Charge density of $La_{0.5}Sr_{1.5}MnO_4$: First results

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$La_{0.5}Sr_{1.5}MnO_4$ is a mixed-valence manganese perovskite and, as a prominent example of correlated electron systems, has been extensively studied during the last years, e.g. [1,2,3]. The occurrence of various electrical and magnetic phenomena, e.g. ferro- and antiferromagnetism, colossal magnetoresistance, etc., makes these materials interesting candidates for many applications in modern technology. The structure is tetragonal (I4/mmm) at room temperature and undergoes a phase transition at 220 K, which was earlier ascribed to charge and orbital ordering at the manganese sites, and can be tested via X-rays by observing superstructure reflections with indices (h/2,k/2,l) and (h/4,k/4,l), respectively. Recent investigations, however, principally claimed a structural distortion to be responsible for the low-temperature superstructure reflection intensities [4]. In order to shed more light on this controversy a charge density study has been performed. Data sets have been recorded both at room temperature and at 10 K using high-energy synchrotron radiation (100 keV photons) in order to minimize absorption and extinction corrections. Details of multipole refinements will be shown as well as first results of densities and topological analyses.

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[4] J. Herrero-Martin et al., Phys. Rev. B83, 184101 (2011).