

**Experiment title:**Local structure and structural coherence across phase transitions in multiferroic hexagonal YMnO₃ and HoMnO₃**Experiment number:**

HC-644

Beamline:

ID11

Date of experiment:

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9

Local contact(s):

Dr. Gavin Vaughan

*Received at ESRF:***Names and affiliations of applicants (* indicates experimentalists):**Sverre M. Selbach^{1,*}, Sandra H. Skjærvø^{1,*}, Mari-Ann Einarsrud¹, Tor Grande¹ and Simon Billinge²¹Norwegian University of Science & Technology Department of Materials Science NOR - 7491 TRONDHEIM²Columbia University Dept. of Applied Physics and Applied Math. 200 SW Mudd Bldg. 500 W 120th St USA - 10025 NEW YORK**Report:**

The purpose of the measurements is to study structural coherence in hexagonal manganites across the structural trimerization phase transition at ~1300 K through Pair Distribution Functions (PDF) obtained from X-ray total scattering can probe the intermediate range and reveal possible structural disorder in presumed displacive phase transitions.

Three high temperature total scattering measurements on YMnO₃ were performed upon both heating and cooling, with temperature setpoints from 100 to 1200 °C. The samples were sintered polycrystals glued onto the top of quartz capillaries to avoid the strong background observed for initial attempts with powder contained in platinum capillaries. A standard air gun was used to heat the sample.

The measurements were succesful in terms of collecting PDFs, which could be easily fitted to the $P6_3cm$ space group of YMnO₃ with PDFGui both for setpoints 100 and 1000 °C (Figure 1 a) and b)). The lattice parameter c goes through a minimum at ~1000 °C [1]. Unfortunately lattice parameter c refined from the PDFs (Figure 1 c)) show that even at setpoint 1200 °C the true sample temperature was ~300 K lower than the setpoint temperature. The discrepancy in setpoint and sample temperature was also directly evident from the XRD diffraction patterns as a superreflection characteristic for the low temperature phase was still visible with setpoint temperature 1200 °C.

The target temperature was not reached and the structural coherence across the trimerization structural transition at ~1300 K could thus not be characterized. A proposal for continuation of this experiment using a Linkam heater, which allows better temperature control, is submitted.

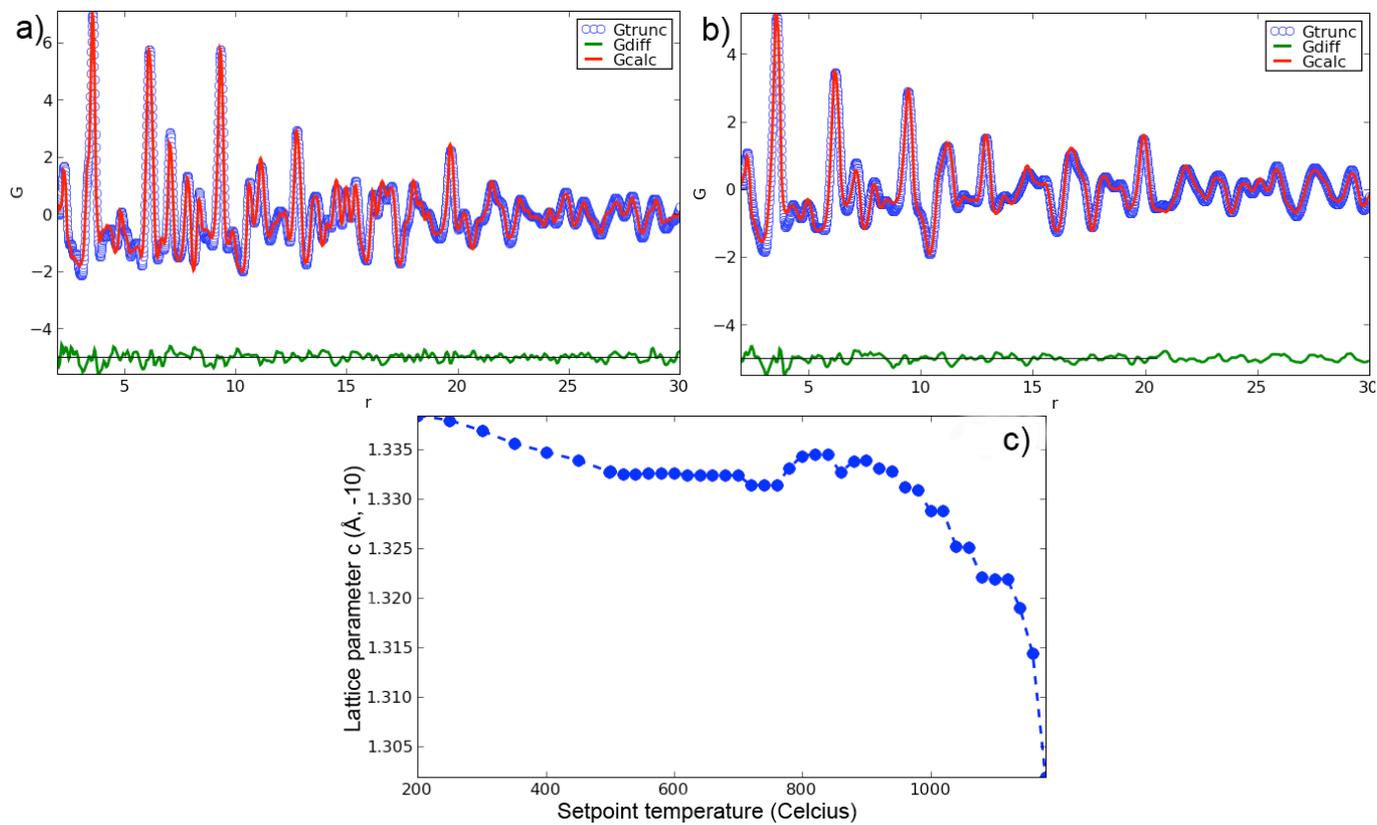


Figure 1. Fitted PDFs of YMnO₃ collected at setpoint temperature a) 100 °C and b) 1000 °C. c) Lattice parameter *c* of YMnO₃ refined from the PDFs as a function of temperature.

References

- [1] A.S. Gibbs, K.S. Knight, P. Lightfoot, Phys. Rev. B 83 (2011) 094111.