Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Lattice Distortion due to Charge-ordering effects in single-layer $\mathbf{La_{0.5}Sr_{1.5}MnO_4}$ DEREK LARSON, F. BRIDGES, University of California, Santa Cruz, A. MEHTA, S. LAROCHELLE, M. LATIMER, SSRL, Stanford CA. — We report measurements of the local structure of the single-layer manganite $La_{1-x}Sr_{1+x}MnO_4$ (x = 0.5) using polarized EXAFS at the Mn K-edge. Earlier diffraction data suggested a quadrupling of the simple perovskite unit cell, most likely from a charge/orbital ordering effect. From a careful analysis of the single crystal diffraction pattern, space group symmetry of the ordered structure is deduced to be B2mm (special space group settings employed to keep Mn-O planes perpendicular to the c-axis). In this space group symmetry there are 3 distinct Mn sites, but the diffraction data indicates that two of them are related by a pseudo-glide and the distinction between them is very subtle. For the EXAFS analysis we have imposed the glide symmetry and therefore assumed a more symmetric space group Bbmm, which contains only two unique Mn sites. We have further assumed that the predominant effect of the charge/orbital ordering is on the basal Mn-O bonds. Bbmm symmetry allows for 4 unique basal Mn-O bond distances, however, the EXAFS analysis shows that they are clustered in two distinct groups. Combining these results with analysis of single crystal diffraction data indicates that the primary mode of distortion of the basal Mn-O bonds is driven by the Jahn-Teller effect. (That is, each Mn has two close basal O neighbors and two distant basal O neighbors.) Support: NSF DMR0301971, and BES/DOE.

Frank Bridges
University of California, Santa Cruz

Date submitted: 27 Mar 2013 Electronic form version 1.4