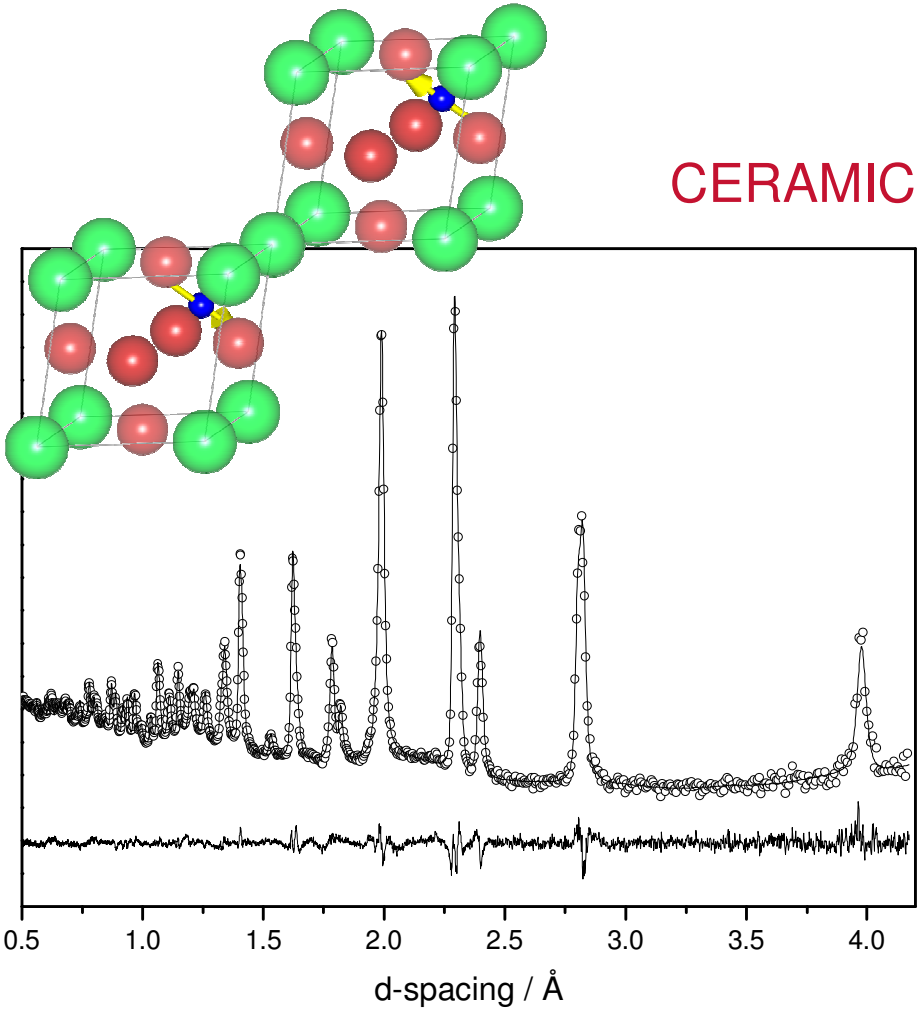
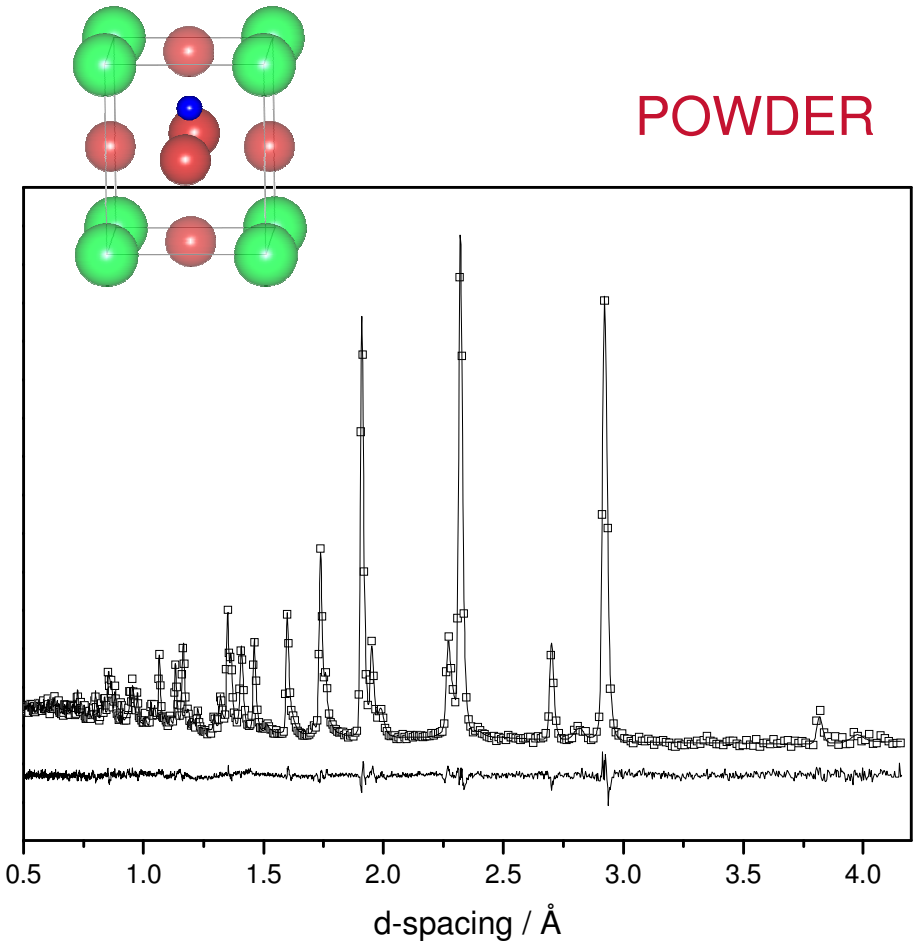
Stress state affects phase

