



Experiment title:

Local structure and structural coherence across phase transitions in multiferroic hexagonal YMnO_3 and HoMnO_3

Experiment number:

HC-1766

Beamline:

ID22

Date of experiment:

from: 17 June 2015 at 08:00 to: 20 June 2013 at 08:00

Date of report:

Received at ESRF:

Shifts:

9

Local contact(s):

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The purpose of the measurements is to study the structural evolution of lead-free relaxor perovskites in the system $(1-x)\text{Bi}_{0.5}\text{K}_{0.5}\text{TiO}_3-x\text{BiFeO}_3$ (BKT-xBFO) across their temperature induced ferroelectric transitions. Pair distribution functions were obtained from the total scattering functions. The beam time was very successful with perfectly working beam, detector and sample environment (hot air blower). Results from this experiment are included in a manuscript soon to be submitted, and the remaining results will be published in at least one follow-up paper. Room temperature PDF of the end member BKT fitted with a crystallographic model with PDFgui and fitted by reverse Monte Carlo simulation with RMCProfile is shown in Figure 1.

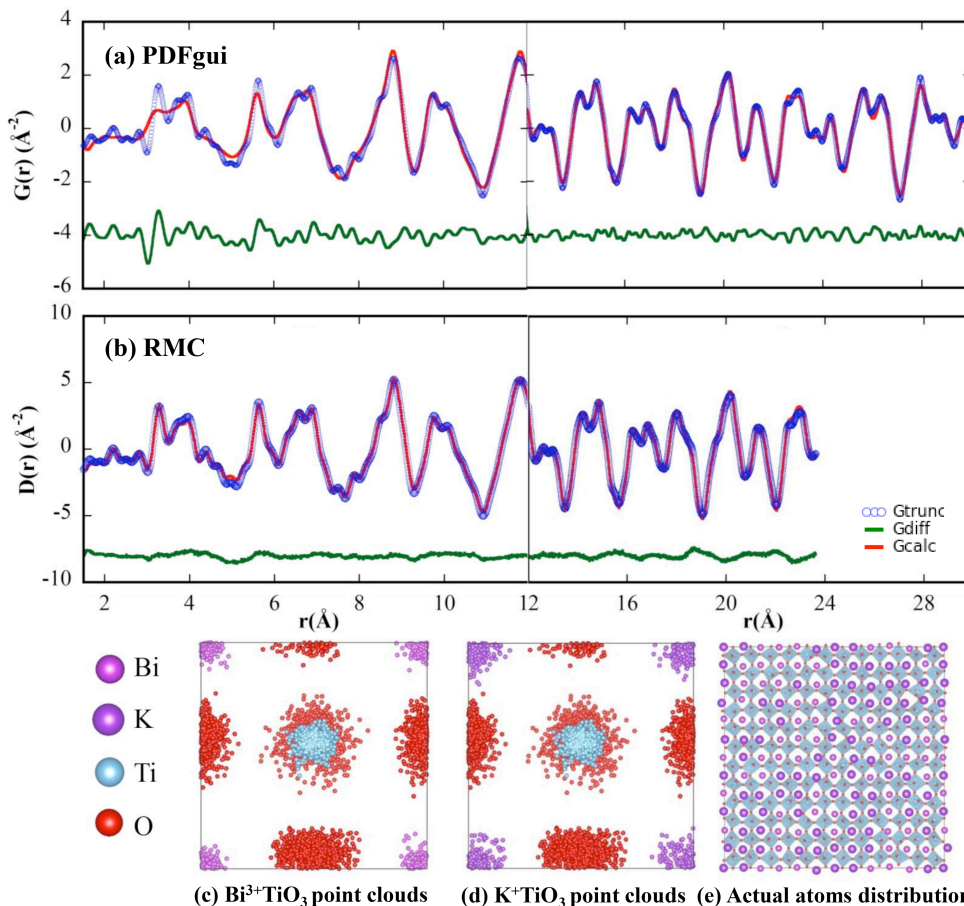


Fig. 1: (a) PDF data of BKT fitted with P4mm A-site-mixed structural model. (b) RMC simulation with experimental and calculated data. Open circles: experimental data; red solid lines: calculated data; the green difference curves shown below each plot. (c) Folded RMC point clouds model only show Bi^{3+} cations. (d) Folded RMC point clouds model only show K^{+} cations. (e) Actual RMC configurations of $12 \times 12 \times 12$ supercell of BKT.