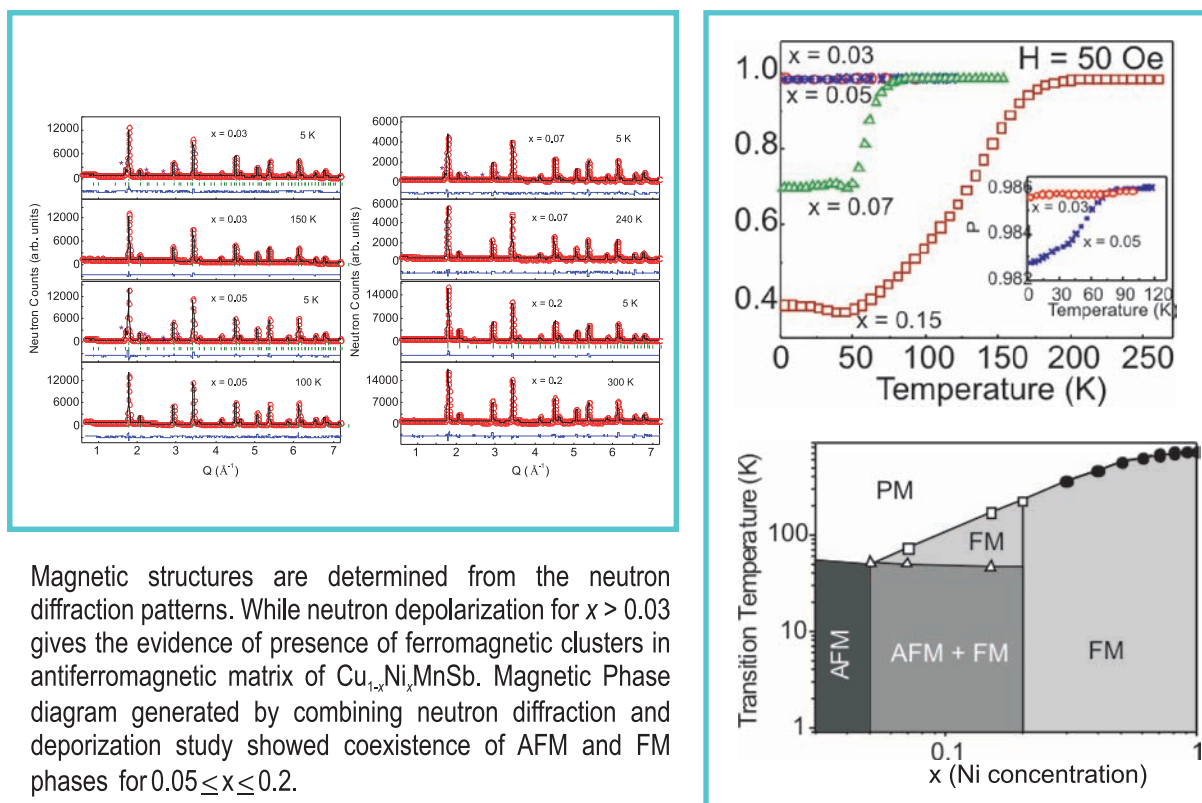


The polarized neutron spectrometer (PNS) is used for magnetic scattering studies. This spectrometer can be used in different modes, such as (a) diffraction mode (2-axis configuration), (b) polarization analysis mode (3-axis configuration in scattering geometry), and depolarization mode (3-axis configuration in transmission geometry). The instrument has been used for studying mixed ferrites, 3d-based alloys, uranium / thorium / cerium based intermetallic compounds, amorphous magnets, CMR perovskites, quasi 1-D spin chain compounds, etc.

S. M. Yusuf and L. Madhav Rao, Neutron News 8 (1997)12
S. M. Yusuf and L. Madhav Rao, Pramana- J. Phys. 47 (1996)171

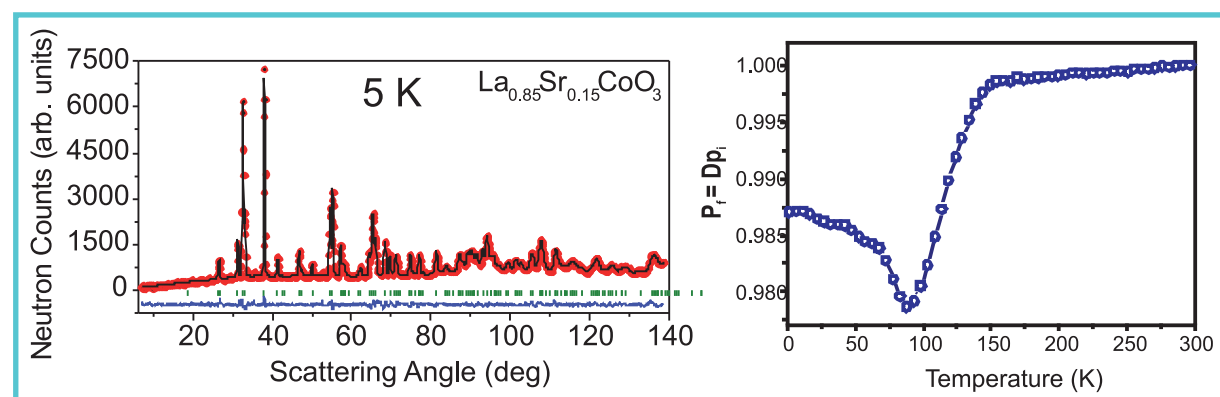
Selected Examples

■ Magnetic Phase diagram of Half Heusler Alloys $\text{Cu}_{1-x}\text{Ni}_x\text{MnSb}$



Magnetic structures are determined from the neutron diffraction patterns. While neutron depolarization for $x > 0.03$ gives the evidence of presence of ferromagnetic clusters in antiferromagnetic matrix of $\text{Cu}_{1-x}\text{Ni}_x\text{MnSb}$. Magnetic Phase diagram generated by combining neutron diffraction and depolarization study showed coexistence of AFM and FM phases for $0.05 \leq x \leq 0.2$.

■ Nature of Magnetic Ordering in Perovskites Cobaltite $\text{La}_{0.85}\text{Sr}_{0.15}\text{CoO}_3$



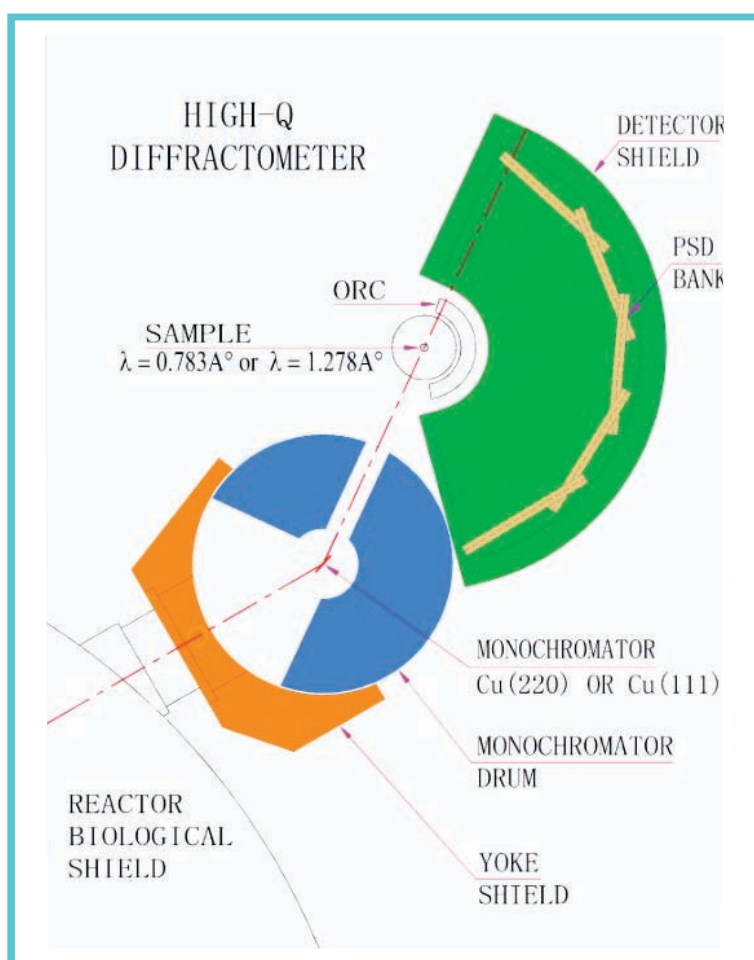
In order to investigate the nature of magnetic ground state, neutron diffraction study has been performed (using PD-2). The diffraction patterns do not show any magnetic signal down to 5 K. The study rules out any long-range magnetic ordering down to 5 K. Neutron depolarization study establishes the presence of magnetic clusters below 150 K.

Selected Publications

1. S. M. Yusuf, R. Ganguly, K. Chakraborty, P.K. Mishra, S.K. Paranjpe, J.V. Yakhmi and V.C. Sahni, Phys. Rev. B 68 (2003) 104421
2. S. M. Yusuf, K. R. Chakraborty, R. Ganguly, P. K. Mishra, S. K. Paranjpe, J. V. Yakhmi and V. C. Sahni, J. Magn. Magn. Mater. 272-276 (2004) 1288
3. S. M. Yusuf, J. M. De Teresa, P. A. Algarabel, J. Blasco, M. R. Ibarra, A. Kumar, C. Ritter, Physica B 385 (2006) 401
4. J. M. De Teresa C. Ritter, P.A. Algarabel, S.M. Yusuf, J. Blasco, A. Kumar, C. Marquina, M.R. Ibarra, Phys. Rev. B 74 (2006) 224442
5. M. Halder S. M. Yusuf, A. Kumar, A. K. Nigam and L. Keller, Phys. Rev. B 84 (2011) 094435

High - Q Diffractometer

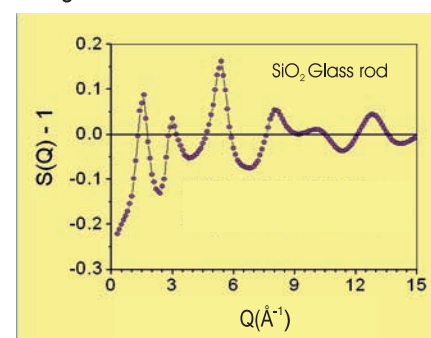
This High-Q diffractometer is a conventional neutron powder diffractometer with high $Q_{\text{max}} (=15 \text{ \AA}^{-1})$ with $\lambda = 0.783 \text{ \AA}$ and is used mainly to understand short range order in glasses, liquids and disordered crystals.