UNIVERSITY OF LEEDS

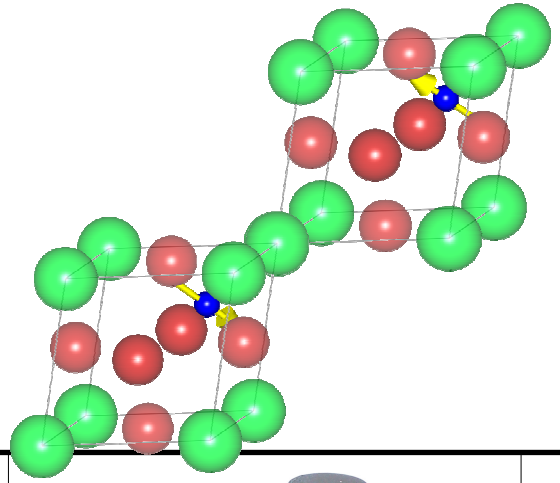
Two fabrication methods induce radical change in crystallography

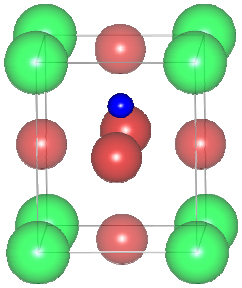




Stress state affects phase

UNIVERSITY OF LEEDS

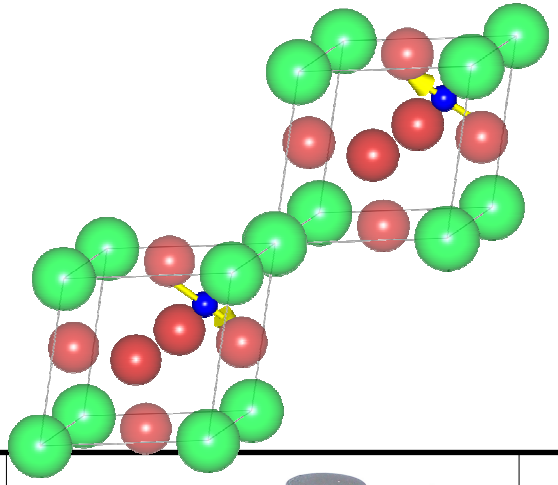


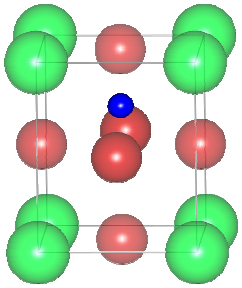


Form	Bulk 		Powder 	
Phase	R3c	P4mm	R3c	P4mm
Phase fraction	0.876	0.124	0.084	0.916
Moment per Fe^{3+}/ μ_B	3.234 ± 0.02	0	0	0
(c-a)/a (P4mm) / %		3.1		18.9
Primitive unit cell volume / 10^{-30} $Å^3$	62.74	63.24	62.50	65.88

Phase transformation ???

UNIVERSITY OF LEEDS





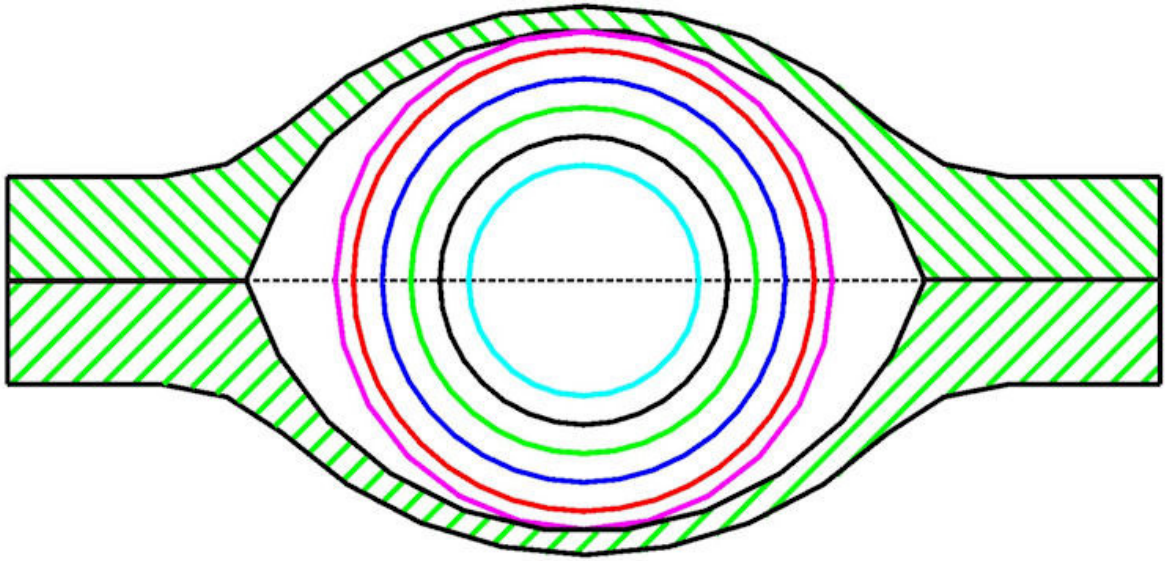
Form	Bulk 		Powder 	
Phase	R3c	P4mm	R3c	P4mm
Primitive unit cell volume / 10^{-30} Å^3			62.50	65.88

