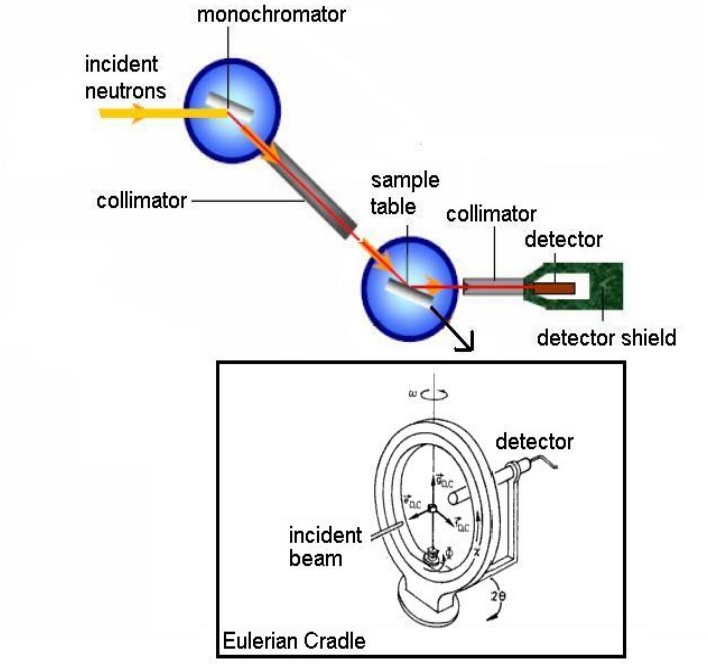
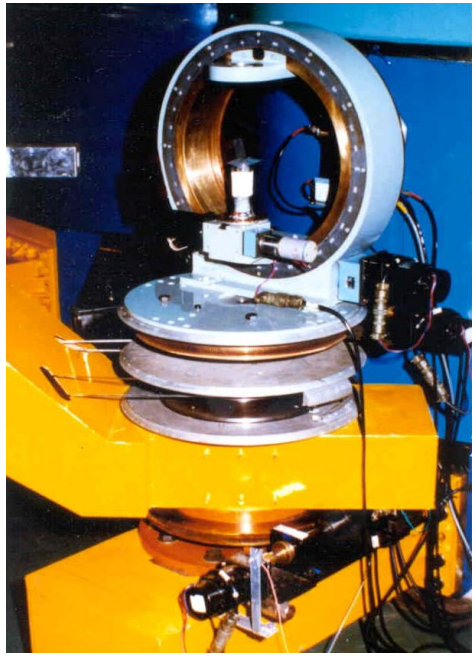
Single crystal neutron diffractometer

The four circle diffractometer is located at T1011 beam line of the Dhruva reactor. In a four circle diffractometer, 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 diffractometer. 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.





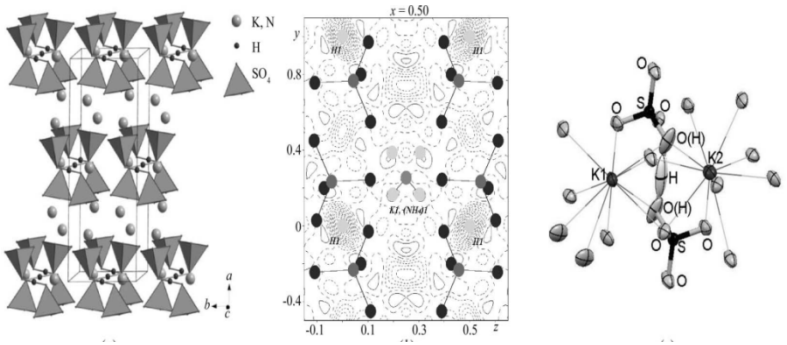
Description of the instrument

Four Circle Eulerian geometry
Monochromator: Cu220
Wavelength :0.995Å
Flux at the sample: 5×10^5 n/cm^2/sec
Detector: BF_3 counter
Computer controlled data collection