Instrument parameters

Beam hole, no	HS1019
Monochromator	Cu (220): $\lambda = 0.783 \text{ \AA}$ Cu (111): $\lambda = 1.278 \text{ \AA}$
Flux at sample (n/cm ² /sec)	2×10^6 ($\lambda = 1.278 \text{ \AA}$) 3×10^5 ($\lambda = 0.783 \text{ \AA}$)
Sample size	40 mm high & 5-10 mm dia
Scattering angle	$3^\circ < 2\theta < 140^\circ$
Detector	10 (1-d PSDs) at 5 positions
Q range	$0.3 - 15 \text{ \AA}^{-1}$
$\Delta Q/Q$	2.5 %

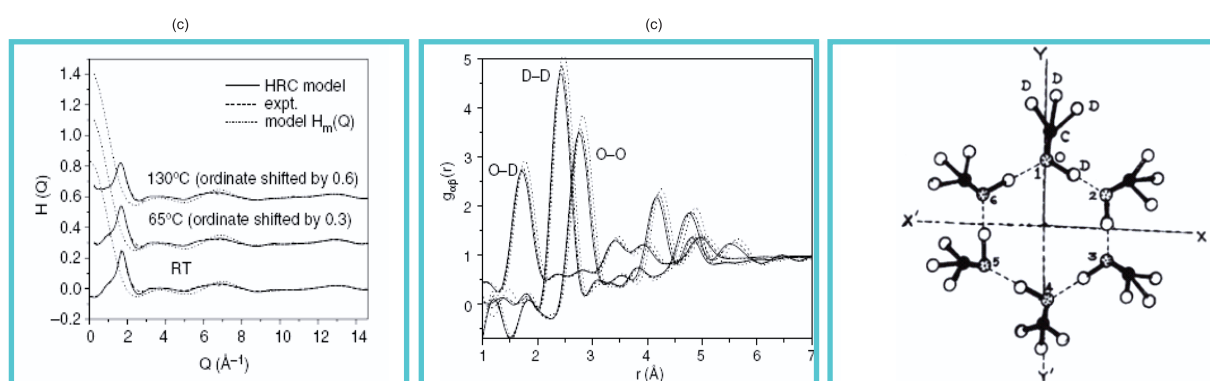
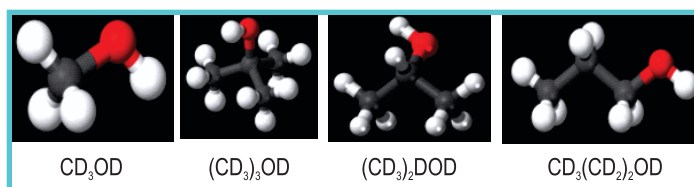
Hi-Q diffractometer is a multi-PSD based instrument covering Q-range up to $15 \text{ \AA}^{-1}$. It has been used for structural studies of a number of molecular fluids, chalcogenide glasses, borate glasses, phosphate glasses, tellurite glasses, sulphide glasses, amorphous carbon and also in studies of local structure determination from disordered crystalline systems. This diffractometer has also been used to study high pressure structural phase transitions in α -Resorcinol, NbO_2F etc., using a home made piston cylinder type pressure cell using EN45 steel as the cell material.



Selected Examples

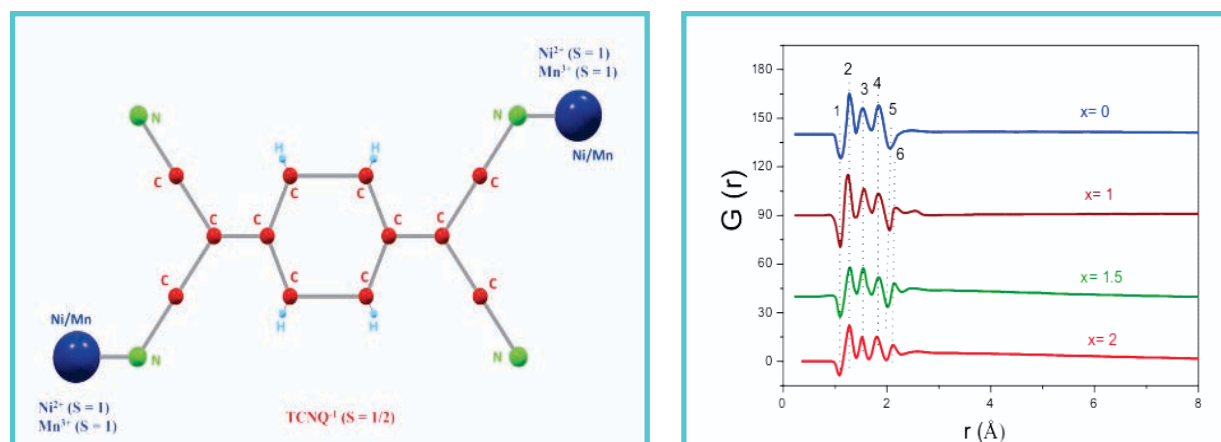
■ H-bonded simple alcohols

Simple alcohols show molecular association via H-bonding. We studied the structures of Methanol, t-Butanol, 2-Propanol and 1-Propanol. We found that under ambient conditions the first 3 alcohols show intermediate range ordering (a pre-peak is seen in the $H(Q)$ function) and also this ordering is via these molecules forming a molecular cluster of Hexagon like benzene via H-bonding. On the other hand 1-propanol is found to have linear clusters. We studied the temperature evolution of CD_3OD on the coexistence curve at 25, 65 and 130°C. We found that on the coexistence line the Hexamer clusters in CD_3OD remain intact. These clusters are dynamically formed and their life time is higher than interaction time of neutron with the system in diffraction experiments. At high temperatures Ornstein-Zernike behaviour is observed at low Q values in $H(Q)$.



■ $Ni_xMn_{0.67(2-x)}[TCNQ](OH)_3$ ($0 \leq x \leq 2$) amorphous molecular magnets

We studied the $Ni_xMn_{0.67(2-x)}[TCNQ](OH)_3$ amorphous molecular magnetic compounds. These compounds are formed by a charge transfer from Ni/Mn metal ions to TCNQ ligand. The Ni-rich studied compounds are magnetic at room temperature and show small values of coercive field and remanence. The magnetization data suggest that Ni^{2+} ($S=1$)/ Mn^{3+} ($S=1$) spins and the $TCNQ^{\cdot-}$ ($S=1/2$) spins order ferri-magnetically for all compounds. We used the program MCGR, for a quantitative analysis of the observed total neutron scattering in order to get an insight of inter atomic distances. The obtained total pair distribution functions are analyzed to find the C-H, C-N, C-C, Ni-N and Mn-N bond distances in the compounds. These distances are found to be 1.1, 1.2, (1.5, 1.7), 2.1 and 2.0 Å respectively. Note the negative peaks corresponding to C-H and Mn-N bond lengths.



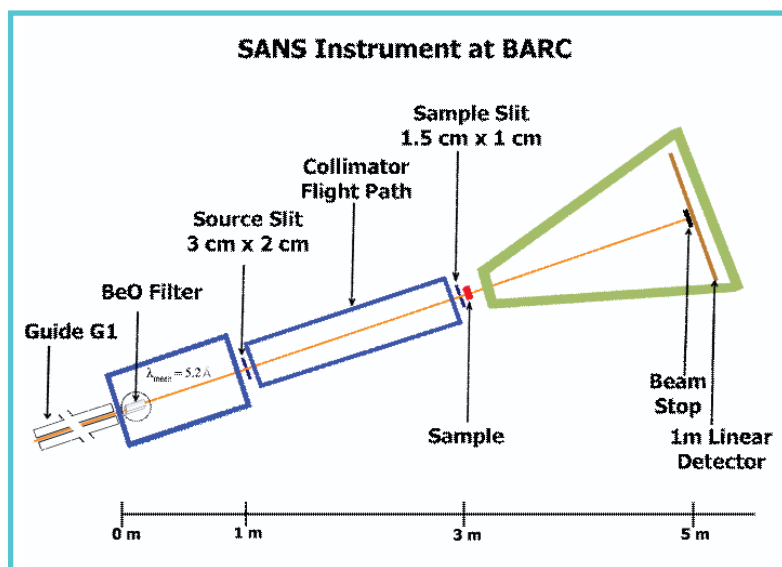
Selected Publications

1. A.Sahoo, P. P. Nath, V. Bhagat, P. S. R. Krishna and R. N. Joarder, Phys. Chem. Liquids, 48 (2010) 546
2. A. Sahoo, S. Sarkar, P. S. R. Krishna and R. N. Joarder, Pramana-Journal of Physics, 74 (2010) 765
3. A. Sahoo, S. Sarkar, V. Bhagat and R. N. Joarder, J. Phys. Chem. A 113 (2009) 5160

Small-angle Neutron Scattering Diffractometer

This SANS diffractometer is installed at the end of one of the guides, G1. The diffractometer is suitable for studies of inhomogeneities of the sizes in the range 10–200 Å.

○ 0.6 wt%
□ 1.0 wt%
△ 2.0 wt%

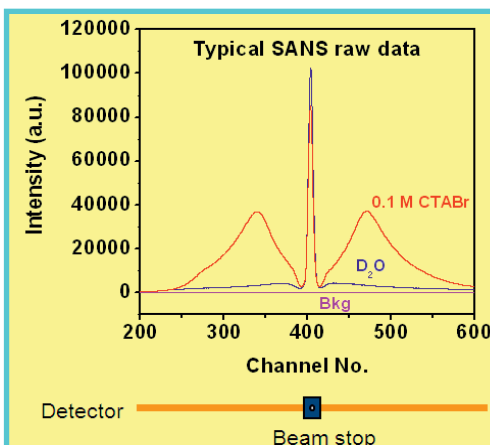


This is a conventional slit-geometry SANS diffractometer. It makes use of BeO filter as a monochromator. The beam passes through two slits S1 and S2 before it is incident on the sample. The angular distribution of neutrons scattered by the sample is recorded using a 1-m linear position sensitive detector.

The SANS diffractometer is widely used to investigate the structure (shape and size) of different kinds of mesoscopic systems such as micellar solutions, magnetic fluids, protein solutions and colloidal suspensions.

Instrument Parameters

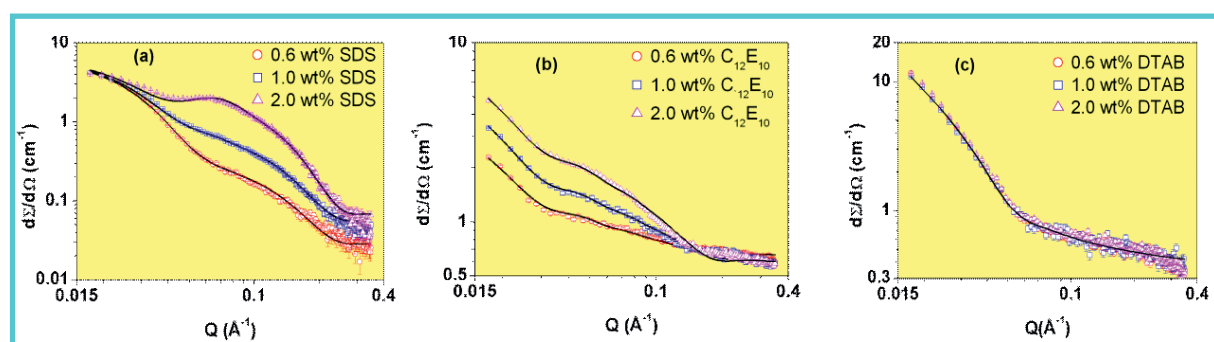
Beam port	Guide G1
λ^* (guide cut-off)	2.2 Å
Monochromator	BeO Filter at 77 K
$\lambda_{\text{cut-off}}$	4.7 Å
λ_{average}	5.2 Å
$(\Delta\lambda/\lambda)$	~15 %
Flux at sample	2.2×10^5 n/cm ² /sec
Source slit (S1)	3 cm x 2 cm
Sample slit (S2)	1.5 cm x 1 cm
Distance S1 & S2	2 m
Angular divergence	$\pm 0.5^\circ$
Detector (D)	linear He ³ -PSD
Distance S2 & D	1.85 m
Q range	0.017 – 0.35 Å ⁻¹



V. K. Aswal and P. S. Goyal, Current Science 79 (2000) 947

Selected Examples

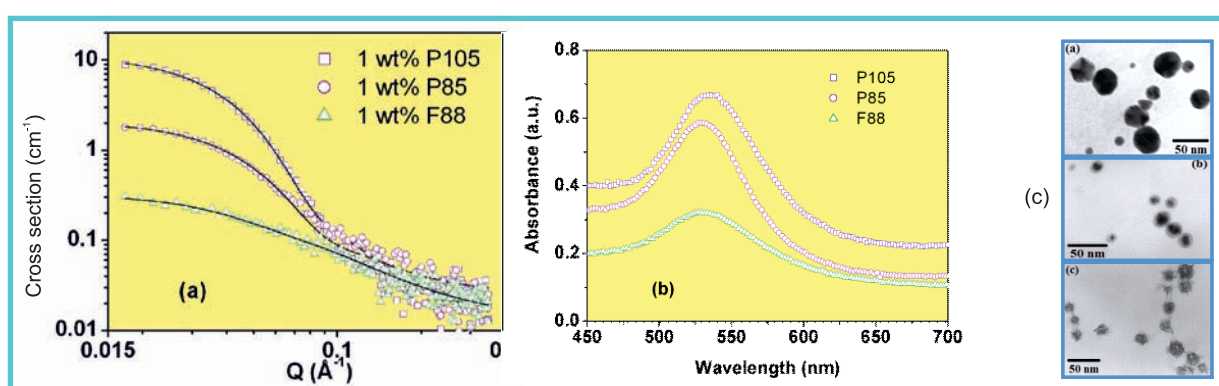
Interaction and resultant structure of nanoparticle-surfactant complexes



SANS data of interaction of 1 wt% anionic silica nanoparticles (15nm) with (a) anionic SDS micelles (both nanoparticles and micelles are visible), (b) nonionic $C_{12}E_{10}$ micelles (nanoparticles contrast matched) and (c) cationic DTAB micelles (micelles contrast matched).

