

[o.m2.p5] Models of the Crystal Structures of Phases in Doped Lanthanum Manganites. V.E. Naish, T.V. Novoselova, *Institute for Metal Physics, Ural Division of Russian Academy of Science, Ekaterinburg, GSP-170, Russia.*

Keywords: manganites, crystal structure, distortion modes.

On the phase diagram in $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ there are three main phases: two orthorhombic phases O' and O* with the same space group $\text{Pnma} = \text{D}_{2h}^{16}$ and one rhombohedral R one with $\text{R}\bar{3}\text{c} = \text{D}_{3d}^6$ space group. The structures of all these phases are just weak distortion of perovskite cubic structure. Such distortion modes have two main mechanisms to occur by:

- 1) the octahedra rotation (tilting ψ or antitilting ϕ) about cubic axes x, y, z or their combination type of $\psi 00$, $\psi \psi 0$, $\psi \psi \psi$, $\psi \psi \phi$ and so on;
- 2) the Jahn-Tellers distortions, formed by Q_2^α or Q_3^α ($\alpha = x, y, z$) modes with wave vectors of M or R type from Brillouin zone.

It has been found that Pnma space group of orthorhombic phase might be realized with the only combination of that distortion modes, $\text{O} = \phi\phi\psi + \text{Q}_2^z(\text{M})$ namely. Thus, the structures of the manganites orthorhombic phases have strict and definitive notation in positions of Pnma group; just two current parameters are in the notation of all atom coordinates, whose numerical value might be obtained from the fitting procedure of theoretical profiles of scattering intensities and experimental ones. It has been brought to light that the difference between two orthorhombic structures O' and O* (the same Pnma space group) appeared to be merely quantitative one: at O' \rightarrow O* phase transition the Jahn-Teller contribution to the distortion becomes sharply reduced.

The structure of rhombohedral R phase with $\text{R}\bar{3}\text{c}$ group has been found to be formed by tilting modes only without Jahn-Teller ones assistance, $\text{R} = \phi\phi\phi$ namely. The only current parameter is in the notation of atom coordinates for this structure.

In spite of the fact that a lot of works¹⁻³ discussed the fascinating structural properties of manganese perovskites does exist yet, we pretend to clarify and systematise the set of the phases on the phase diagram in lanthanum manganites.

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[o.m2.p6] Charge ordering and antiferromagnetism in $\text{Pr}_{0.8}\text{Na}_{0.2}\text{MnO}_3$. M. Dlouha¹, S. Vratislav¹, Z. Jiráček², K. Knižek², ¹*Faculty of Nuclear Physics and Physical Engineering, Prague and* ²*Institute of Physics, Prague, Czech Republic.*

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The manganites $\text{Pr}_{1-x}\text{Na}_x\text{MnO}_3$ ($x=0-0.2$) have been synthesized and investigated by the neutron diffraction. All the systems show a perovskite structure with the tilt pattern of the Pnma type. Similarly to related systems with substituted divalent alkali earths, the increasing monovalent sodium substitution generates charge carriers and changes gradually the magnetic groundstate from the layered A-type antiferromagnetism in PrMnO_3 ($T_N=91$ K) through canted arrangements for $x\sim 0.05$ to the pure ferromagnetism for $0.10\leq x\leq 0.15$ ($T_C\sim 125$ K). An interesting feature is the detection of charge and orbital ordering ($T_{CO} \sim 225$ K) followed by the "pseudo" CE type antiferromagnetic order ($T_N=175$ K) in the compound with highest possible sodium concentration $x=0.2$ (the actual $\text{Mn}^{3+}/\text{Mn}^{4+}$ ratio in this sample was determined by the cerimetric titration to 64%:36%). The structure consists of two sublattices – one is composed of Mn^{3+}O_6 octahedra with a characteristic tetragonal elongation, which are oriented alternatively in the [101] and [10-1] directions; the other one is formed by the mixed valence ($\text{Mn}^{3+}/\text{Mn}^{4+}$) O_6 octahedra elongated along the [010] direction. As a result, the lattice metrics remains pseudocubic – $a=5.430$, $b/\sqrt{2}=5.427$, $c=5.446$ at 10 K, compared to $a=5.437$, $b/\sqrt{2}=5.439$, $c=5.450$ at 300 K. This is in distinction to the charge ordered manganites with ideal $\text{Mn}^{3+}/\text{Mn}^{4+}$ ratio of 50%:50% (e.g. $\text{Pr}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$) where a marked tetragonal contraction along the b axis is encountered. On the other hand, the structural and magnetic arrangement of $\text{Pr}_{0.8}\text{Na}_{0.2}\text{MnO}_3$ at low temperatures is analogous to the structure observed previously in the $\text{Pr}_{1-x}\text{Ca}_x\text{MnO}_3$ manganites with similar $\text{Mn}^{3+}/\text{Mn}^{4+}$ content ($x\sim 0.35$)¹⁻³. A novel finding on the present compound is a reorientation of the magnetic axis of the "pseudo" CE arrangement from the [010] to [001] direction below ~ 50 K.

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