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High Resolution X-ray Diffraction Study of $La_{2-x}M_xCuO4$, M=Sr, Ba

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Beamline(s): X7A

Introduction: The title materials represent prototype layer superconducting perovskite compounds. Stripe phases are presumed to influence the properties for M=Ba. For M=Sr, recent evidence suggests that stripes may also enter into the picture for this system. Initially, the low temperature structures for these two systems were shown to be different. More careful work demonstrates that there are similarities here too. The M=Ba system transforms essentially completely to a low temperature tetragonal phase (LTT). For M=Sr there is a partial (~10%) transformation to LTT. The accurate determination of structure represented here is a prerequisite for analyzing the relationships among superconductivity, magnetism, and stripes.

Methods and Materials: Powder samples prepared using standard procedures, including pairs of oxygen isotope exchanged specimens, were examined using high resolution x-ray diffraction. Diffraction work at NSLS X7A utilized powder on a flat plate holder in a refrigerator capable of 20-400K. The data was obtained using a detector placed after a crystal analyzer. X-ray wavelength was in the range 0.07-0.09 nm, selected by a Si (111) crystal double monochromator. Beamline-specific fitting programs were utilized to fit the diffraction peaks (see Figure 1).

Results: Phases were identified by studying the region of the orthorhombic 020/200 peak region. For M=Ba, $x \geq 0.09$, samples transform essentially completely from the orthorhombic Bmab space group (LTO1 phase) to LTT via a first order transition near temperature $T_1 \cong 60$ K. It was found that, for M=Ba and Sr, $x > 0.03$, the orthorhombic LTO1 phase (Bmab space group) contains as a minority phase ~8-16% low temperature tetragonal ($P4_2/ncm$, LTT) phase. For each sample, there is a temperature range (~100 K) for which the fraction of LTT in LTO1 changes slowly. The LTO1/LTT transformation can be viewed as a two-step transition. At some high temperature a fraction (on the order of 10%) of the nominally LTO1 sample transforms to LTT. Over a range of temperatures this phase mixture is stable. Then, within a few degrees of T_1 the sample goes completely to LTT. (La_2CuO_4 shows no evidence for even a partial transformation to LTT). Several pairs of oxygen isotope-exchanged samples (M=Sr) were also examined to search for structural differences, which might contribute to the unusual reported isotope effects (M. K. Crawford et al.) in these materials.

Conclusions: The two-step transformation toward LTT can be interpreted in light of low temperature transmission electron diffraction (TEM). The partial transformation toward LTT above temperature T_1 may be a nucleation of a minority LTT phase at the LTO1 twin boundaries. At T_1 (M=Ba) the remaining material rapidly transforms completely to LTT. For M=Sr we see only the partial transformation. When comparing oxygen exchanged M=Sr samples we can discern no difference in the fraction of LTT at low temperature, nor any difference in crystallographic characteristics of the two coexisting phases. Since no perceptible structural differences were observed among these samples, we conclude that the isotope effects are intrinsic lattice effects.

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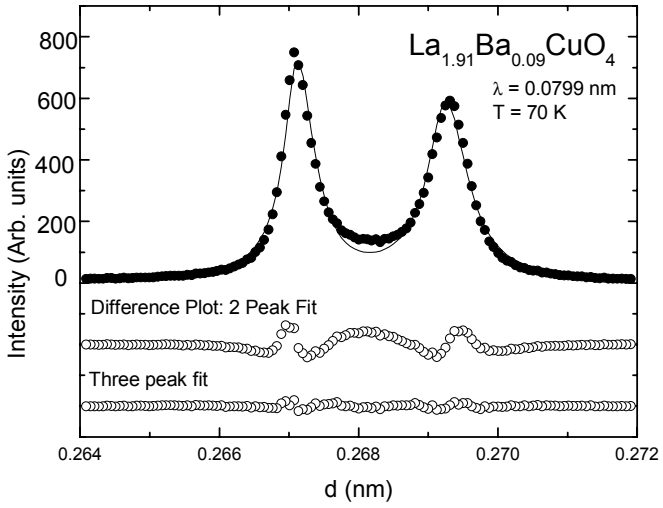

Figure 1. Example of fitting to the LTO1 020/200 and LTT 200 above the bulk transformation temperature T_1~60K. The solid line represents a two-peak fit; the three peak fit accounts very well for the data (see difference plots). The two sharp peaks accounting for ~90% of the total intensity are LTO1. The broad peak between is characteristic of LTT 200, both in shape and position