SANS has been used to study the interaction of silica nanoparticles with three different types of surfactants (Figure 1). It is found that the interaction of anionic silica nanoparticles with anionic, cationic and nonionic surfactants is very different and each case leads to different microstructures. The dominant repulsion in the case of silica nanoparticles with anionic SDS micelles prevents any physical interaction of the two components. The strong attractive interaction of nanoparticles with cationic DTAB micelles leads to the aggregation of particles and is characterized by a fractal structure. For nonionic micelles $C_{12}E_{10}$, the non-electrostatic interaction between nanoparticle and micelles gives rise to the adsorption of micelles on individual particles.

Role of self-assembly of block copolymer in gold nanoparticle synthesis



(a) SANS data of self-assembly of F88, P85 and P105 block copolymers, (b) SPR peaks of the gold nanoparticles and (c) TEM of gold nanoparticles synthesized from these block copolymers.

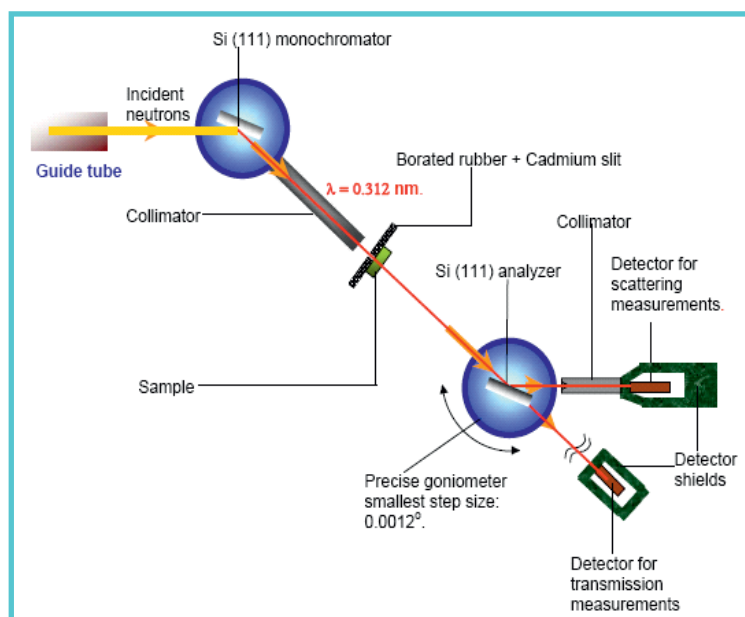
The synthesis of gold nanoparticles from hydrogen tetrachloroaurate (III) hydrate ($HAuCl_4 \cdot 3H_2O$) has been carried out using three different block copolymers P85 [$EO_{26}PO_{39}EO_{26}$], F88 [$EO_{103}PO_{39}EO_{103}$] and P105 [$EO_{37}PO_{56}EO_{37}$], which not only have varying molecular weight but also differ in hydrophobicity to hydrophilicity ratio. The yield is found to be in the order $P105 > P85 > F88$ and is related to the higher tendency of block copolymer to self-assemble leading to greater yield of gold nanoparticles. The formation rate is also found faster for the system having higher yield. The P105 block copolymer having highest tendency of self-assembly forms the nanoparticles with largest sizes whereas the size of the nanoparticles decreases for P85 and F88 mostly consists of block copolymer cross-linked small gold nanoparticles.

Selected Publications

1. A.J. Chinchalikar, V.K. Aswal, J. Kohlbrecher and A.G. Wagh, Eur. Phys. J. E 35 (2012) 55
2. J. Bhattacharjee, V. K. Aswal, P. A. Hassan, R. Pamu, J. Narayanan and J. Bellare, Soft Matter 8 (2012) 10130
3. S. Kumar and V.K. Aswal, J. Phys.: Condensed Matt. 23 (2012) 035101
4. D. Ray, V. K. Aswal and D. Srivastava, J. Nanosci. Nanotechnol. 11 (2011)1905
5. S. De, V.K. Aswal and S. Ramakrishnan, Langmuir 26 (2010)17882

Double Crystal based SANS Instrument

This is a double crystal based medium resolution small-angle neutron scattering instrument built and commissioned at the guide tube laboratory. The instrument consists of a non-dispersive (1, -1) setting of (111) reflections of silicon single crystals with sample between the two crystals.



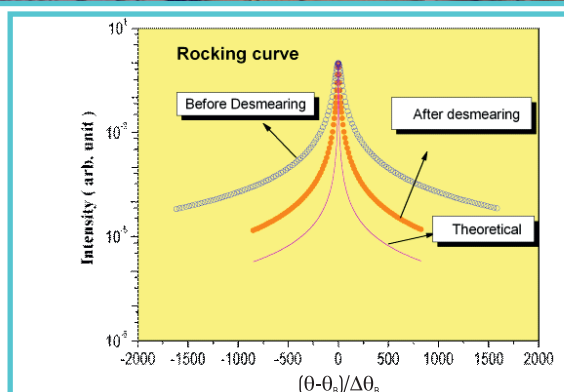
Instrument parameters

Beam port	Guide G1
Monochromator	Si(111)
Wavelength	3.12 Å
($\Delta \lambda / \lambda$)	~1 %
Flux at sample	500 n/ cm ² /sec
Analyser	Si(111)
Q range	0.0003-0.0173 Å ⁻¹
Real space resolution	200 - 10000 Å
Detector	BF ₃



This facility is widely used to investigate the mesoscopic inhomogeneities in ceramics, metallurgical alloys, naturally occurring porous media like rock etc.

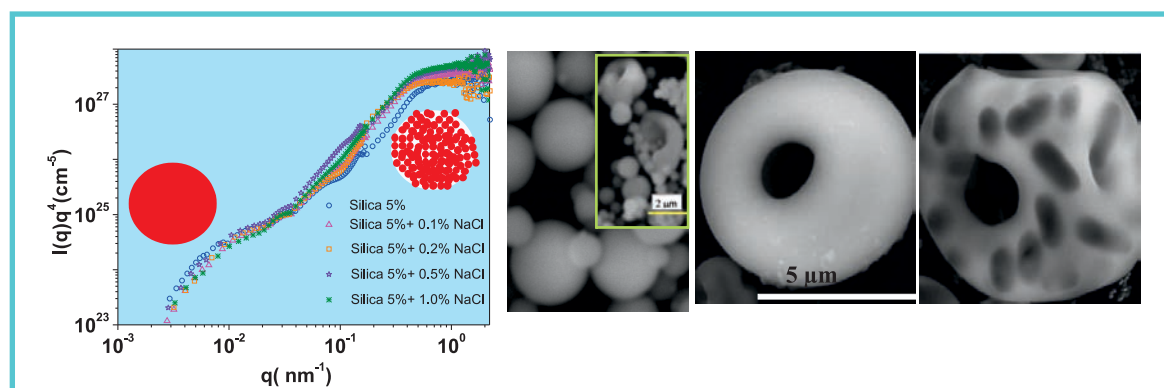
In this kind of double crystal based instruments, unlike the pinhole collimation instruments, the collimation is performed in the reciprocal space only and the resolution in wave vector transfer Q is independent of the beam cross section. Because of the non-dispersive setting of both the crystals, the width of the rocking curve is independent of the divergence of the incoming beam.



S. Mazumder, D. Sen, T. Saravanan and P. R. Vijayaraghavan, J. Neutron Research 9 (2001) 39
S. Mazumder, D. Sen, T. Saravanan and P. R. Vijayaraghavan, Current Science 81 (2001) 257

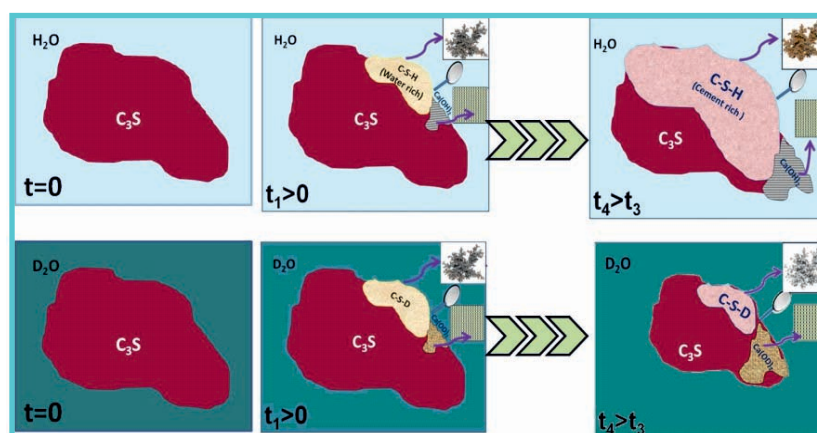
Selected Examples

■ Evaporation induced self assembly of colloidal nanoparticles during spray drying



Spray drying, an indispensable industrial process for long time to obtain dry particles from solution phase, has obtained a special attention in nano-technology in recent time because of evaporation induced self assembly. SANS profiles (left) from spray dried (under slow drying condition) silica grains are shown. Correlation between the jammed nanoparticles inside the grains gets modified with electrolyte concentration in the dispersion phase prior to drying. Morphology of the assembled grains under slower and faster drying conditions are shown (SEM micrographs). Individual nanoparticles are not visible from SEM due to resolution constraint. However, SANS profiles clearly reveal their structure and correlation at intermediate /higher q . Two level structure is also discernible from SANS data. Sphere to doughnut like morphological transition occurs at faster drying condition.

