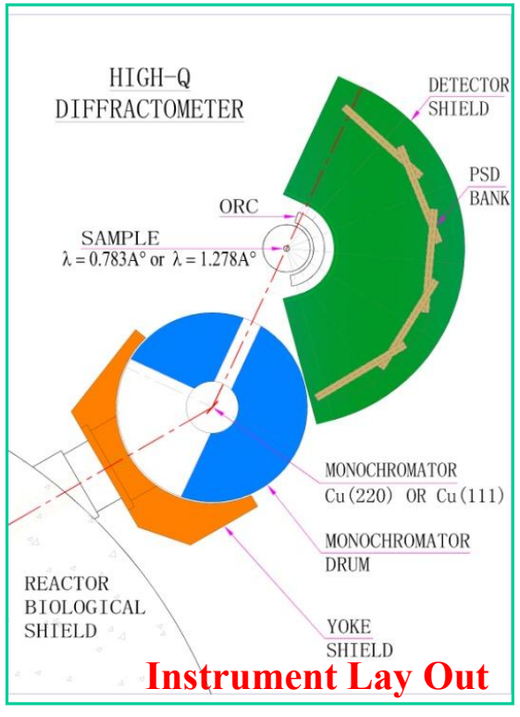
High-Q Diffractometer



Instrument Lay Out

Instrument Details	
Beam Hole	HS - 1019
Monochromator	Cu (220): λ = 0.783 Å Cu (111): λ = 1.278 Å
Flux at sample (n/cm²/sec)	2 ×10⁶ (λ = 1.278 Å) 3 ×10⁵ (λ = 0.783 Å)
Sample size	40 mm high & 5-10 mm dia
Scattering angle	3° < 2θ < 140°
Detector	10 (1-d PSDs) at 5 positions
Q range	0.3 – 15 Å^{-1}
ΔQ/Q	2.5 %

High-Q diffractometer is used to extract short and intermediate range order from:

- Various types of glasses
- Molecular Liquids
- Disordered crystals (local structure)
- High pressure structural phase transistions

Future plans:

It is currently under upgradation to have various resolution and throughput options

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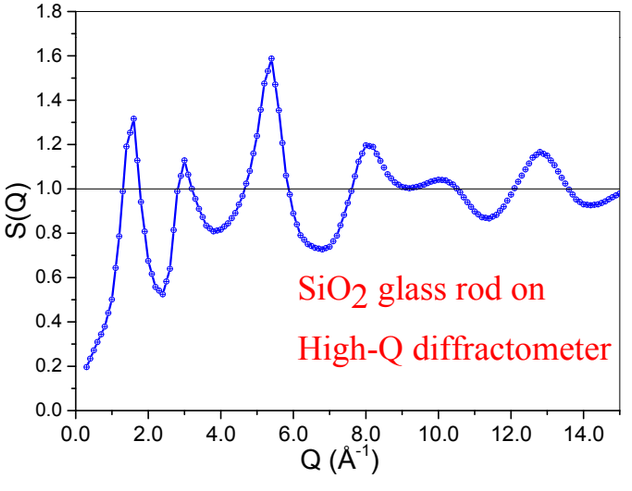

Sample Environment Available:

CCR (4 K – 300 K)
CCR (20 K – 450 K)
Furnace (300 K – 1400 K)
Pressure (10^{-4} GPa – 2.5 Gpa)

Defect topology and annihilation by cooperative movement of atoms in neutron-irradiated graphite

