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|   | <b>Experiment title:</b><br>Local structure and structural coherence across phase transitions in multiferroic hexagonal YMnO <sub>3</sub> and HoMnO <sub>3</sub> | <b>Experiment number:</b><br>HC-1179 |
| <b>Beamline:</b><br>ID11  | <b>Date of experiment:</b><br>from: 02 May 2014 at 08:00 to: 04 May 2014 at 08:00  | <b>Date of report:</b>               |
| <b>Shifts:</b><br>6   | <b>Local contact(s):</b><br>Dr. Gavin Vaughan  | <i>Received at ESRF:</i>             |
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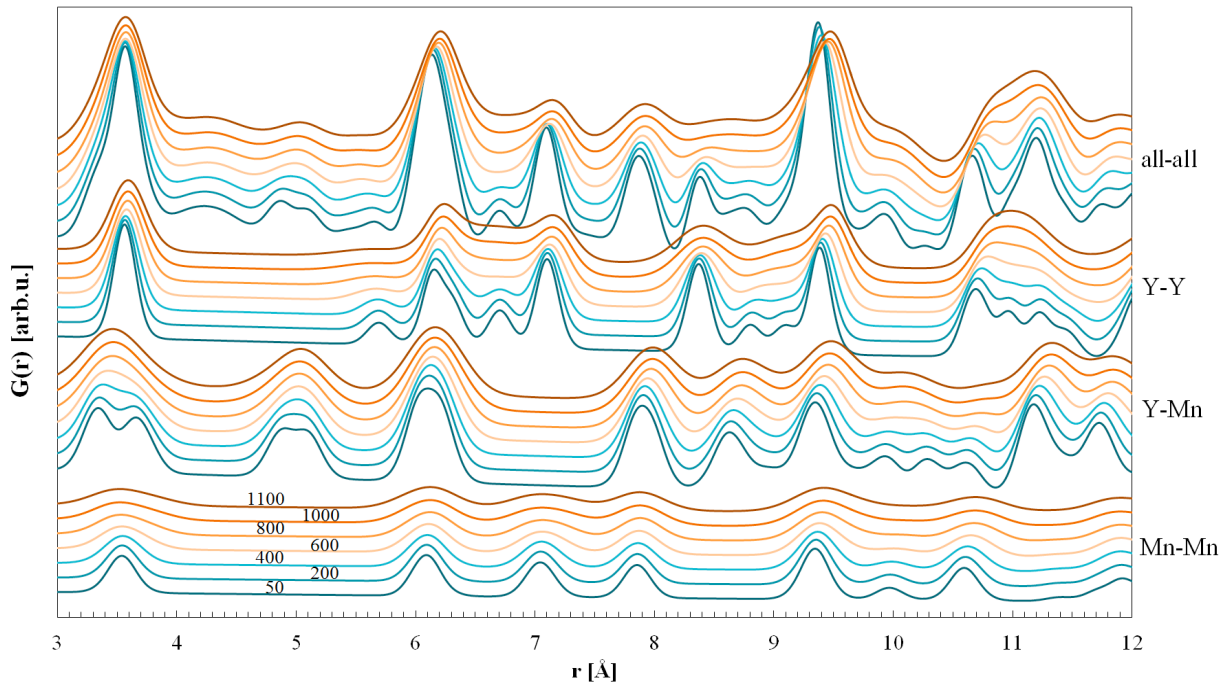
## Report:

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). This was a continuation of HC644.

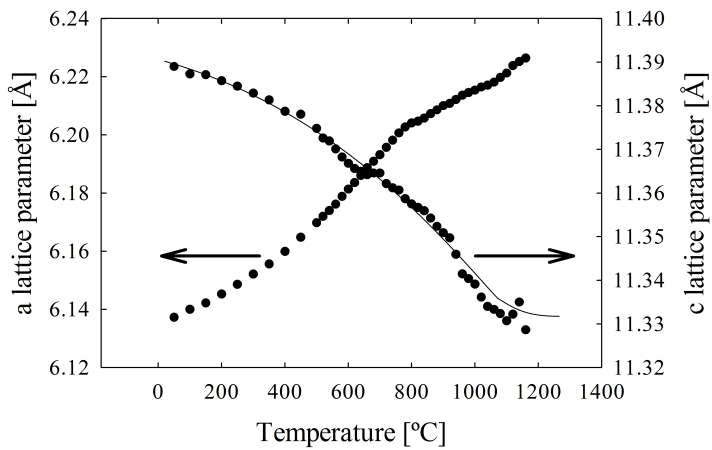
High temperature total scattering measurements on YMnO<sub>3</sub> were performed upon both heating and cooling, with temperature setpoints from 100 to 1160 °C. The samples were sintered polycrystals glued onto the top of sapphire capillaries to minimize the background. In this experiment much better temperature control was obtained with a Linkam heating camera compared to the hot air blower used in the preceding experiment HC644. However, the background from the Linkam heating camera was difficult to mask and remove completely by background subtractions, and this resulted in substantial noise at low  $r$  in the final  $G(r)$ .

We have successfully fitted the high temperature PDFs with PDFgui, but the data was not of sufficient quality to obtain reliable oxygen positions, and the lowest  $r$ -region could not be fitted due to the noise. For these reasons we have conducted parallel total scattering measurements with spallation source neutrons and we intend to publish the ESRF data together with the neutron data.

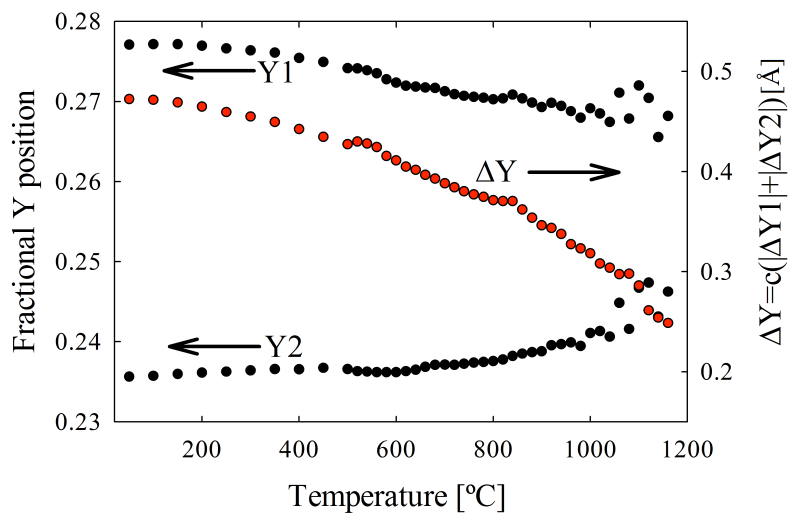
We include preliminary figures from the HTPDF collected at ID11 in May 2014 here:



Partial PDFs have been simulated from the structure obtained by fitting the total PDFs. The setpoint temperatures are given in Celsius.



Lattice parameter evolution obtained from fitting the data with PDFgui.



Refined Y positions from fitting PDFs with PDFgui.