■ Isotope effect in the temporal evolution of mesoscopic structure during cement hydration



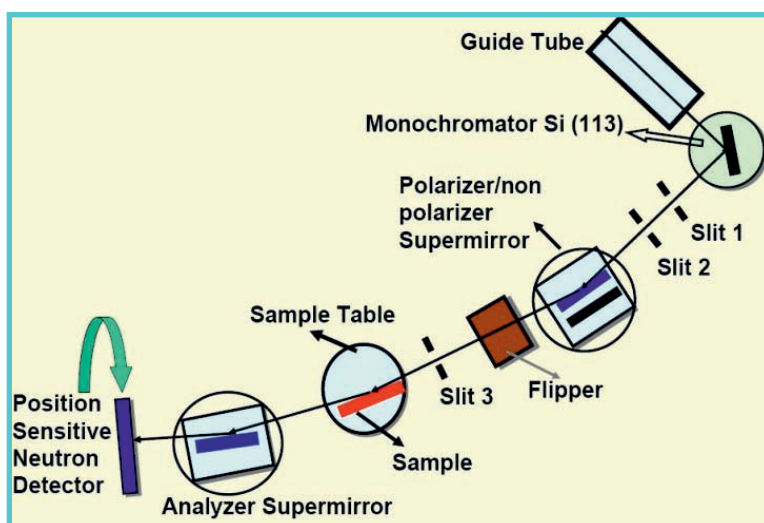
To improve the lifetime of cement and its macroscopic properties (such as compressive strength, permeability, elastic modulus etc.), it is important to understand the mechanisms determining its hydration and how cement-water mixtures develop their high compressive strength. Temporal evolution of mesoscopic structure of the cement paste has been investigated by small-angle neutron scattering and ultra-small-angle neutron scattering. This reveals temporal oscillations, strongly dependent on the hydration medium (H_2O or D_2O). The investigation contributes towards understanding cement hydration mechanism- an enigma to date.

Selected Publications

1. D. Sen, J. Bahadur, S. Mazumder, G. Verma, P. A. Hassan, S. Bhattacharya, K. Vijai and P. Doshi, *Soft Matter* 8 (2012)1955
2. J. Bahadur, D. Sen, S. Mazumder, B. Paul, H. Bhatt and S. G. Singh *Langmuir* 28 (2012)1914
3. D. Sen, J. Bahadur, S. Mazumder and S. Bhattacharya, *Soft Matter* 8, (2012)10036
4. S. Mazumder, D. Sen, R. Loidl and H. Rauch, *Phys. Rev.B* 84 (2011)134302
5. D. Sen, J. S. Melo, J. Bahadur, S. Mazumder, S. Bhattacharya, S. F. D'Souza, H. Frielinghaus, G. Goerigk and R. Loidl, *Soft Matter* 7 (2011) 5423

Polarized Neutron Reflectometer

The polarized neutron reflectometer is located in Guide Tube laboratory. The reflectometer has been designed for vertical sample geometry. It utilizes a highly collimated monochromatic: polarized or unpolarized beam of neutrons.



Instrument Parameters

Monochromator	Si(113)
Wavelength	2.5 Å
$\Delta Q/Q$	0.141 - 0.411
Polarizer	FeCo/TiZr supermirror
Flux at sample	10^4 n/cm ² /sec
D.C. flipper efficiency	92 %
Detector	linear He ³ PSD
Reflectivity	$1 - 10^{-4}$



The reflectometer uses a linear position sensitive detector, which helps to collect the off-specular reflectivity data in addition to specular reflectivity data from the thin film samples, in a single setting.

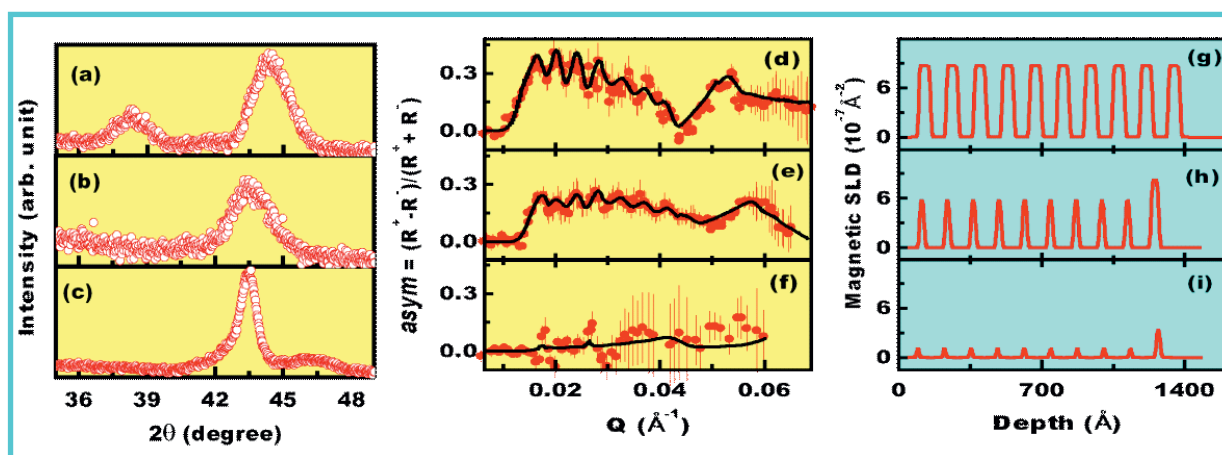
This facility has been widely used for structural and magnetic characterization of thin film samples, using specular and off-specular techniques.

Reflectivity is intrinsically sensitive to the difference of the refractive index (or contrast) across any interface. For the case of specular reflection, the intensity of the reflected beam is related to the depth dependence of the index of refraction averaged over the lateral dimensions of the sample. Polarized neutron reflectometry is a unique technique to study the depth profile of magnetic moment in multilayer. Off-specular or diffuse neutron reflectivity is a widely used technique to understand surface (interface) morphology.

S. Basu and S. Singh, J. Neutron Research 14 (2006) 109

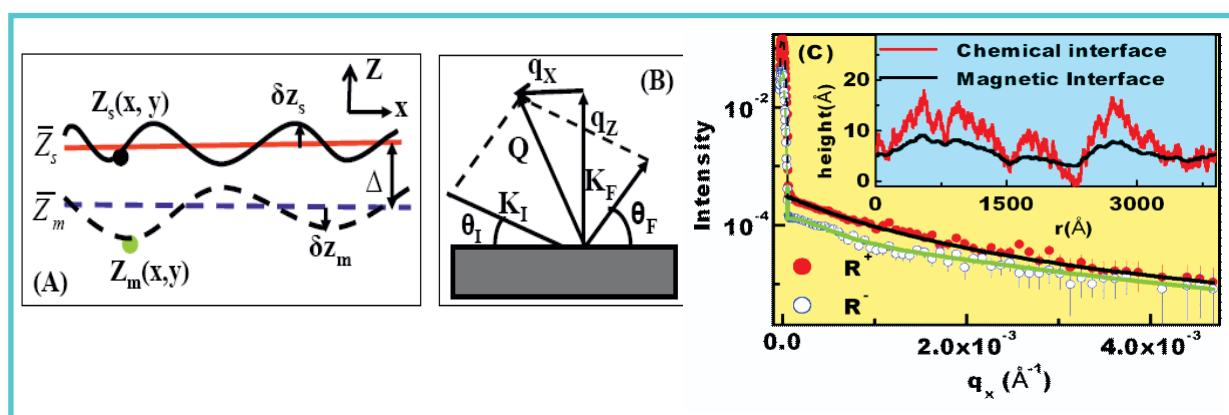
Selected Examples

■ Kinetics of Alloy formation at the Interfaces in a Ni-Ti multilayer



Rapid alloying and modification of electronic and magnetic properties of Ni-Ti multilayer was studied using XRD, X-ray reflectivity and polarized neutron reflectivity (PNR). Fig. (a), (b) and (c) are XRD data from Ni-Ti multilayer for as-deposited, annealed at 300°C and 400°C, respectively. PNR measurements from as-deposited (d) sample and sample annealed at 300°C (e) and 400°C (f). Magnetic scattering length density (SLD) depth profile obtained from PNR for as-deposited (g) sample and sample annealed at 300°C (h) and 400°C (i). The study suggested formation of alloying at interface which are magnetically dead.

■ Separation and correlation of structural and magnetic roughness in a Ni thin film.



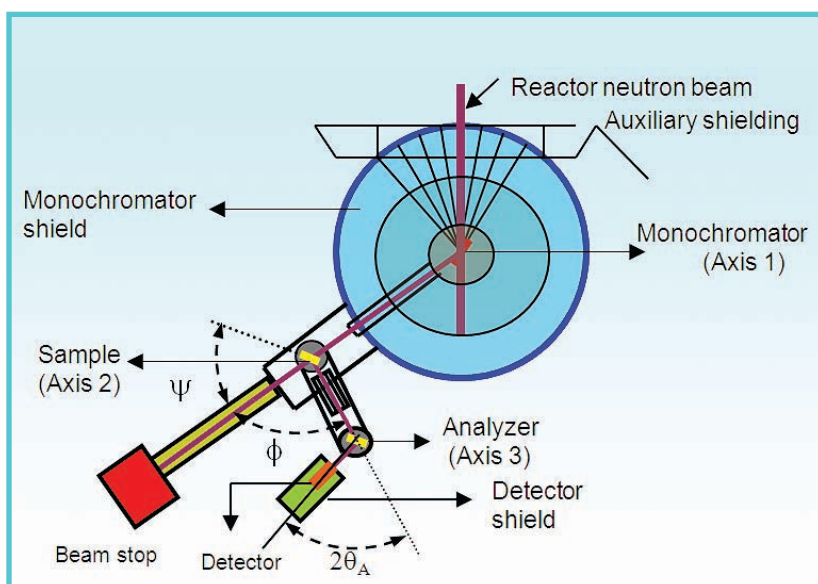
Magnetic and structural roughness of the film is separated quantitatively using polarized diffuse (off-specular) neutron reflectivity (PDNR) measurements. Fig (A) depicts the interface model suggesting different chemical (Z_s) and magnetic (Z_m) boundary used to analyze PDNR data. Fig. (B) show the scattering geometry for PDNR. Fig. (C) show the PDNR data. The results suggested that the magnetic interface shows a higher in-plane correlation length with smooth surfaces (inset of Fig. (C)) as compared to chemical interface.

Selected Publications

1. D. Bhattacharya, S. Basu, Surendra Singh, S. Roy and B. N. Dev, Appl. Surf. Science 263 (2012) 666
2. S. Singh, S. Basu, M. Gupta, C. F. Majkrzak, and P. A. Kienzie, Phys. Rev. B 81 (2010) 235413
3. S. Singh, S. Basu, D. Bhattacharya and A. K. Poswal, J. Appl. Phys. 107 (2010) 123903
4. S. Singh, S. Basu, Pramod Bhatt and A. K. Poswal, Phys. Rev. B 79 (2009) 195435
5. S. Singh and S. Basu, J. Phys.: Condensed Matt. 21 (2009) 055010

Triple Axis Spectrometer

This instrument is used to study inelastic neutron scattering from single crystals / polycrystalline samples.



Instrument Parameters

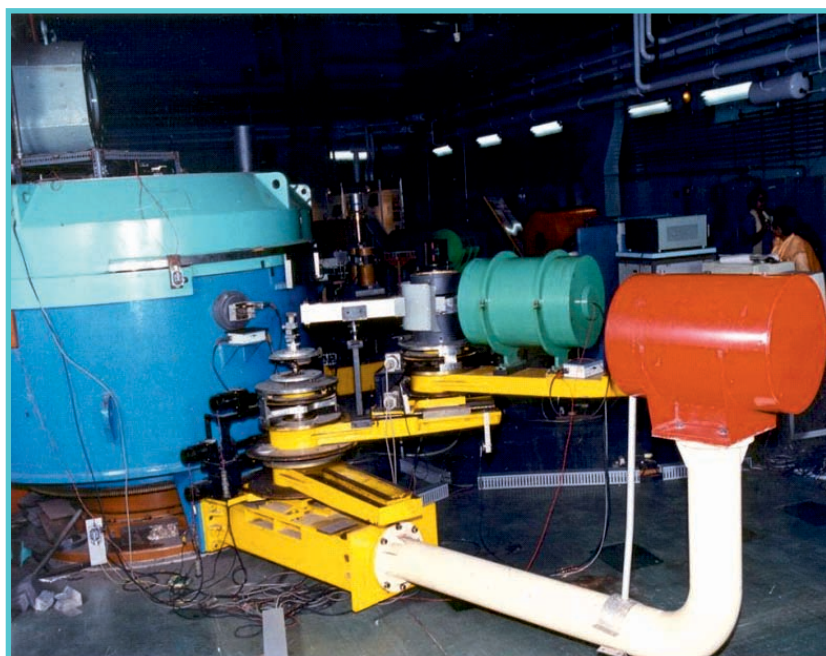
Beam hole no.	T1007
Monochromator	Cu(111)
ΔE range	3 – 200 meV
Q range	1 – 10 $\text{\AA}^{-1}$
λ range	0.6 – 2.3 $\text{\AA}$
Beam size	50 mm x 50 mm
Flux at sample	10^6 n/cm ² /sec
Analyzer	PG(0002)
Scattering angle	10 – 100°
Detector	BF ₃ Counter

This instrument has been successfully employed for measurements of phonon dispersion curves, phonon density of states, crystal field excitations and quasielastic scattering.