Contact Scientists: rchitra@barc.gov.in
rajul@barc.gov.in

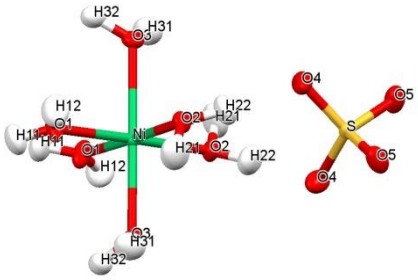
DST–RFBR project sponsored by DST

A) Proton Conductors: electrolytes in fuel cell



- Single crystals neutron diffraction investigation On (K0.9(NH4) 0.1)3H(SO4)2 were conducted at Dhruva
- A correlation between the kinetics of the Hydrogen Bond strength and kinetics of the superionic phase transition could be established

B) α-Nickel sulphate hexahydrate crystals:

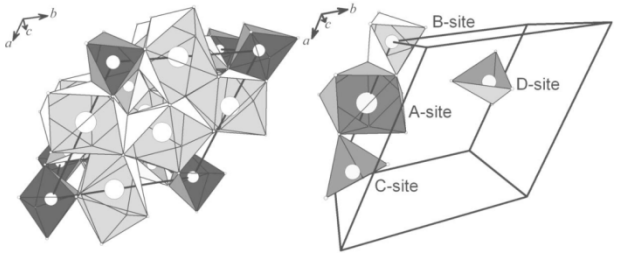


•Single crystals of α-NSH (α-Nickel sulphate hexahydrate) were grown from two different aqueous solution one of them containing an excess of sulphuric acid (H_2SO_4).

•Single crystal neutron diffraction were performed on both the crystals.

•The structural data showed subtle difference in the SO_4 geometry and also the intramolecular separation between the $(SO_4)^{2-}$ and $[Ni(H_2O)_6]^{2+}$ ions of NSH molecule. This difference in geomerty was found due to the solvent effect altering the solvent properties of water leading to the fine tuning of interionic interaction between $(SO_4)^{2-}$ and $[Ni(H_2O)_6]^{2+}$ ions in solutions phase and this feature is carried over in crystalline phase.

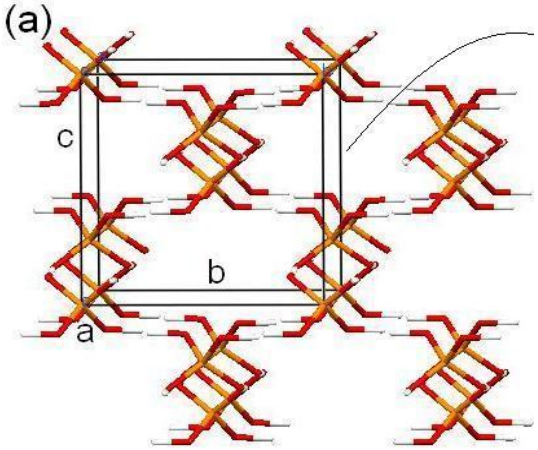
C) Piezoelectrics langasite family



The crystal structures of LGS, LGT, LGST and LGZrT crystals were obtained from single-crystal neutron diffraction

It was shown that significant change in the D site affects the orientation of the A site along the [100] direction leading to a change in the piezoelectric property

Hydrogen bonded NLO crystals



network of H-bonded chains of anions $H_2PO_4^-$

- NH4+ ion has a dual behaviour; it has a hydrogen bonding tendency as well as a pseudo-alkali character.
- The N–H–O hydrogen bond strength determines which of these two tendencies of the NH4+ ion dominates in a given structure

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The Changes of Thermal, Dielectric, and Optical Properties at Insertion of Small Concentrations of Ammonium to $K_3H(SO_4)_2$ Crystals , Selezneva, E.V., Makarova, I.P., Grebenev, V.V.,Chitra, R., Choudhury, R.R.Crystallography Reports,63(4), pp. 553-562, 2018

A single crystal neutron diffraction study on mixed crystal $(K)_{0.25}(NH_4)_{0.75}H_2PO_4$: tuning of short strong hydrogen bonds by ionic interactions,Choudhury, R.R., Chitra, R.Bulletin of Materials Science 41(1),8, 2018

Effect of cationic substitution on the double-well hydrogen-bond potential in $[K_{1-x}(NH_4)x]_3H(SO_4)_2$ proton conductors: A single-crystal neutron diffraction study,Choudhury, R.R., Chitra, R., Selezneva, E.V., Makarova, I.P.
Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 73, pp. 863-867. 2017