Direct Measurements – PEARL

UNIVERSITY OF LEEDS

Powder sample placed within tungsten carbide gaskets

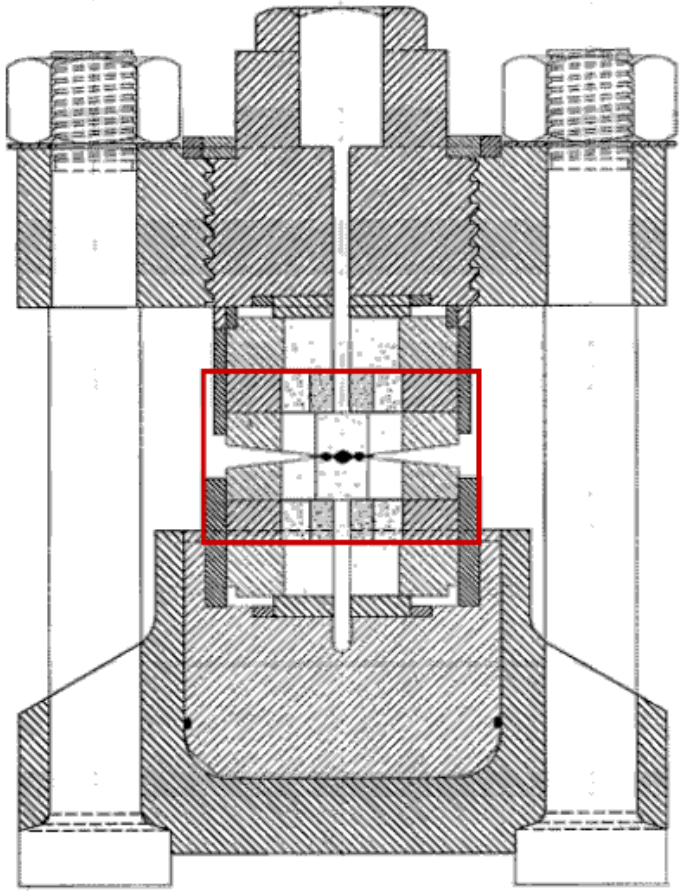
- Max diameter 4.3 mm
- Metallic lead sphere used as pressure marker
- Deuterated methanol/ethanol used as pressure medium