The geometry of the triple axis spectrometer allows measurements of the scattering function $S(Q, E)$ in single crystals at well defined values of momentum transfer Q and energy transfer E .

Principal components of this instrument are:

- Monochromator that produces the monoenergetic neutron beam
- Positional spectrometer that sets the angles
- Analyzer that measures the outgoing energy
- Various arms of the spectrometer can be moved by means of worm-gear Assemblies

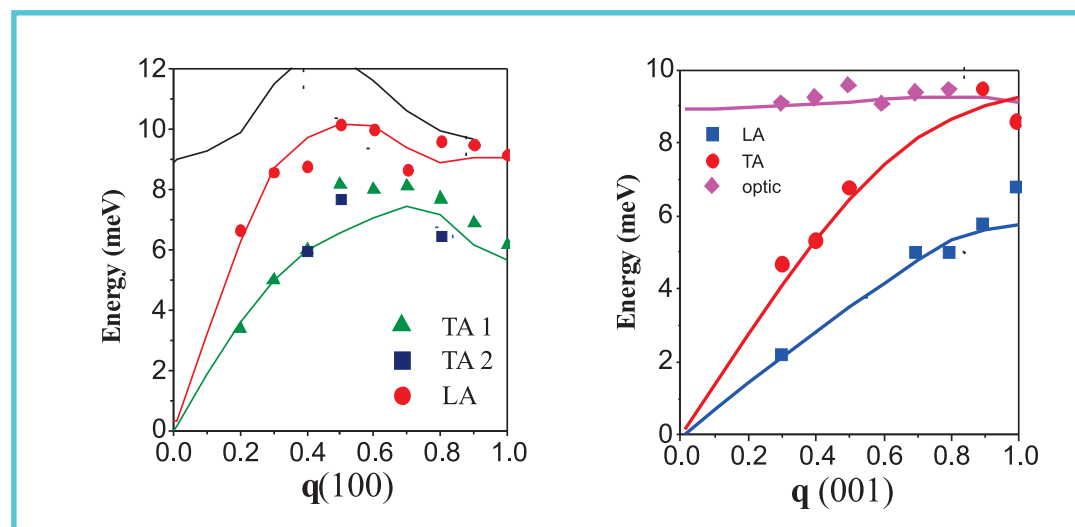


The shielding wedges of the monochromator shield are lifted automatically to allow for continuous variation of the monochromator settings.

S.L. Chaplot, R. Mukhopadhyay, P.R. Vijayaraghavan, A.S. Deshpande and K.R. Rao, Pramana - J. Phys. 33 (1989) 595

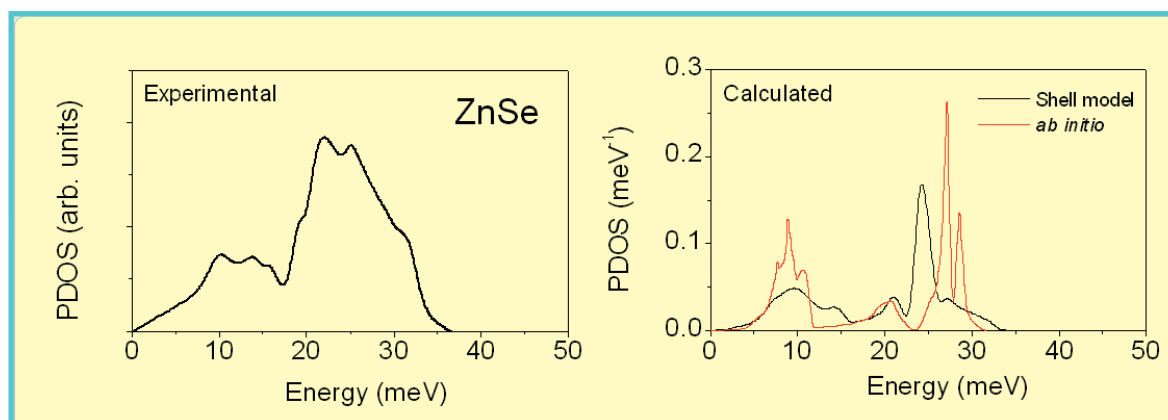
Selected Examples

■ SrWO_4 : alkaline earth tungstate, with a rich phase diagram



Measured (symbols) and calculated (solid line) low energy phonon dispersion curves along two directions in SrWO_4 . Phonon dispersion curves show good agreement with calculations. Interatomic potential model as used in phonon calculations has also been used for molecular dynamics simulation to study pressure-driven transitions.

■ ZnSe : II–VI semiconducting material



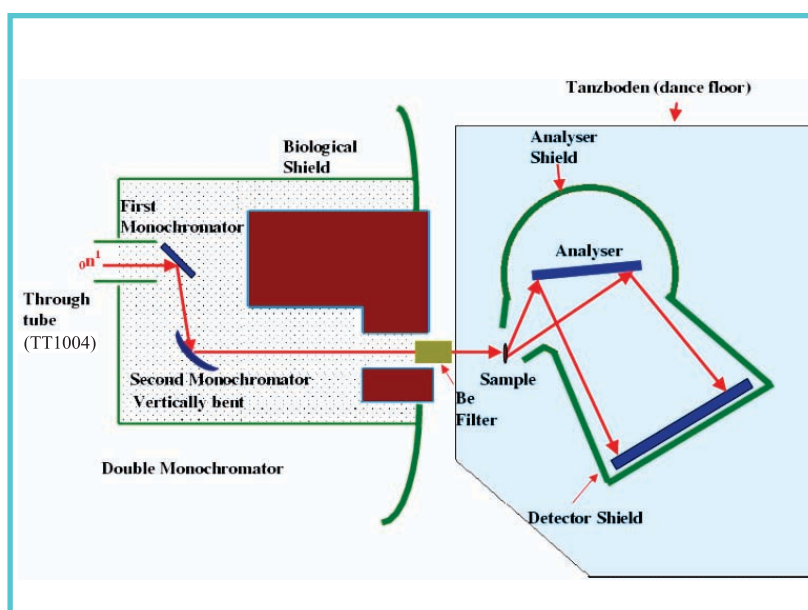
The phonon density of states of ZnSe was determined and interpreted with lattice dynamical computations (*ab initio* as well as a potential model). Vibrational (phonon spectra and Grüneisen parameters), and thermal (negative thermal expansion and non-Debye specific heat) properties have been calculated and found to be in good agreement with available experimental data. This model has been further employed to study the pressure-induced solid–solid phase transitions exhibited by these compounds. An investigation of the pressure dependence of the phonon frequencies shows that the existence of the (experimentally undetected) SC16 phase as a thermodynamically stable high pressure phase is impeded due to dynamical instabilities.

Selected Publications

1. T. Basak, M.N. Rao, M.K. Gupta and S.L. Chaplot, J. Phys.: Condensed Matt. 24 (2012) 115401
2. V. K. Sharma, S. Gautam, S. Mitra, M.N. Rao, A.K. Tripathi, S.L. Chaplot, and R. Mukhopadhyay, J. Phys. Chem. B 113 (2009) 8066

Quasi Elastic Neutron Scattering instrument

This instrument is used to study Stochastic Motion (like Diffusion) in Condensed Matter. 'Quasi' means near elastic. Provides information about the time scale and geometry of diffusive motion as also the potential experienced by the species.

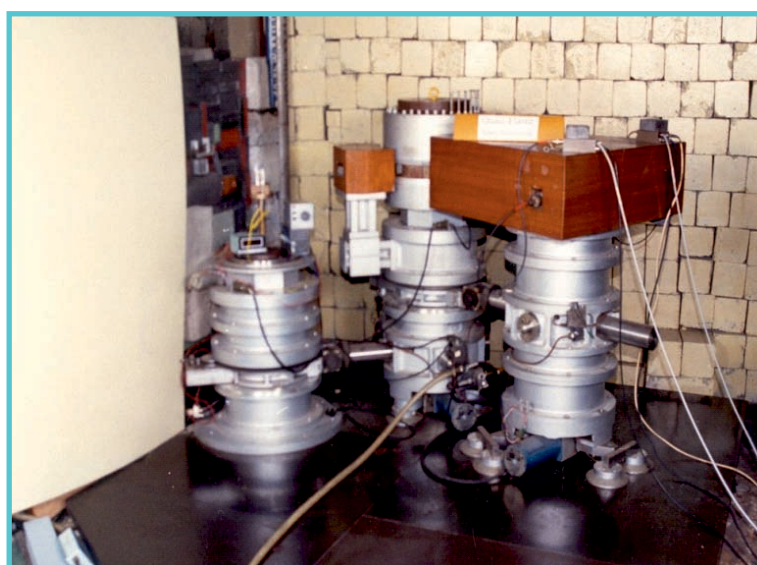


Instrument Parameters

Beam hole no.	TT1004
Monochromator (2 nos. in tandem) crystals (2nd one vertically focused): PG (0002) (100 x 80 mm ²)	
$\lambda_{\text{incident}}$	1.3 – 4.7 Å
Scattering angle	$2\theta < 80^\circ$
Flux at sample	$5 \times 10^5 \text{ n/cm}^2/\text{sec}$
Analyser (MARX Mode)	PG(0002)
ΔE_{range} (for $E_i = 4 \text{ meV}$)	2.3 meV
$\Delta E/E$	4 %

Some distinct features of this instrument are mentioned below:

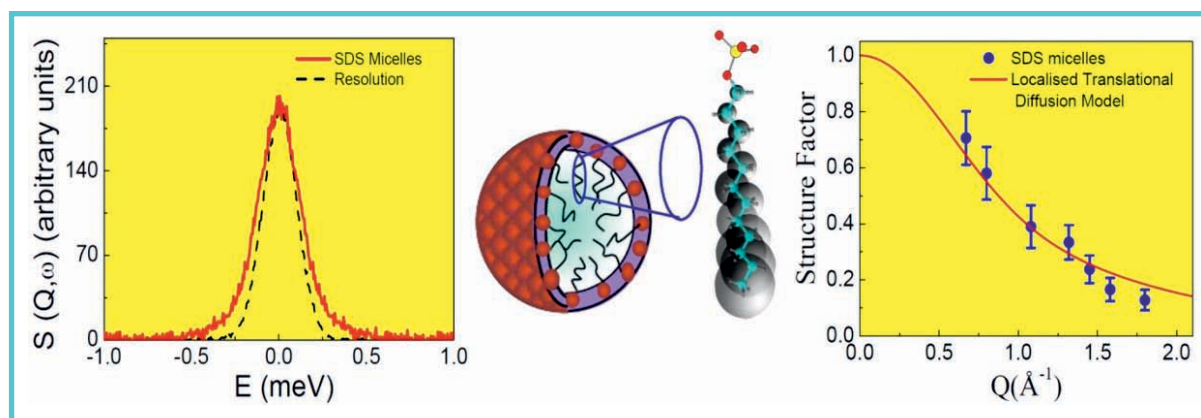
- Virtue of Double Monochromator, neutrons of different incident energy can be obtained at a fixed sample position
- The instrument works in Multi angle Reflecting X-tal mode (MARX) thereby facilitating complete energy spectrum for one instrumental configuration.
- Provision to change in the distance between different axes to obtain different energy resolutions.
- The out-of-pile portion of the instrument is on a 'tanzboden' facilitating easy maneuvering.



