Oral Contributions

[MS27 - 04] Jahn-Teller Symmetry Switching in LaMnO3. 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].

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As the parent compound of the $La_{1-x}A_xMnO_3$ (A = Ca, Sr, Ba) series of colossal magnetoresistive (CMR) compounds [1], $LaMnO_3$ has attracted significant attention over recent years. Its orthorhombic to pseudocubic transition at TJT = 750 K is often taken to be a fine example of an orbital order-disorder transition [2], where the Jahn-Teller (JT) distorted MnO_6 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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