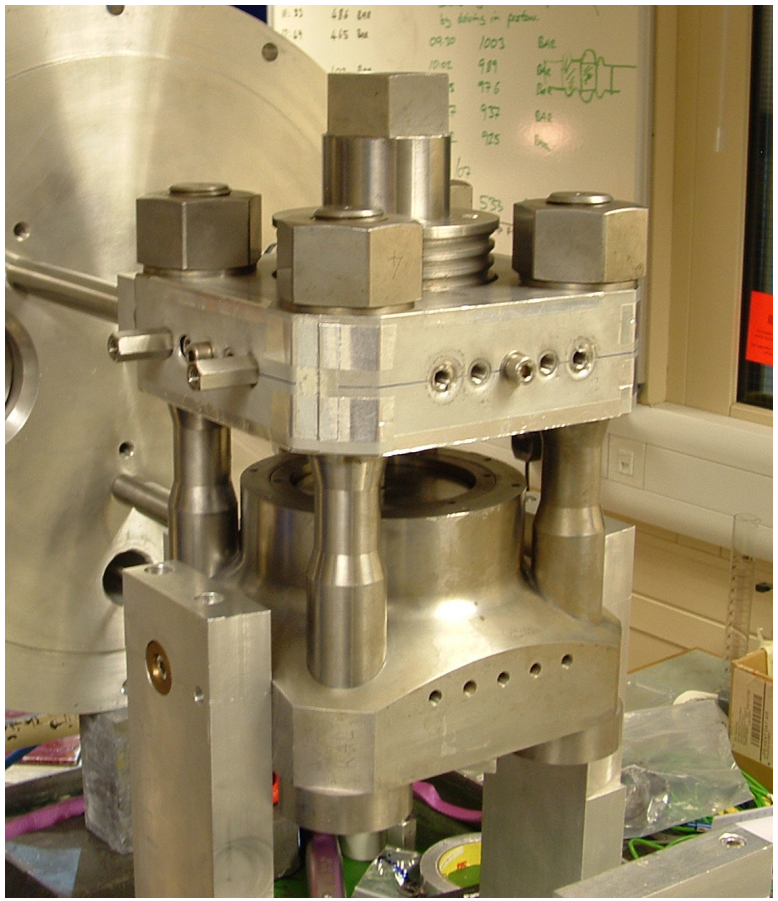


Experimental set-up

UNIVERSITY OF LEEDS

Gasket assembly loaded into Paris Edinburgh Cell

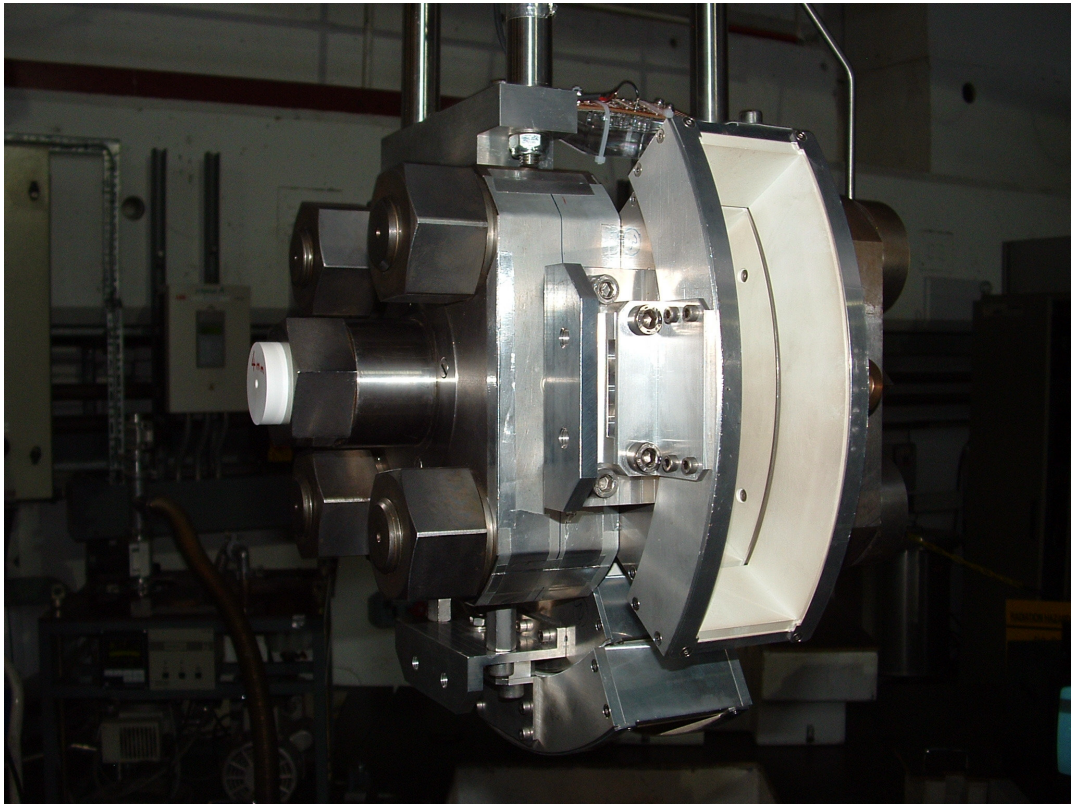




Experimental set-up

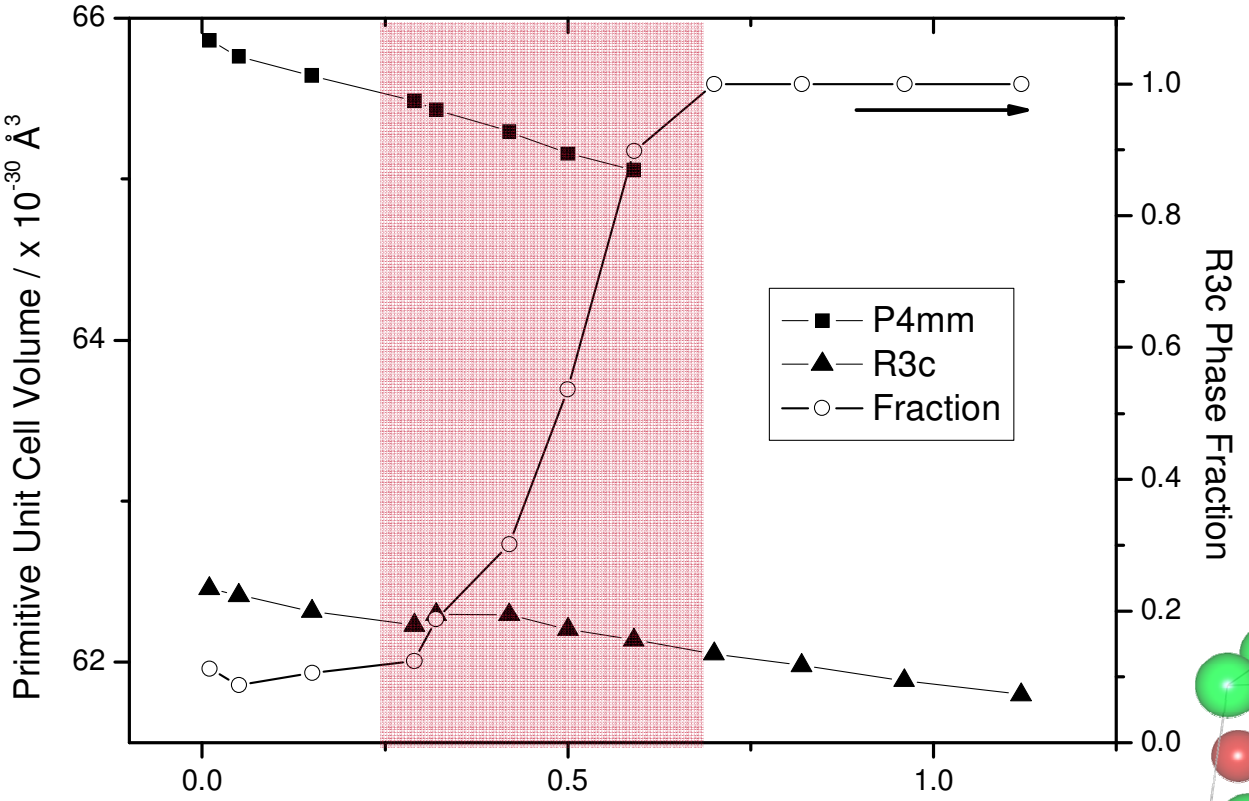
UNIVERSITY OF LEEDS

Pressure cell loaded into shield assembly and craned into neutron beamline