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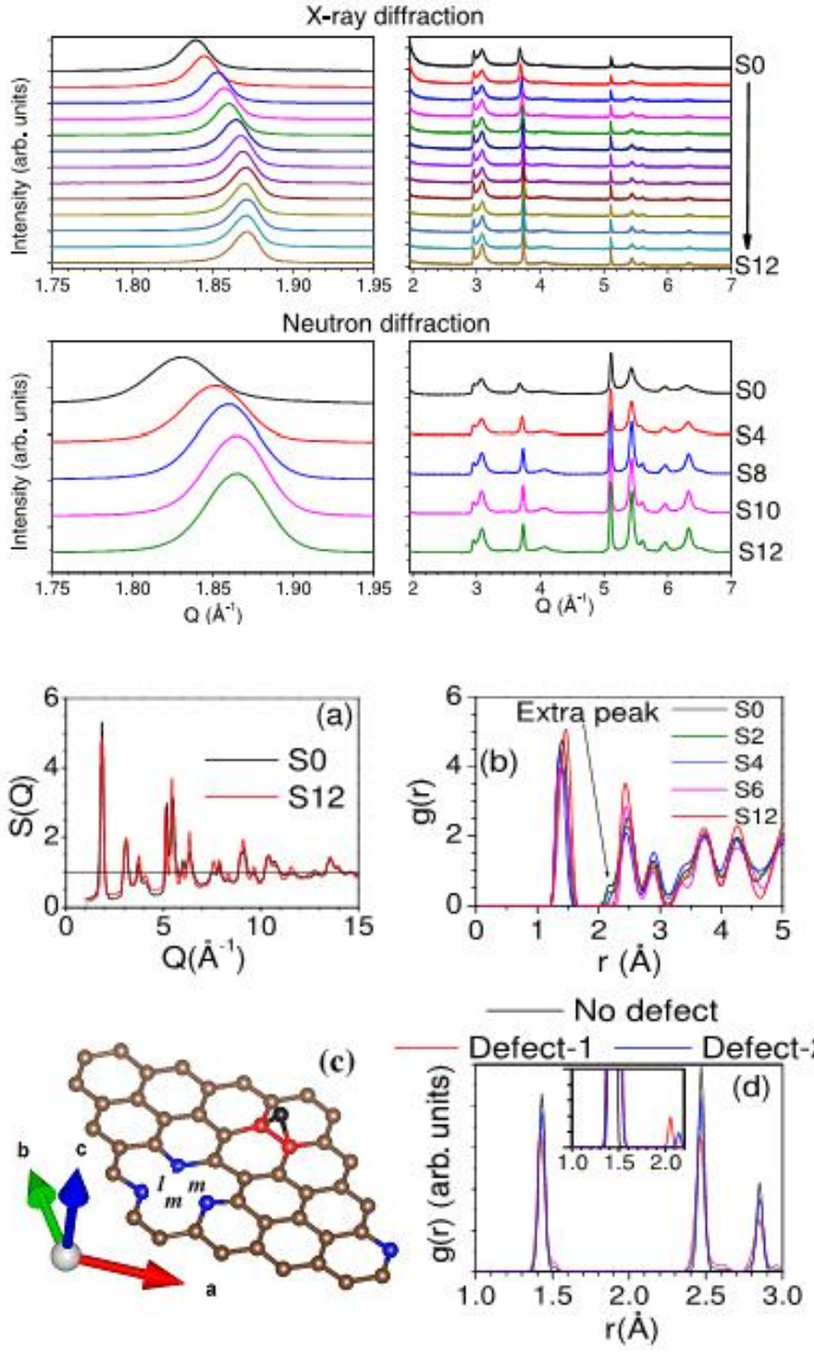
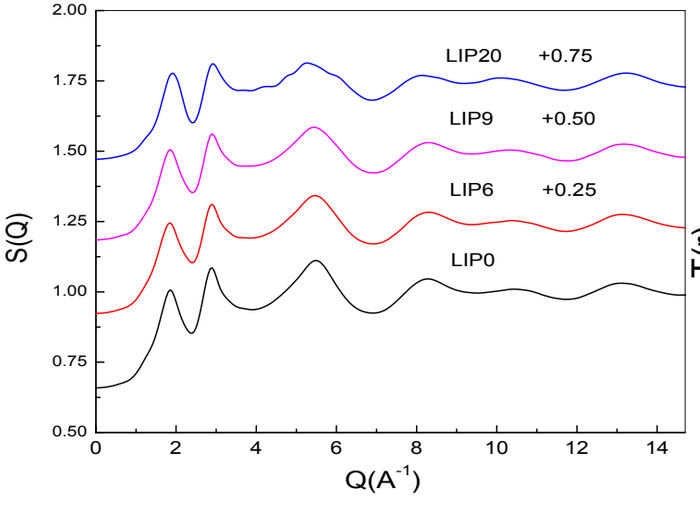
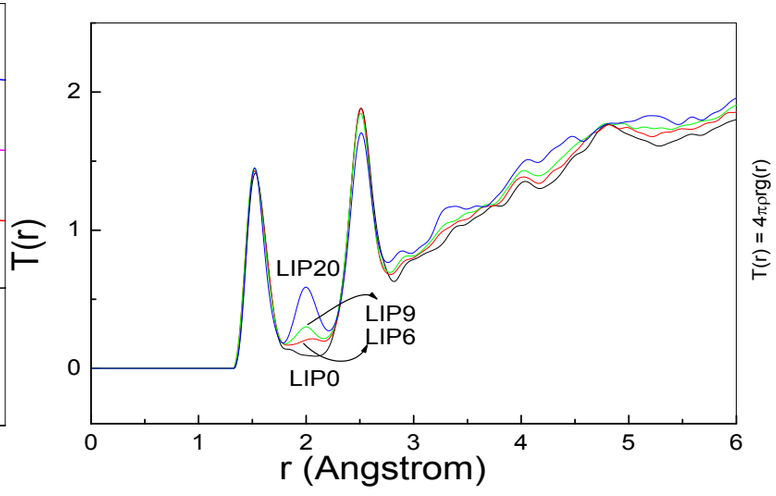
Graphite has been used as a neutron moderator or reflector in many nuclear reactors. The irradiation of graphite in a nuclear reactor results in a complex population of defects. Heating of the irradiated graphite at high temperatures results in annihilation of the defects with release of an unusually large energy, called the Wigner energy. From various experiments on highly irradiated graphite samples from the CIRUS reactor at Trombay and *ab initio* simulations, we have identified various 2-, 3-, and 4-coordinated topological structures in defected graphite, and provided a microscopic mechanism of defect annihilation on heating and release of the Wigner energy. The annihilation process involves cascading cooperative movement of atoms in multiple steps involving an intermediate structure. Our work provides insights in understanding of the defect topologies and annihilation in graphite which is of considerable importance to wider areas of graphitic materials including graphene and carbon nanotubes.

