Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Enhanced local lattice distortions with the antiferromagnetic transition in the multiferroic $LuMnO_3$ DESPINA LOUCA, University of Virginia, THOMAS PROFFEN, Los Alamos National Laboratory, SEUNG-HUN LEE, University of Virginia, SANG-WOOK CHEONG, Rutgers University — The ferroelectric hexagonal manganite, $LuMnO_3$, has been investigated via neutron scattering and the pair density function analysis to determine the nature of the local atomic distortions with the antiferromagnetic transition, T_N, of the Mn ions. While in previously reported neutron diffraction data, it was shown that all atomic coordinates changed based on symmetry considerations with T_N, we hereby show that it is the ferroelectric motion of the Lu ions coupled with O distortions that exhibits a strong temperature dependence below T_N as reflected in the Lu-O bonds. This suggests an enhancement of the net electric polarization below T_N. At the same time, the motion of the apical O1 and O2 ions distorts the MnO_5 bipyramids, leading to more buckling of the ab-layers. However, the Mn ions do not appear to distort significantly away from their equilibrium position. The oxygen distortions induced with the spin reorientations below T_N may be the cause for the Lu ion displacements through electrostatic interactions and this in turn produces coupling to the electric dipole moments.

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Date submitted: 14 Nov 2008 Electronic form version 1.4