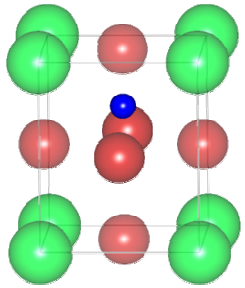


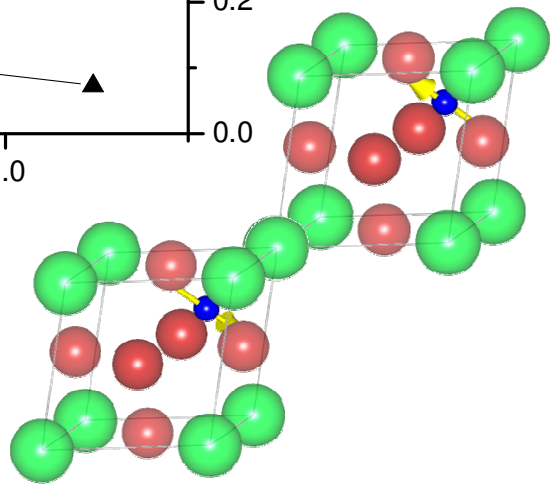
Direct Measurements - Results

UNIVERSITY OF LEEDS



Paramagnetic
Tet, P4mm



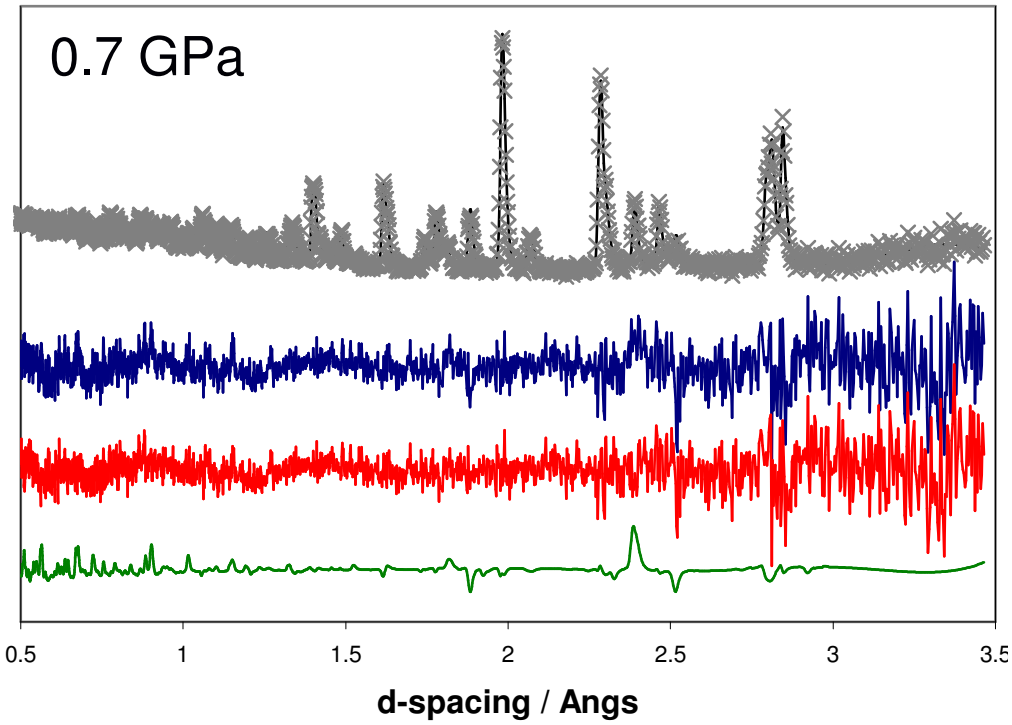


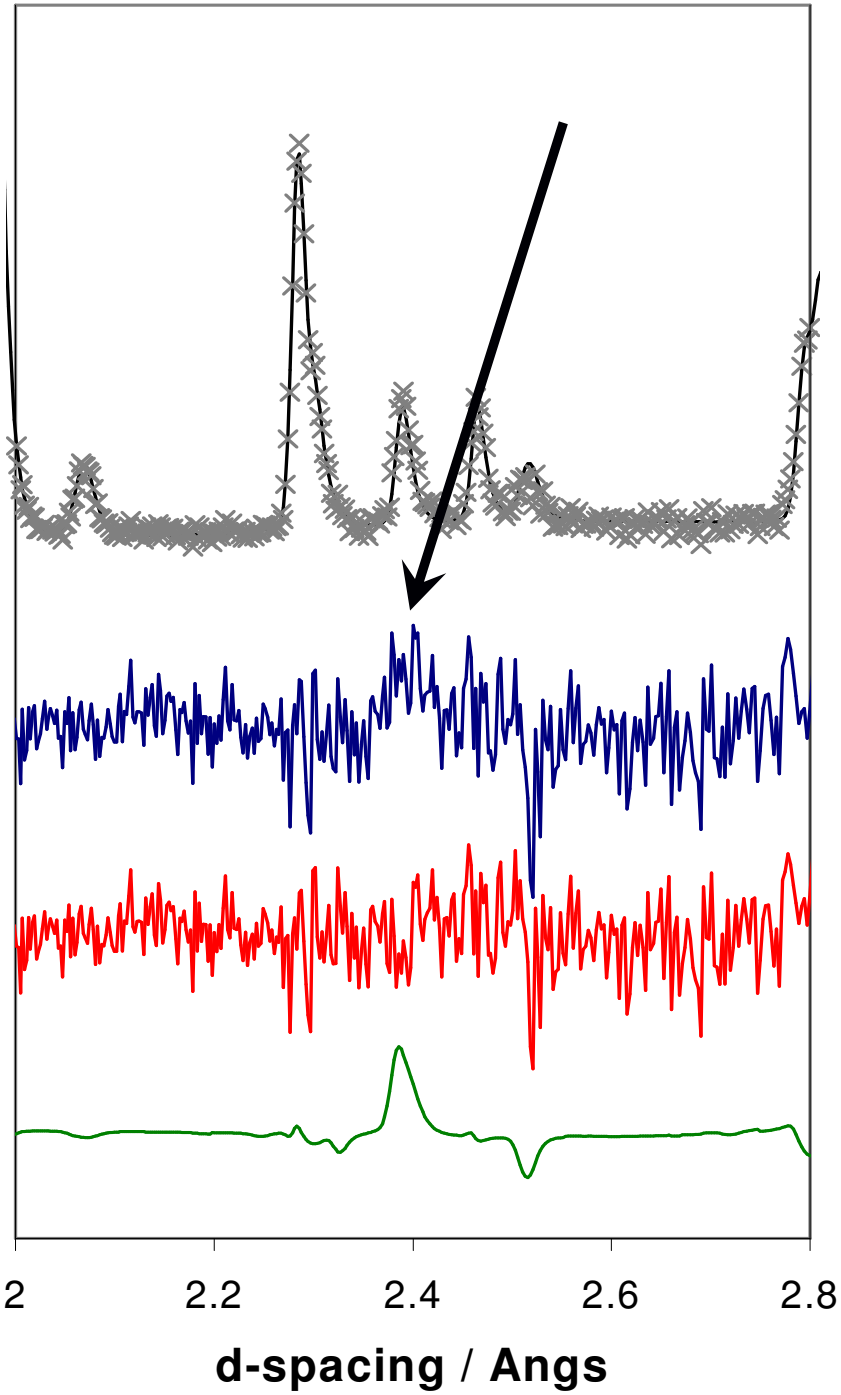
Antiferromagnetic