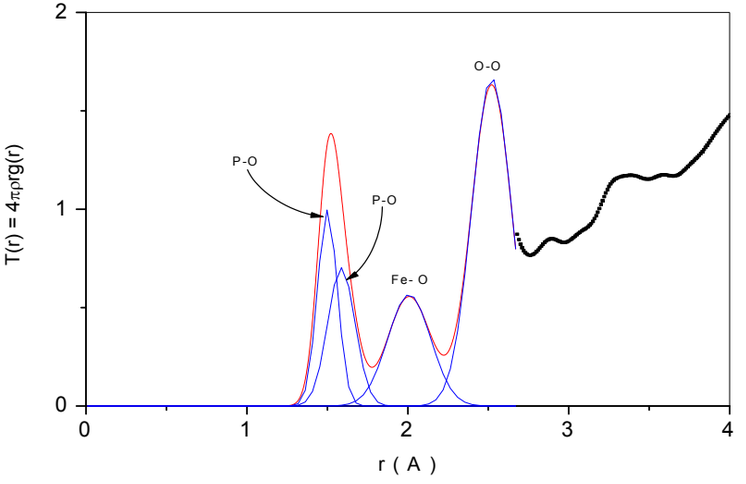
Sample No.	Radial distance (cm)	Thermal neutrons ($\times 10^{20}$ neutrons/cm^2) ($E < 0.625$ eV)	Epithermal neutrons ($\times 10^{19}$ neutrons/cm^2) (0.625 eV $< E <$ 0.82 MeV)	Fast neutrons ($\times 10^{18}$neutrons/cm^2) ($E >$ 0.82 MeV)	Displacement per atom (dpa) ($\times 10^{-3}$)
S0	0	22.06	37.69	19.99	64.5
S1	5	20.37	25.12	13.17	42.9
S2	10	18.53	16.46	8.50	28.0
S3	15	16.62	10.49	5.29	17.7
S4	20	15.09	7.38	3.70	12.5
S5	30	12.94	4.30	2.03	7.2
S6	40	10.11	1.72	0.084	2.4
S7	50	7.58	0.67	0.034	0.9
S8	60	5.38	0.29	0.016	0.4
S9	70	3.44	0.08	0.0063	0.1
S10	80	1.71	0.05	0.0033	0.07
S11	90	0.75	0.03	0.0013	0.04



Structure of (1-x)($PbO-P_2O_5$)- x(Fe_2O_3) glasses – Candidates for radioactive waste loading







These glasses are candidates for Radioactive waste loading as they offer 4 orders of magnitude higher leaching resistance to the conventional borosilicate glasses.