R. Mukhopadhyay, S. Mitra, S.K. Paranjpe, B.A. Dasannacharya, Nucl. Instr. Meth. A 474, (2001) 55
S. Mitra and R. Mukhopadhyay, Current Science 84 (2003) 653

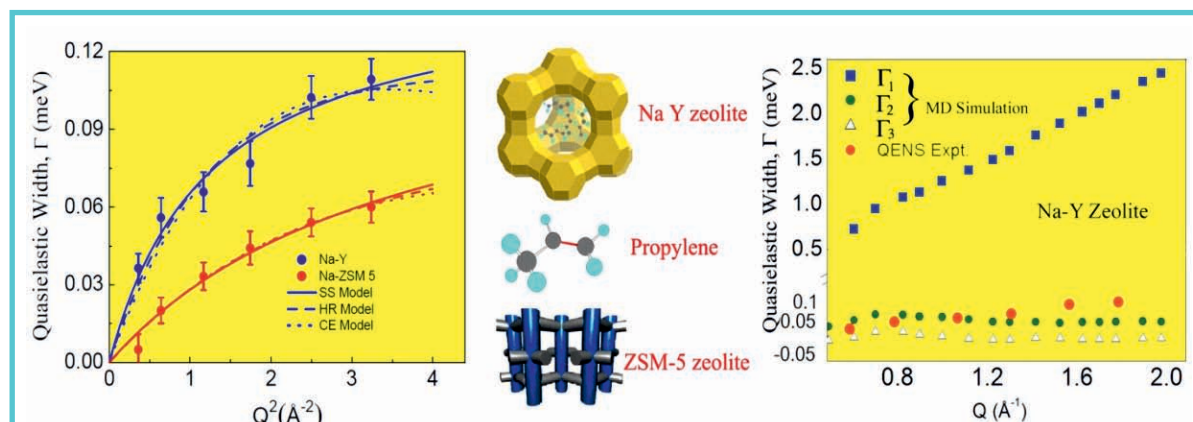
Selected Examples

Internal Dynamics in Ionic Micellar Solutions



Internal dynamics of micellar assemblies are important in understanding various properties such as the mechanism in releasing the solubilized drugs, micellar breaking time, etc. Dynamics of various ionic micellar solutions including sodium dodecyl sulfate (SDS) have been investigated using QENS technique. A model in which the hydrogen atoms undergo localised translational diffusion confined within spherical volumes successfully describes internal dynamics of the SDS molecules. This volume increases linearly along the SDS chain (as shown in the schematic above) such that the hydrogen atoms closer to the head group move within smaller spheres with lower diffusion constant than the hydrogen atoms away from the head group.

Diffusion of Molecules Adsorbed in Zeolite



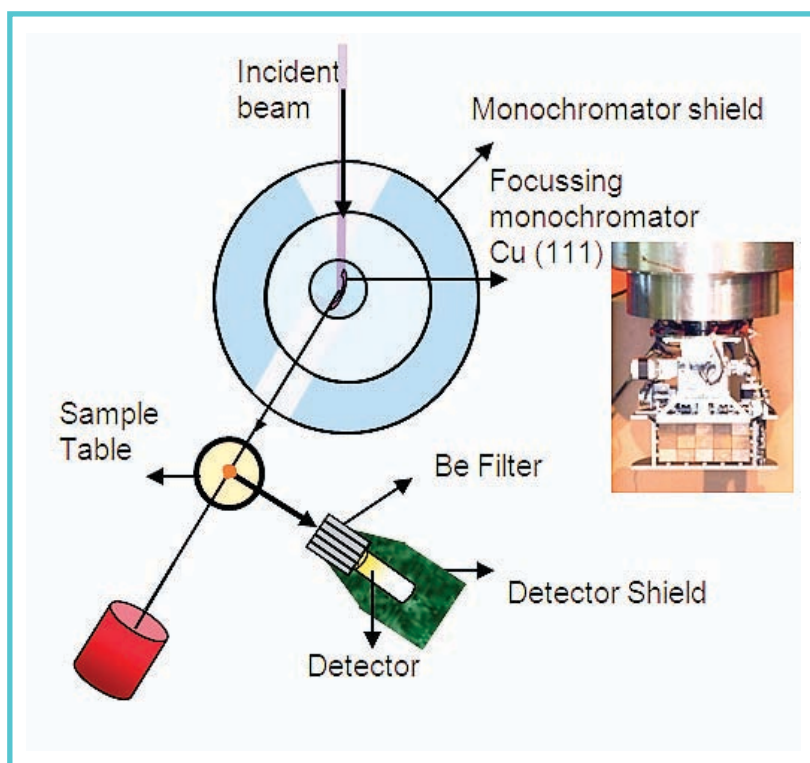
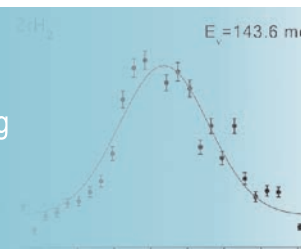
Catalysis and molecular sieving properties of zeolites mainly depend upon the diffusivity of the adsorbed molecules. The dynamics of adsorbed species is indeed complex and depend upon a number of factors like the size and shape of the molecule, host structure, guest-host interaction, and temperature. The effect of host structure (Na-Y and ZSM-5 zeolite) on dynamics of adsorbed species (propylene) has been investigated. QENS data showed that the translational motion of propylene is slower in ZSM-5 zeolite than in Na-Y zeolite. MD simulation results show translational motion exists in three different time scales in both the systems, only one of which corresponds to that observed through the QENS measurements.

Selected Publications

1. V.K. Sharma, S. Mitra, V. G. Sakai, P.A. Hassan and R. Mukhopadhyay, *Soft Matter* 8 (2012) 7151
2. V. K. Sharma, S. Mitra, V. G. Sakai and R. Mukhopadhyay, *J. Phys. Chem. B* 116 (2012) 9007
3. V. K. Sharma, S. Mitra, Amit Kumar, S. M. Yusuf, F. Juranyi and R. Mukhopadhyay, *J. Phys: Condensed Matt.* 23 (2011) 446002
4. S. Mitra, V. K. Sharma, V. G. Sakai, J. Peter Embs and R. Mukhopadhyay; *J. Phys. Chem. B* 115 (2011) 9732
5. V.K. Sharma, S. Gautam, S. Mitra and R. Mukhopadhyay, *Z. Phys. Chem.* 224 (2010) 133

Filter Detector Spectrometer

This instrument is used to study inelastic neutron scattering from condensed matter.



Instrument Parameters

Beam hole no.	HS1017
Monochromator	Doubly focusing Cu(111)
ΔE range	15 – 200 meV
Q range	1 – 10 $\text{\AA}^{-1}$
λ range	0.6 – 2.8 $\text{\AA}$
Flux at sample	2×10^7 n/cm ² /sec
Analyzer	Be filter
Scattering angle	10° – 100°
Detector	BF ₃ Counter



The scattered neutron beam from the sample is filtered by polycrystalline Be made of beryllium blocks interleaved with cadmium. The neutron scattering cross section of Be exhibits a sharp drop at a neutron energy of 5 meV. Thus, neutrons whose energy is less than 5 meV are allowed to pass through the filter and all others are scattered out of the beam.

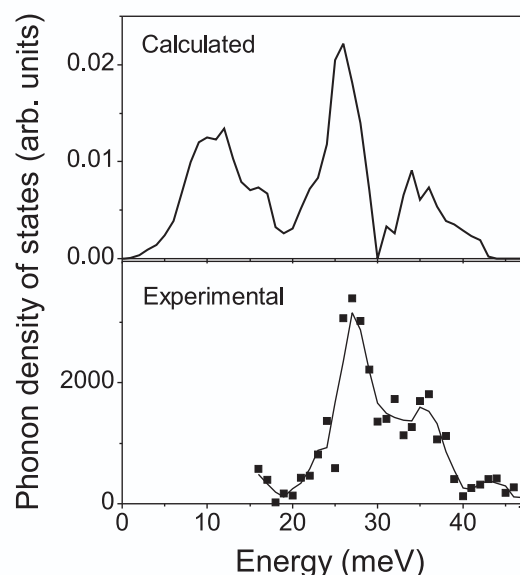
Principal components of this instrument are:

- (i) Monochromator that produces the monoenergetic neutron beam. Continuous variation of the incident neutron energy is allowed for by lifting of the shielding wedges of the monochromator shield
- (ii) Positional spectrometer that sets the scattering angle.
- (iii) Analyzer that measures the outgoing energy.

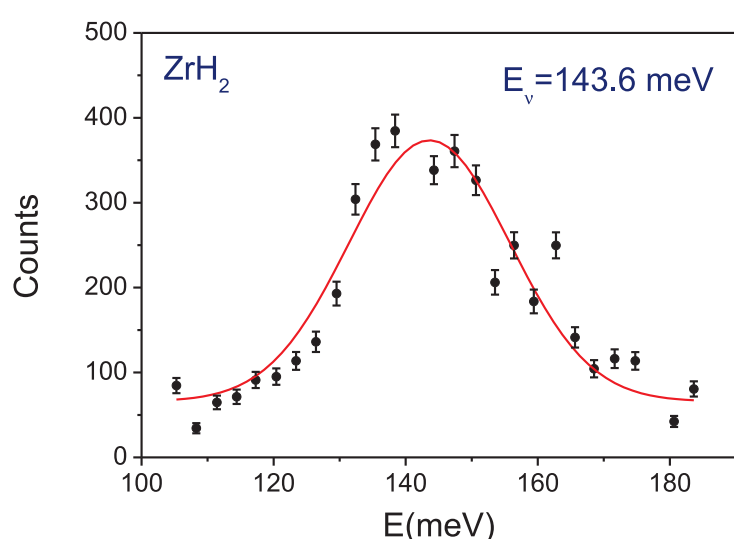
Selected Examples

■ Phonon density of states in $\text{ZnS}_{0.58}\text{Se}_{0.42}$

$\text{ZnS}_{1-x}\text{Se}_x$ is a promising solid solution (for the fabrication of blue light emitting diodes) on account of the miscibility of its parent compounds (ZnS and ZnSe) over a wide range of composition. IR reflection and Raman spectra have revealed that this system exhibits a two-mode behavior (one LO-TO pair (27-31 meV) corresponds to ZnSe-like vibrations, and the other LO-TO pair (35-43 meV) to ZnS-like ones). Two additional unexplained modes were observed in the energy range 37-40 meV in the region between the ZnS-like modes. Phonon density of states measurements and lattice dynamical calculations confirms that these are resonance modes of Se in ZnS.

