Structural, magnetic, and transport properties of $La_{1-x}Ca_xMnO_3$ at high temperatures

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Doped manganese oxides are strongly correlated systems where the order parameter is believed to comprise spin, charge, and lattice degrees of freedom [1]. Souza *et al.* [2] showed that in the high-temperature regime (300 K < T < 850 K), the system $La_{1-x}Ca_xMnO_3$, x = 0.30, undergoes a structural phase transition from orthorhombic (*Pnma*) to rhombohedral (*R-3c*) space group, close to T_{O-R} = 710 K. They also found that for T > $T_{O-R,}$ the temperature dependence of the electrical resistivity ρ(T) is well described by an adiabatic polaron mechanism while for T < $T_{O-R,}$ it still obeys the polaron model but in the non-adiabatic regime. Here, we have extended our understanding to the samples with x = 0.20, 0.25, 0.34, 0.40, and 0.45 by performing high-resolution x-ray diffraction (HRXRD), ρ(T), and magnetization experiments as a function of temperature. Measurements of HRXRD indicate that the sample $La_{0.55}Ca_{0.45}MnO_3$ exhibits only a partially structural phase transition from *Pnma* (low T) to *R-3c* (high T) at T_{O-R} = 767 K. Increasing the temperature further, both phases coexist from T_{O-R} to the highest measured T ~ 900 K. We have also found that the phase transition at T_{O-R} = 767 K is not observed in ρ(T) measurements, probably due to the percolative nature of the electronic mechanism. Furthermore, it is also observed that the transport mechanism in samples with x = 0.20, 0.25, and 0.34 obeys the polaron model. However, increasing the charge carriers (x = 0.40 and 0.45) results in a different transport mechanism. We suggest that such result is closely related to the temperature dependence of the unit-cell parameters. The thermal expansion coefficient for the *Pnma* phase, x = 0.45, is temperature independent whereas the sample with x = 0.30 shows a linear temperature dependence. The magnetic results will also be discussed on the light of these interesting results.

Keywords: Electrical resistivity, X-ray diffraction, Structural transition, Thermal expansion coefficient.

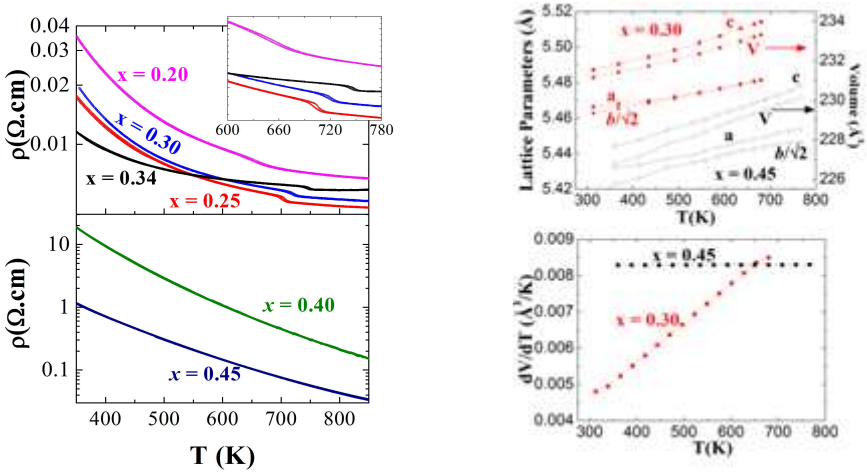

Fig. 1 (Left panel) ρ(T) data for several studied samples. (Right panel) Unit-cell parameters/unit-cell volume (upper) and the thermal expansion coefficients (bottom).

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