Poster Presentations

[MS27-P07] Jahn-Teller Symmetry Switching in $LaMnO_3$.

Callum A. Young,[1]* Edward O. R. Beake,[1] Fabio Denis Romero,[1] Leigh D. Connor,[2] Thomas E. Proffen,[3] Matthew G. Tucker,[4] David A. Keen,[4] Michael A. Hayward[1] and Andrew L. Goodwin[1].

[1]*Department of Chemistry, University of Oxford, Inorganic Chemistry Laboratory, South Parks Road, Oxford OX1 3QR, U.K.*
[2]*Diamond Light Source, Diamond House, Harwell Campus, Didcot, Oxfordshire, OX11 0DE, U.K.*
[3]*Oak Ridge National Laboratory, Oak Ridge, TN 37831-6475, U.S.A.*
[4]*ISIS Facility, Rutherford Appleton Laboratory, Harwell Oxford, Didcot, Oxfordshire OX11 0QX, U.K.*
*callum.young@chem.ox.ac.uk

As the parent compound of the $La_{1-x}A_xMnO_3$ (A = Ca, Sr, Ba) series of colossal magnetoresistive (CMR) compounds [1], LaMnO3 has attracted significant attention over recent years. Its orthorhombic to pseudocubic transition at T_{JT} = 750 K is often taken to be a fine example of an orbital order-disorder transition [2], where the Jahn-Teller (JT) distorted MnO6 octahedra lose their long-range ordering upon heating. The higher temperature pseudocubic phase is of importance as it is this phase that leads into the CMR phase in the doped compounds, so it is crucial that a clear picture of the structure of this phase is developed to aid our understanding of this unusual behaviour.

Here we have employed high-resolution neutron and X-ray total scattering measurements and reverse Monte Carlo (RMC) refinements [3] to develop a large-box model of $LaMnO_3$ across the phase transition. Our results show that rather than being a simple order-disorder transition, the nature of the JT distortion actually changes discontinuously at the transition, with the Mn^{3+} cation off-centering towards an edge. Such a distortion favours a more disordered state, and could account for many experimental observations, including dielectric [4], resistivity [5], magnetic [6], X-ray absorption [7], and volume [8] anomalies, and suggests that the orbital degrees of freedom available are more numerous than initially thought.

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