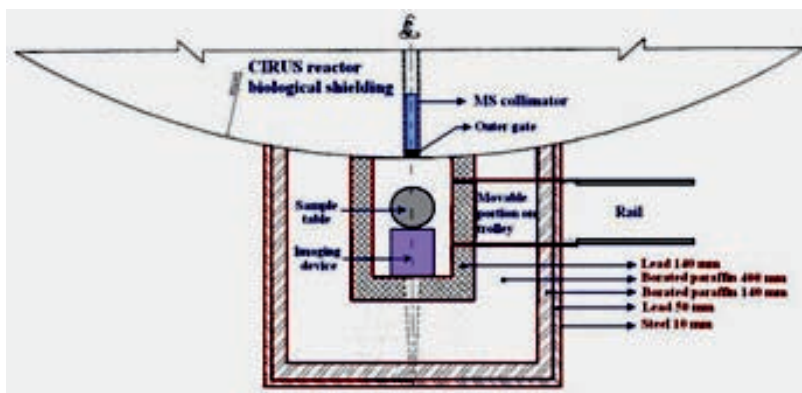
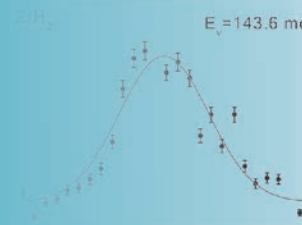


■ Vibration of Hydrogen in Zirconium Hydride (ZrH_2)



The thermal vibration spectrum of zirconium hydride includes (in addition to the band of acoustic frequencies) a sharp "optic" frequency (ν) corresponding approximately to vibrations of the individual hydrogen atoms in an isotropic harmonic well. This implies a set of energy levels for the lattice $E_n = n h \nu$. Peaks corresponding to transitions between these energy levels will be seen in the spectrum of neutrons scattered from zirconium hydride. The first transition is observed as a peak at an energy transfer of about 140 meV.

Neutron Radiography



NR Facility At Beam Hole No. E-18, CIRUS reactor. Schematic (above)
Photograph of the Facility (below).



Facility Details

Collimator: Parallel type, 10 cm ID,
13 cm OD, 120 cm long

Useful beam size: $\sim 15 \text{ cm dia}$

Thermal Neutron Flux: 5×10^8
($\text{n/cm}^2/\text{sec}$)

N/ γ ratio $\sim 3.6 \times 10^5 \text{ cm}^{-2} \text{ mR}^{-1}$

Neutron/gamma ratio: 9×10^5
($\text{n/cm}^2/\text{mR}$)

NR methods employed: Dy 250 μm ,
 $^6\text{LiF-ZnS(Ag)}$ scintillator and CCD
camera based system, Image plates.

Applications

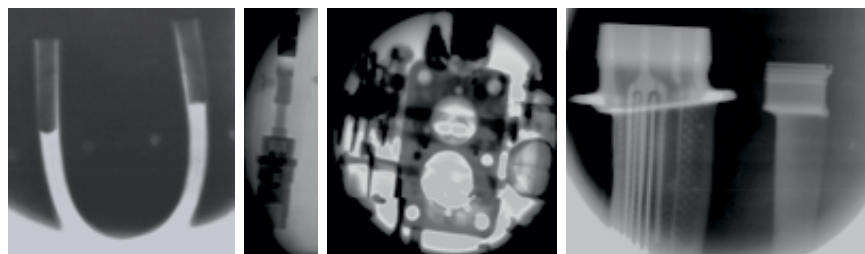
Non-Destructive Testing and
Evaluation of : Nuclear fuel pins, fuel
plates, Control Rods, INSAT-
pyrovalves & cable cutters, electric
detonator, marker shells, Jet turbine
blades

Hydrogen Sensitive Epithermal
Neutron Radiography Real time
electronic imaging,

Neutron radiography with imaging
plates Neutron Induced Beta
Radiography

Thermal neutron radiographs of

- Thick Cu-tube filled with wax,
- INSAT cable cutter,
- automobile carburetor,
- turbine jet blades,
- BNC T-connector,
- USB Pen drive,
- Flower plant (Transfer
radiography with Dy screen,
exposure 9 minutes &
transfer 4.5 minutes on
X-ray film Agfa D-7)

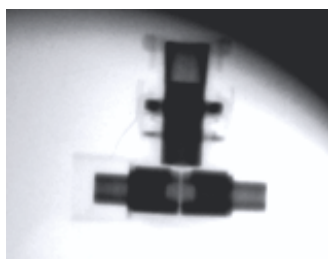


(a)

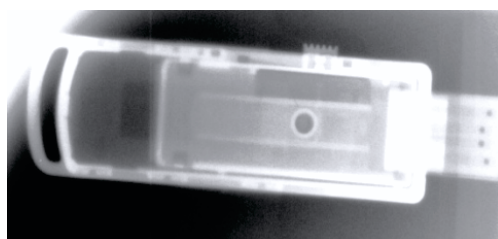
(b)

(c)

(d)



(e)



(f)

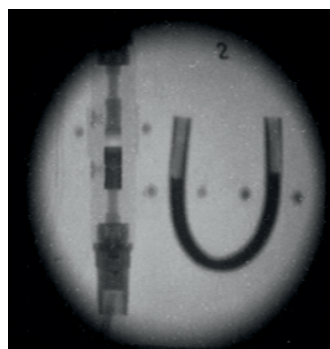


(g)

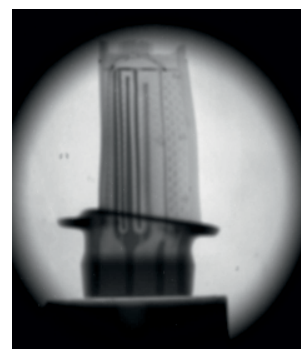
■ CCD based Electronic imaging



In house built electronic imaging system.



INSAT cable cutter and Cu-tube filled with wax



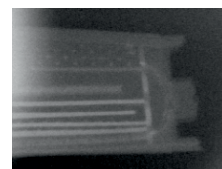
Turbine jet blade.

■ Radiography with Image plates

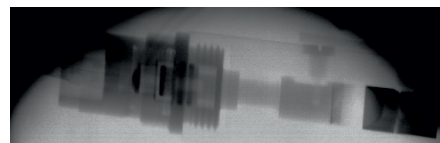


FUJIFILM BAS-5000 Image plate scanner, reader and eraser

Neutron radiographs Fluence: 3×10^9 n/cm²
Exposure time: 10 sec



Turbo jet blade



INSAT cable cutter



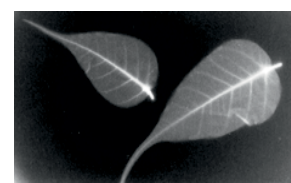
(a)



(b)



(c)



(d)

Neutron Induced Beta Radiography (NIBR) (using Dy foil) of 1000 currency bill showing the a) Mahatma Gandhi security water mark and other features, b) the horizontal strips and circled 1K and 1000 in are not seen with naked eyes and also in UV light. c) Miniature painting of Radha (Indian postal stamp) and its NIB radiograph to the right. d) NIBR of Banyan tree leaves using thermal neutron irradiated In foil. Veins of different thickness are clearly seen

Selected Publications

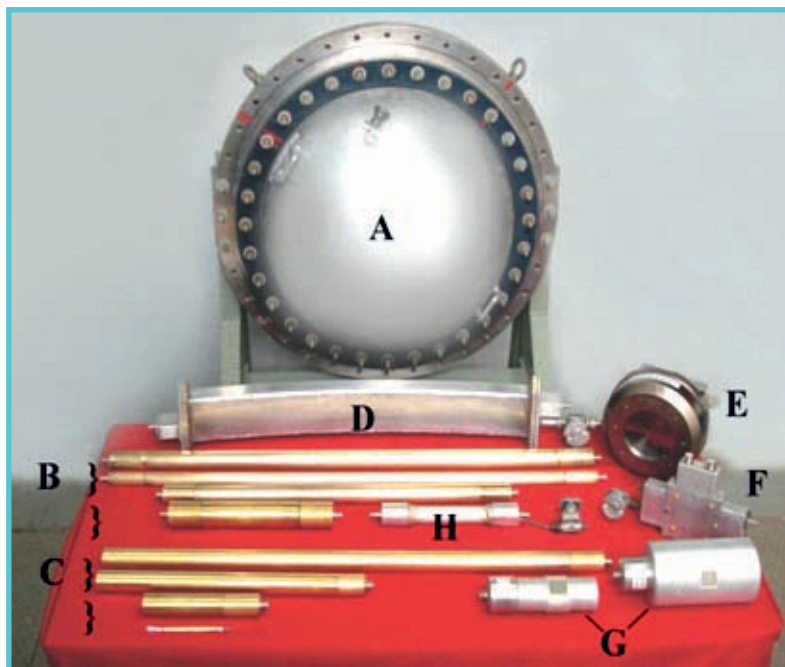
1. A.M. Shaikh, www.ndt.net/article/nde-india2009/pdf/18-C-3.pdf
2. A.M. Shaikh and D. Shylaja, American Institute of Physics Conf. Proc. 1349 (2011)455
3. A.M. Shaikh, www.ndt.net/article/nde-india2011/pdf/1-02A-5.pdf
4. A.M. Shaikh, www.ndt.net/article/wcndt2012/papers/646_wcndtfinal00647.pdf

Development of Neutron Detectors

All Neutron Scattering instruments at NFNBR, Dhruva are equipped with in-house developed detectors. They show stability in operation and long life over the decades.

Various types of neutron and X-ray detectors developed by Solid State Physics Division

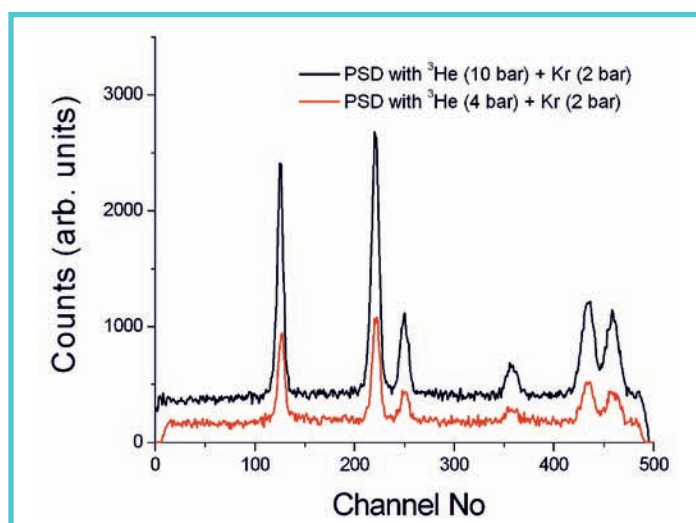
- A: 2-D Position Sensitive Neutron Detector
- B: 1-D Position Sensitive Neutron Detectors
- C: Neutron Proportional Counters
- D: 1-D Curvilinear Position Sensitive Neutron Detector
- E: 2-D Position Sensitive X-ray detector
- F: Microstrip Detector for X-rays and Neutrons
- G: X-ray Proportional counters for Mossbaur experiment
- H: 1-D Position Sensitive X-ray Detector



Detector development involves

- Design of detectors
- Machining of components
- Assembly of detector components
- Evacuation and gas filling
- Testing of detectors at reactor

Development of high efficiency high resolution position sensitive detectors



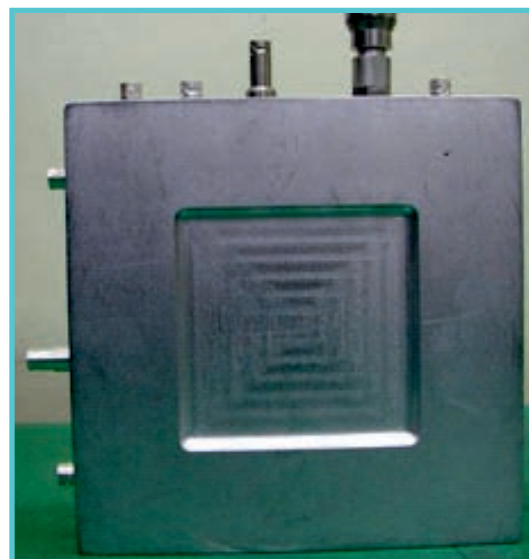
Comparison of neutron diffraction pattern recorded at Hi-Q Diffractometer using PSD with 3He with 4 bar and 10 bar fill pressure. The gain in intensity is evident.