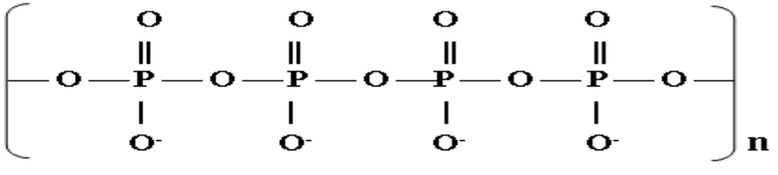


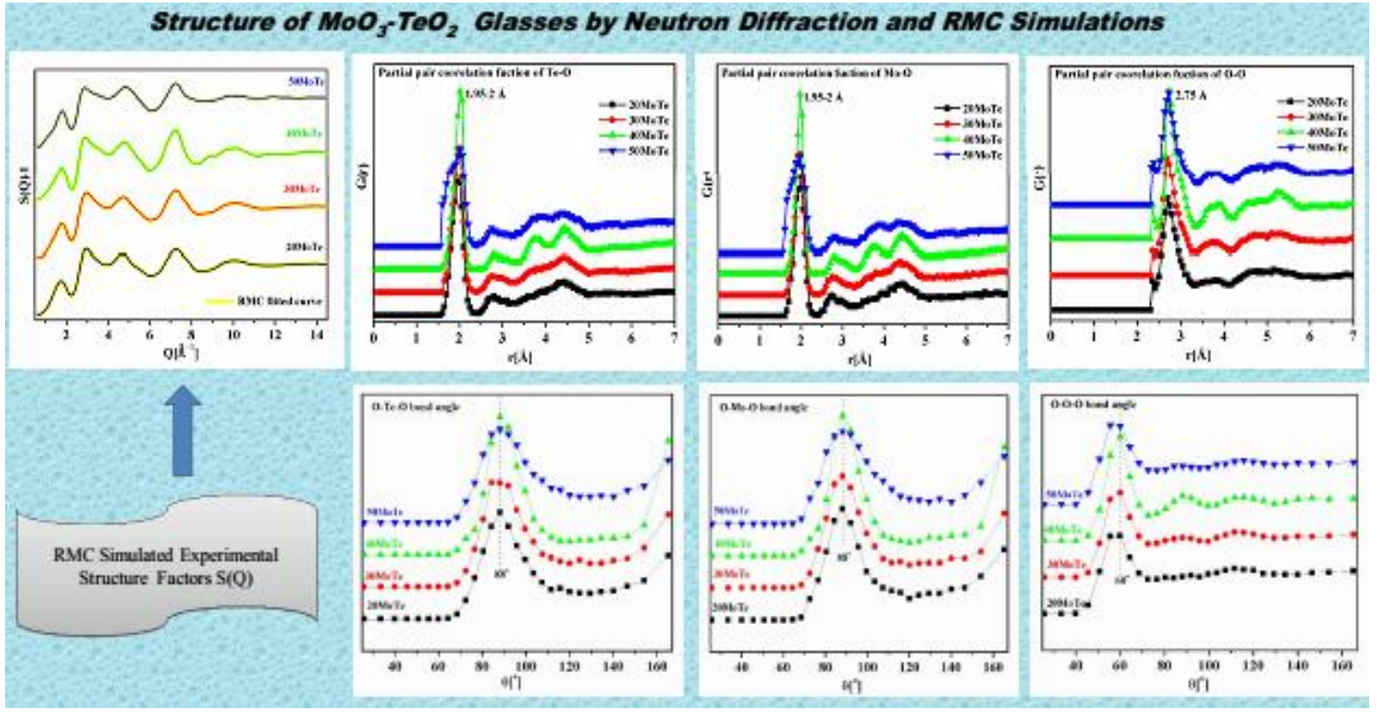
Figure. 1.1: Linear structure of polyphosphate