Rhom, R3c

Effect of pressure
PEARL

Evidence that transforming phase turns on magnetic ordering at ca. 0.4 GPa

- R3c magnetic with Fe mag. ca. 3 μ_B above 0.4 GPa





Why is tet. phase not magnetic??

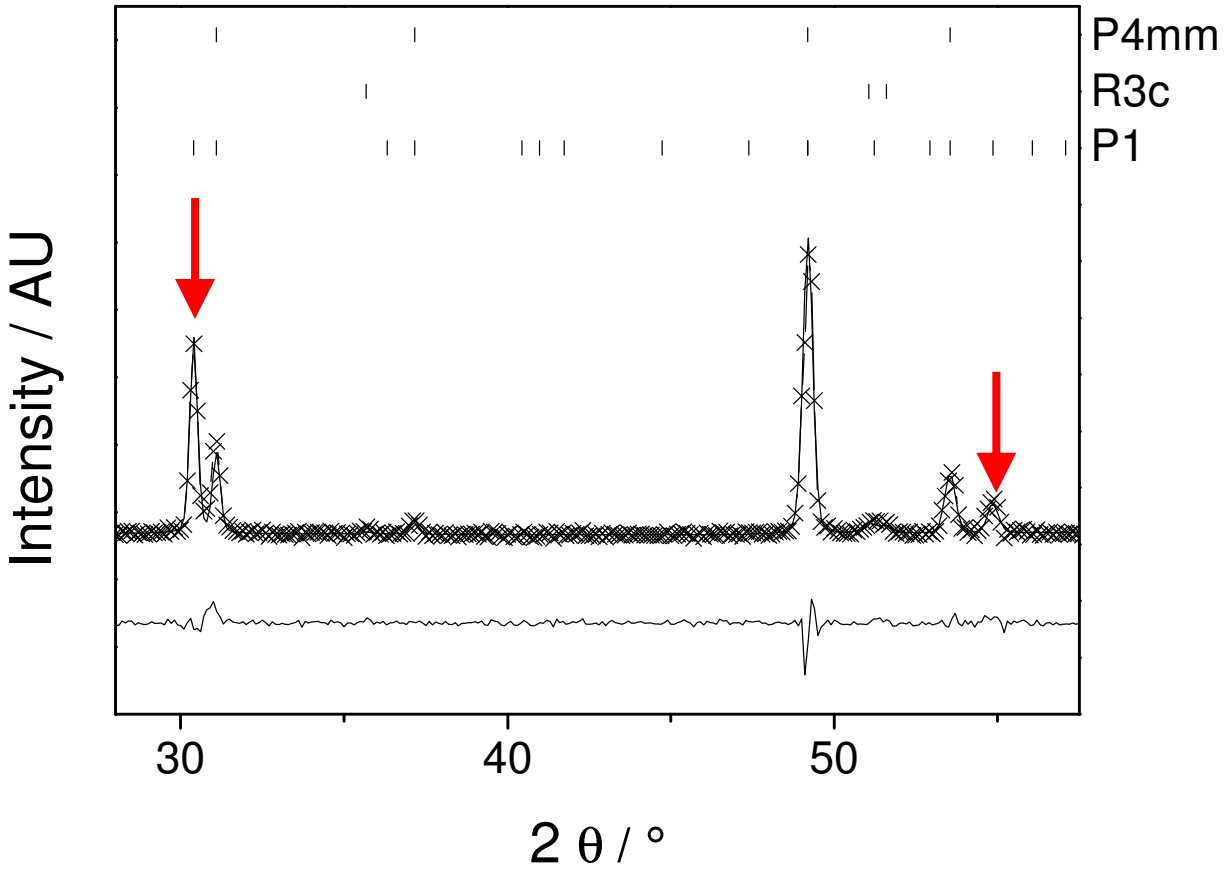
UNIVERSITY OF LEEDS

Why is tet. phase not magnetic??