High efficiency and high resolution position sensitive detectors (PSD) were developed successfully. Challenges like high pressure He3 filling and sealing are skillfully handled.

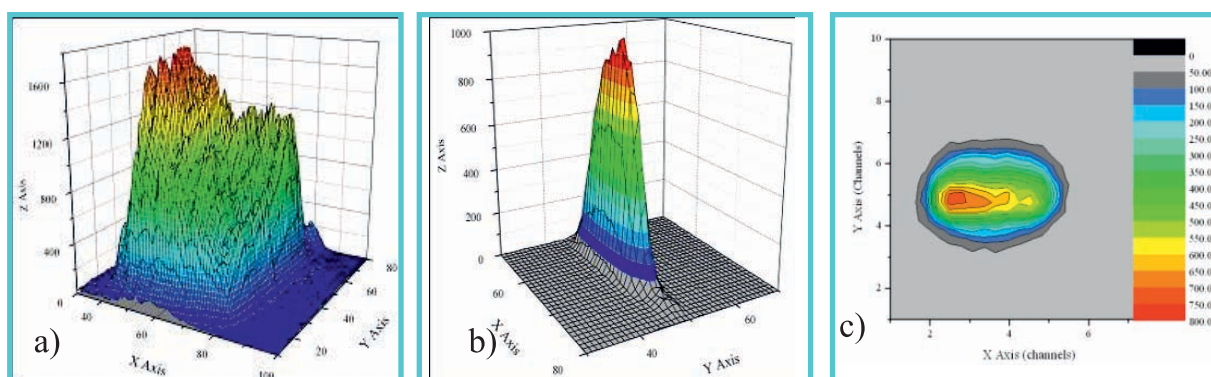
- 15 PSDs fabricated at high pressure (10 bar 3He + 2 bar Kr)
- All PSDs show identical operating parameter
- Position resolution: 4 mm and efficiency: ~90 %
- Hi-Q Diffractometer upgraded with these PSDs arranged in stack of 5 x 3 layers
- Efficiency gain with single PSD is 2.2
- Overall Efficiency gain ~6.5
- Experiment time reduced by same factor.

Neutron imaging beam monitor using delay line based position readout

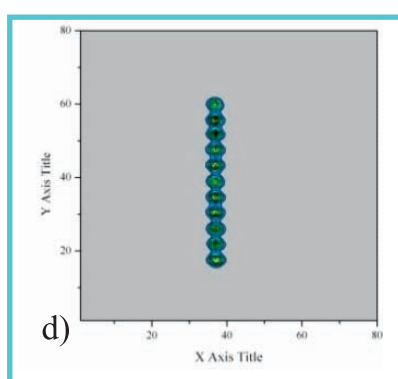
A multiwire based 2D position sensitive detector for beam imaging with sensitive area 10 cm x 10 cm and ^3He as fill gas is assembled and tested using in-house readout electronics. This is used for online monitoring of beam images and intensity profile of various neutron scattering spectrometers at Dhruva.



Delay line readout based neutron imaging beam monitor



Neutron beam images of various spectrometers at Dhruva



Linearity scan of the beam monitor using a neutron beam ~ 2 mm diameter and displacement of ~ 4 mm in Y-direction.

Selected Publications

1. S.S. Desai and Mala N. Rao, AIP Conf. Proc. 1447 (2012) 491
2. S.S. Desai, Shylaja Devan, and P S R Krishna, AIP Conf. Proc. 1349, (2011) 489
3. S.S. Desai and A.M. Shaikh, Rev. Sci. Instr. 78 (2007) 023304
4. S.S. Desai and A.M. Shaikh, Nucl. Instr. Meth. Phys. Res. A 557 (2006) 607
5. S.S. Desai and A.M. Shaikh, J. Neutron Research 14 (2006) 121

Contact Scientists

Location	Instrument	Persons Responsible	Office Address	Contact Ext. No.	Email ID
T1007	Triple Axis Spectrometer (TAS)	1. Mala N. Rao	R. No. 87, Dhruva	24604	mala@barc.gov.in
		2. R. Mittal	R. No. 45, CIRUS	24307	rmittal@barc.gov.in
T1009	Polarisation Neutron Spectrometer (PNS)	1. Amit Kumar	R. No. 87, Dhruva	24604	amitkr@barc.gov.in
		2. Anil Jain	R. No. 89, Dhruva	24306	ajain@barc.gov.in
T1011	Single Crystal Diffractometer (SCD)	1. R. Chitra	R. No. 307, CMPD	24623	rchitra@barc.gov.in
		2. Rajul Choudhury	R. No. 307, CMPD	24623	rajul@barc.gov.in
TT1015	Powder Diffractometer –1 (PD -1)	1. Anil Jain	R. No. 89, Dhruva	24306	ajain@barc.gov.in
		2. A.K. Rajarajan	R. No. 1 - 271S, Mod Lab	20427	rajuak@barc.gov.in
T1013	Powder Diffractometer –2 (PD -2)	1. Amitabh Das	R. No. 86, Dhruva	24292	adas@barc.gov.in
		2. P.S.R. Krishna	R. No. 89, Dhruva	24668	glass@barc.gov.in
TT1015	Powder Diffractometer –3 (PD -3)	1. V. Siruguri	R. No. 52, R5 - Shed	24930	siruguri@barc.gov.in
		2. R. Mukhopadhyay	R. No. 12, Dhruva	24667	mukhop@barc.gov.in
HS1017	Filter Detector Spectrometer (FDS)	1. S.K. Mishra	R. No. 89, Dhruva	24984	skmsspd@barc.gov.in
		2. Mala N. Rao	R. No. 87, Dhruva	24604	mala@barc.gov.in
HS 1019	High -Q Diffractometer (Hi -Q)	1. P.S.R. Krishna	R. No. 89, Dhruva	24306	glass@barc.gov.in
		2. Amitabh Das	R. No. 86, Dhruva	24292	adas@barc.gov.in
TT1004	Quasi -elastic Neutron Spectrometer (QENS)	1. S. Mitra	R. No. 86, Dhruva	24292	smitra@barc.gov.in
		2. V.K. Sharma	R. No. 87, Dhruva	24604	sharmavk@barc.gov.in
G1 -2	Polarised Neutron Reflectometer (PNR)	1. Surendra Singh	R. No. 87, Dhruva	24604	surendra@barc.gov.in
		2. D. Bhattacharya	R. No. 309, CMPD	24070	debarati@barc.gov.in
G1 -1	Small Angle Neutron Scattering Instrument (SANS - 1)	1. V.K. Aswal	R. No. 44, CIRUS	24642	vkaswal@barc.gov.in
		2. Sugam Kumar	R. No. 45, CIRUS	24307	sugam@barc.gov.in
G1 -3	Double Crystal based SANS Instrument (SANS - 2)	1. D. Sen	R. No. 44, CIRUS	24606	debasis@barc.gov.in
		2. J. Bahadur	R. No. 44, CIRUS	24606	jbahadur@barc.gov.in
G2	Multipurpose Test facility				

List of conversion factors used in neutron scattering

	kJ/mol	kcal/mol	meV	cm ⁻¹	rad/sec	Hz	K	Å	m/sec
kJ/mol	1	0.2388	10.36	83.58	1.574 x 10 ¹³	2.505 x 10 ¹²	120.3	2.810	1.408 x 10 ³
kcal/mol	4.187	1	43.39	345.0	6.591 x 10 ¹³	1.049 x 10 ¹³	503.3	1.373	2.881 x 10 ³
meV	0.097	0.0230	1	8.006	1.519 x 10 ¹²	2.418 x 10 ¹¹	11.605	9.045	437.4
cm ⁻¹	1.196 x 10 ⁻²	2.858 x 10 ⁻³	0.124	1	1.884 x 10 ¹¹	2.98 x 10 ¹⁰	1.439	25.68	154.05
rad/sec	6.351 x 10 ⁻¹⁴	1.517 x 10 ⁻¹⁴	6.582 x 10 ⁻¹³	5.309 x 10 ⁻¹²	1	0.159	7.640 x 10 ⁻¹²	1.115 x 10 ⁻⁷	3.547 x 10 ⁻⁴
Hz	3.991 x 10 ⁻¹³	9.536 x 10 ⁻¹⁴	4.136 x 10 ⁻¹²	3.336 x 10 ⁻¹¹	6.238	1	4.800 x 10 ⁻¹¹	4.447 x 10 ⁻⁶	8.895 x 10 ⁻⁴
K	8.314 x 10 ⁻³	1.986 x 10 ⁻³	8.616 x 10 ⁻²	0.695	1.309 x 10 ¹¹	2.083 x 10 ¹⁰	1	30.81	128.4
Å	7.894	1.885	81.807	659.8	1.243 x 10 ¹⁴	1.978 x 10 ¹³	949.4	1	3.956 x 10 ³
m/sec	5.044 x 10 ⁻⁷	1.202 x 10 ⁻⁷	5.227 x 10 ⁻⁶	4.216 x 10 ⁻⁵	7.948 x 10 ⁶	1.265 x 10 ⁶	6.066 x 10 ⁻⁵	3.956 x 10 ⁻³	1

Quantity	Symbol	Unit
Energy	E	kJ, kcal, meV
Optical wave vector	ν/c	cm ⁻¹
Cycles	ω	rad/sec $E = h\omega$
Frequency	ν	Hz $\nu = \omega/2\pi$
Temperature	T	K $E = k_B T$
Wavelength	λ	Å $E = h^2/(2m\lambda^2)$
Velocity	v	m/sec $E = mv^2/2$

$$h = h/2\pi \quad h = 6.616 \times 10^{-34} \text{ J sec} \quad m = 1.675 \times 10^{-27} \text{ kg}$$

Sample Environment Facilities

Low Temperature	:	CCR- 1.5 - 300 K
High Temperature	:	Furnace: 300-2000 K
High Pressure Apparatus	:	A piston-cylinder type high-pressure cell with pressure range up to 25 kbar.
Magnetic Field	:	12 kOe at Room Temperature 1.5 kOe and 2 kOe in vertical and horizontal direction With CCR up to 7 Tesla and T=1.5 to 300 K

For further information about facilities and proposals for experiments contact**Dr. R. Mukhopadhyay**

Head, Solid State Physics Division

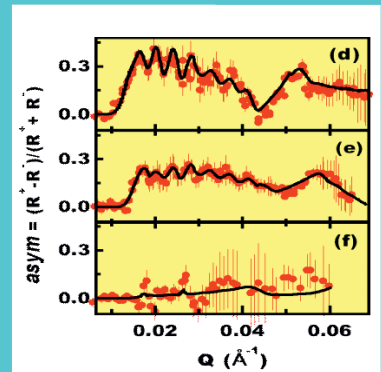
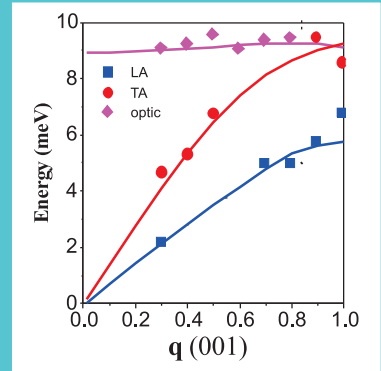
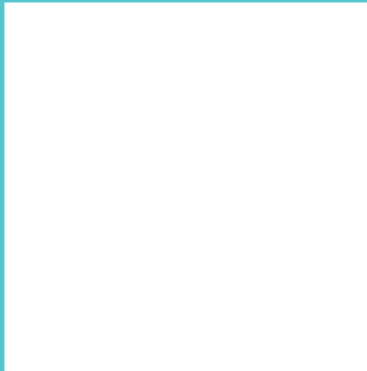
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