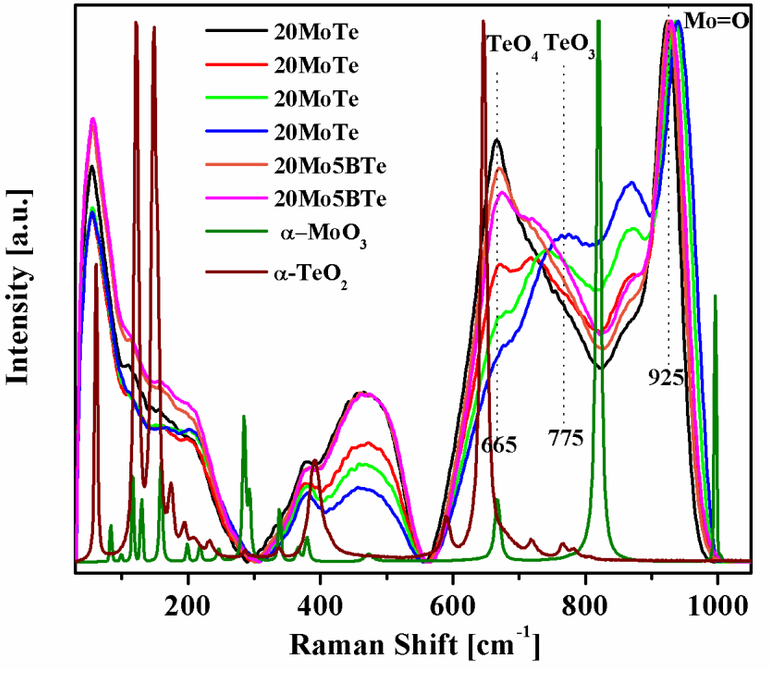
Key findings:

- **PO_4 tetrahedra are the basic building blocks**
- **Fe-O co-ordination is 5.75 to 5.95 (ionic bond)**
- **Fe helps in cross linking the poly phosphate chains**
- **Increasing Fe content makes the whole network connected in a 3D network compared to 1D chains increasing the structural rigidity and improving the mechanical & leaching properties.**

Sourabh Wajhal, P.S.R. Krishna & A.B. Shinde (2020)

Structure-Property Correlations in Molybdenum Tellurite glasses by Neutron Diffraction

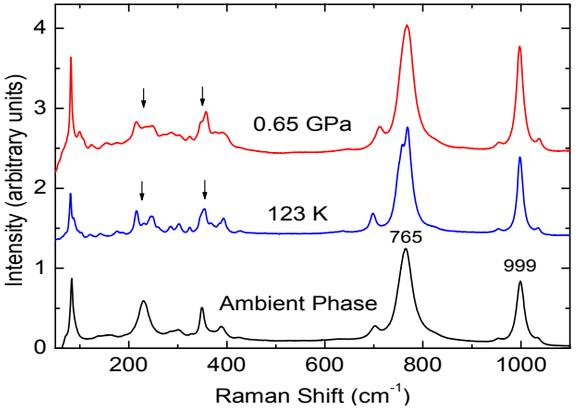




- Density decreases from 5.251 to 4.994 g cm^{-3} with increase in MoO_3 mol% due to the replacements of heavier TeO_2 (159.60 u) with lighter MoO_3 (143.5 u).
- Glass transition temperature decreases from 323°C to 309°C with increase in MoO_3 content from 20 to 50 mol%. The addition of B_2O_3 enhances T_g due to higher bond enthalpy of B-O compared to Te-O linkages.
- Raman spectroscopy indicate the structural transformation: TeO_4 → TeO_3 .
- RMC simulations confirm the existence of MoO_4 and TeO_4 units with significant concentrations of penta- and hexa-Te-O and Mo-O structural units.
- Bond angle distribution functions for O-Te-O and O-Mo-O linkages have a maxima at ~90°.