UNIVERSITY OF LEEDS

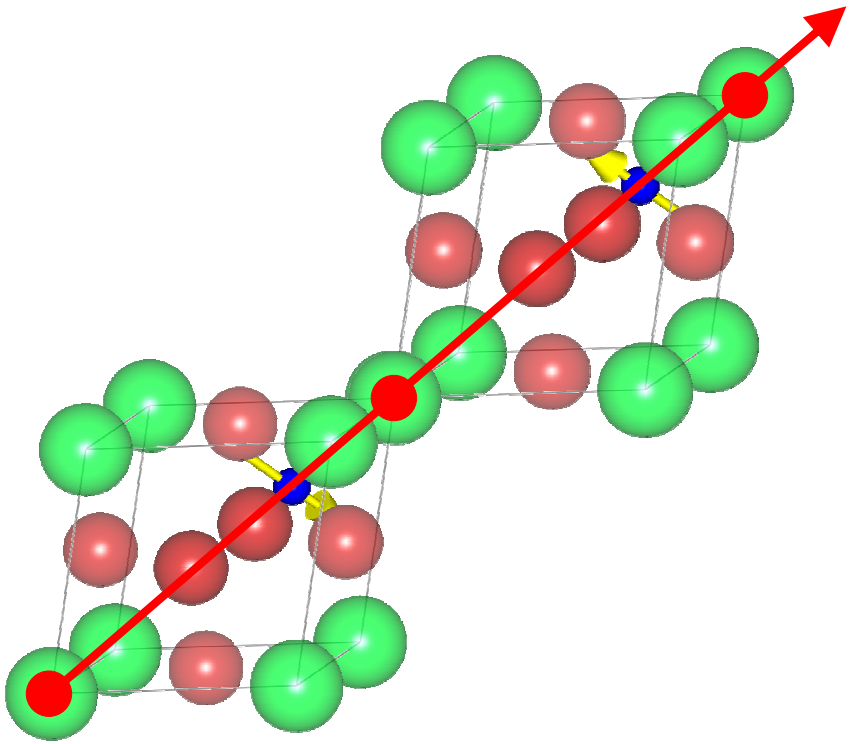
It is – but not at room temperature

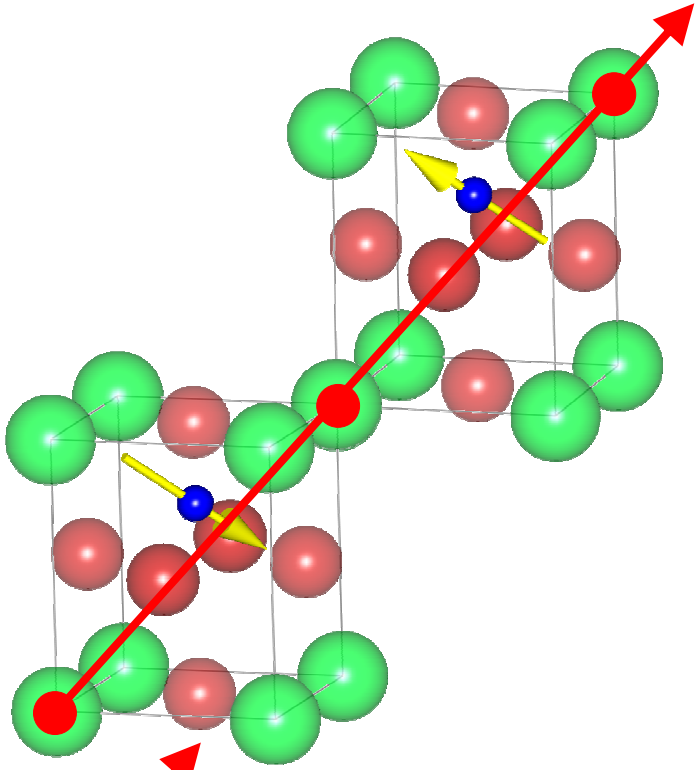
- Neutron diffraction measurements at 4 K