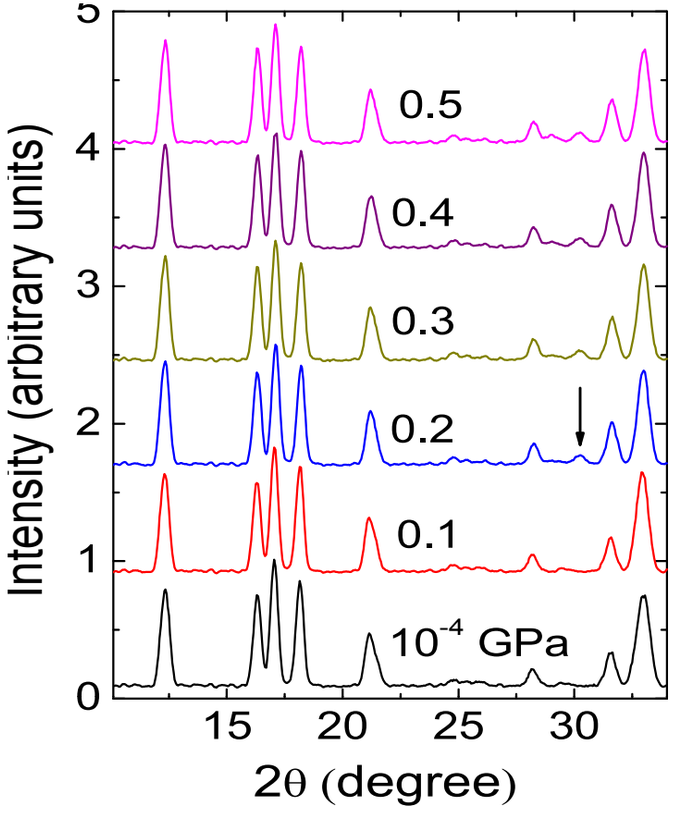
***Mater. Res. Express 6, 075211*, [2019]**

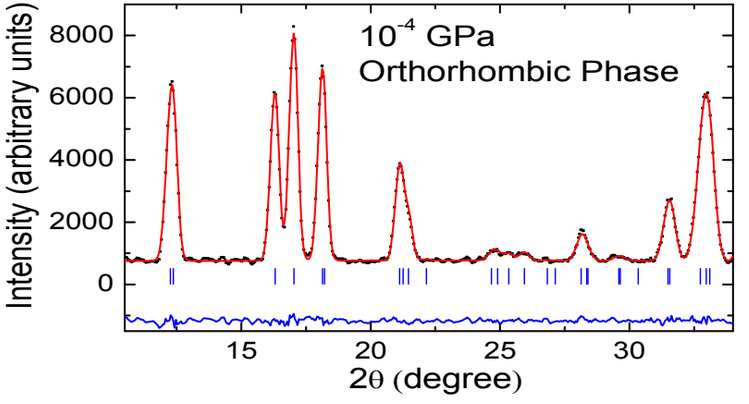
High Pressure Phase Transition Studies in $TaVO_5$

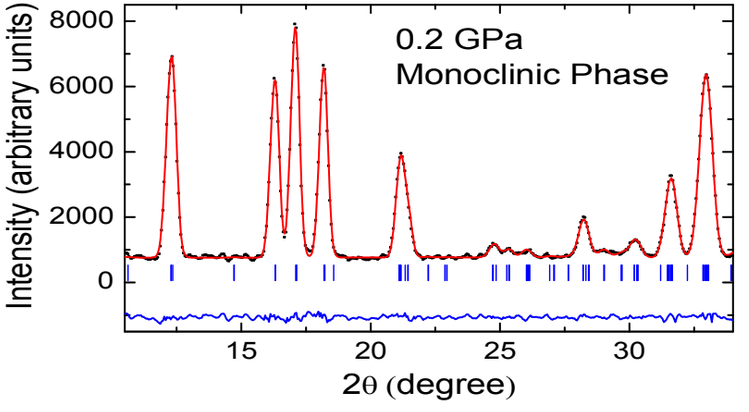


Refined unit cell parameters and residuals observed in Rietveld refinements.
At ambient pressure,
space group *Pnma*
a = 11.856(2) Å, b = 5.5110(9) Å
c = 6.632(1) Å

At 0.2 GPa,
space group $P2_1/c$
a = 13.7404 Å, b = 5.4928 Å
c = 13.8141 Å, β = 120.127°







The data obtained before the first Bragg peak of the pressure cell is used for presentation and Rietveld analysis. Essentially the contribution in this 2θ range is from the sample only.

***Inorganic Chemistry, 57, 6973-6980*, [2018]**