Magnetic and nuclear structures

UNIVERSITY OF LEEDS





Rhombohedral, R3c

T_N = 540 K

Magnetic order

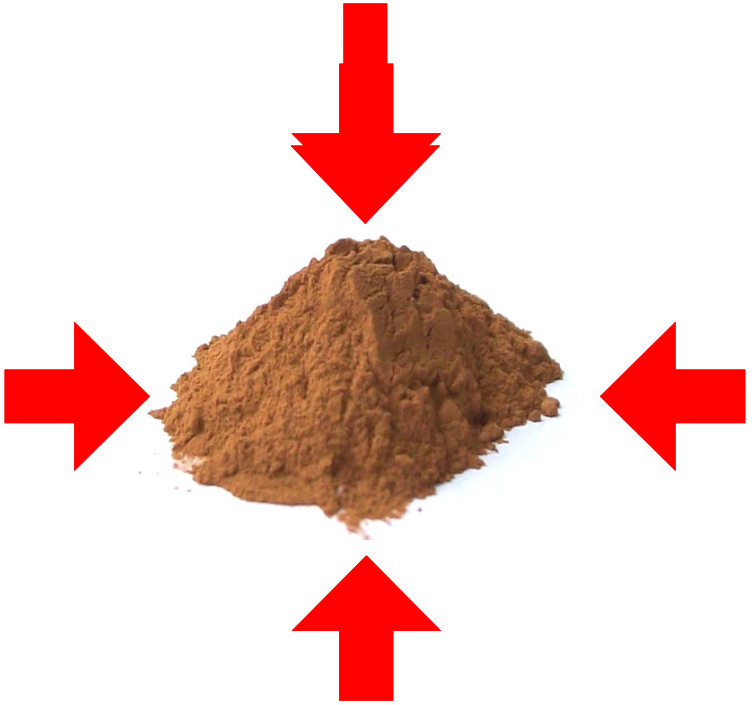
Electric order

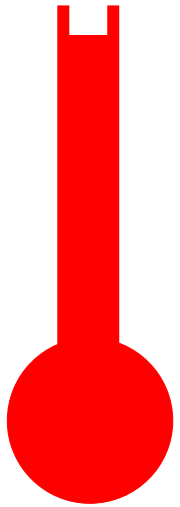
Tetragonal, P4mm

T_N = 220 K

Conclusions

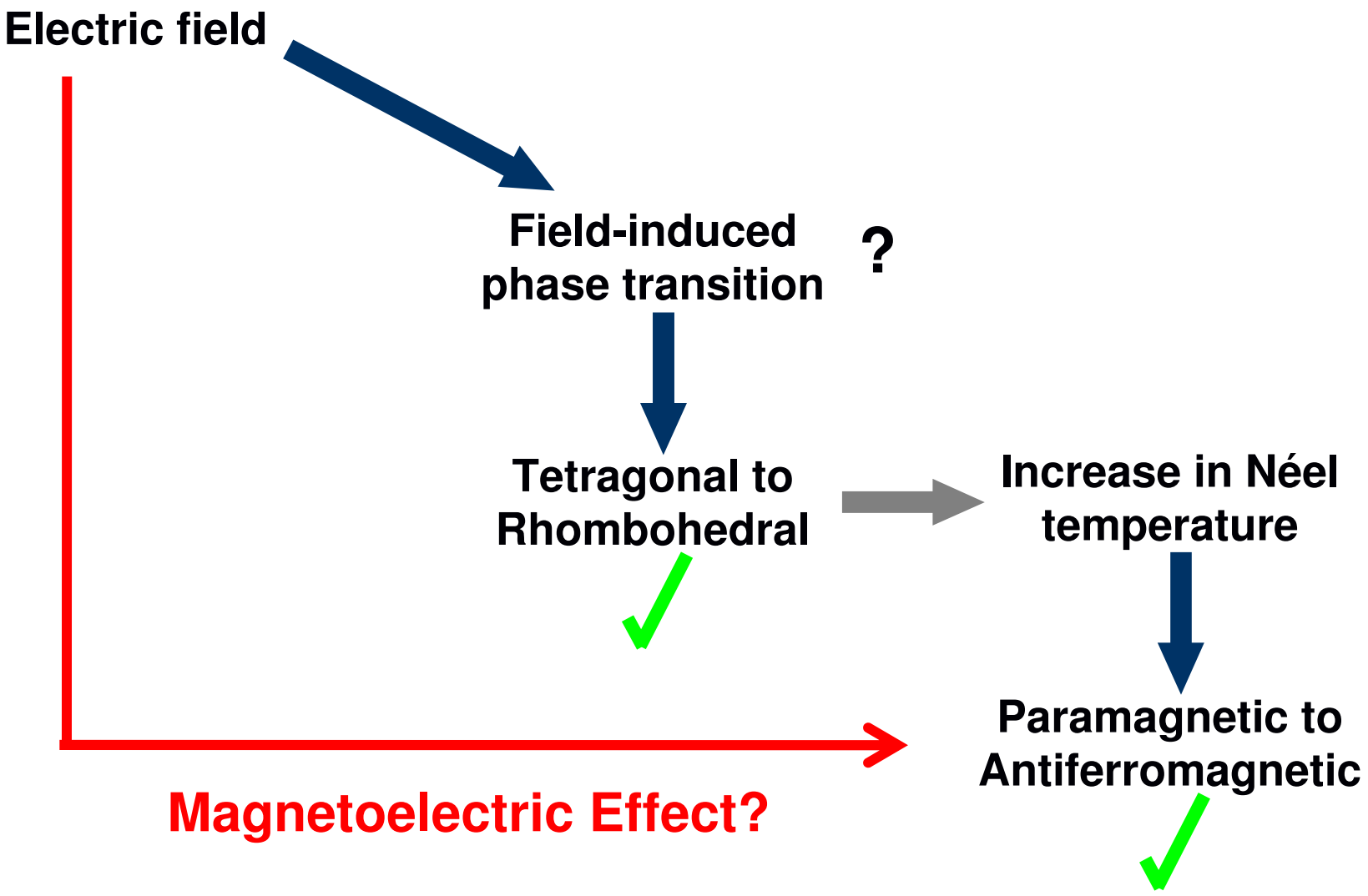
UNIVERSITY OF LEEDS





What next

UNIVERSITY OF LEEDS



Upcoming experiments

UNIVERSITY OF LEEDS

In-situ hydrostatic pressure experiments – PEARL, ISIS, UK

- Reversibility
- Wider d-space range – better magnetic refinement
- Finer steps in applied pressure

Effect of electric field on magnetic ordering – HMI, Berlin

- Apply electric field in situ with polycrystalline materials