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Features of Structural Transformations in La1-xCaxMn0.98Fe0.02O3+δ (x = 0.05 −0.50)

The lanthanum manganite compounds doped with a divalent impurity are the materials with colossal magnetoresistance and widely used in different fields of modern engineering. In lanthanum manganites manganese has a mixed valence: Mn3+ and Mn4+. Mn3+ is the Jahn-Teller ion with a degenerated orbital state of electrons. The main feature of the compounds with Jahn-Teller ions is strong correlation between lattice and electron subsystems. These compounds are characterized by strong lattice distortions.

The features of structural transformations in La1-xCaxMn0.98Fe0.02O3+δ (x = 0.05 −0.50) as a function of Ca concentration have been studied by Mössbauer spectroscopy and X-ray diffraction analysis. For x = 0.05 and 0.10 the rhombohedral phase (space group R-3c) has been shown to be synthesized. Beginning from x = 0.20 the structure of the origin synthesized samples is orthorhombic (space group Pnma). Varying the heat treatment conditions it is possible to transit from one phase to another. The phases are subsequently suppressed with an increase in a Ca concentration. For Ca concentrations less than 20% all set of the phases with reversible structural transitions PnmaII ↔ PmnaI ↔ R-3c can be obtained under heat treatment like in the Ca-undoped compound LaMn0.98Fe0.02O3+δ. The rhombohedral phase is suppressed for x = 0.20. When a Ca concentration higher than 20%, the PnmaII phase is suppressed, as a result, only the PnmaI phase remains which is stable under any heat treatment.

Mössbauer spectra for the PnmaI and R-3c phases have relatively narrow lines and were processed by single doublet. Spectra for the PnmaII phase represent strongly broadened quadrupole-splitting (QS) doublets. A large QS value is related to the strong lattice distortion due to the Jahn-Teller effect. Since the spectra for the PnmaII phase have a smooth shape, they were processed by the QS distribution.

Doping with divalent Ca occupying trivalent La positions generates vacant oxygen sites in the lattice. Therefore already during synthesis a part of Jahn-Teller Mn3+ ions transfers to Mn4+ and oxygen coming with Mn4+ should occupy first of all these oxygen sites. Under oxidation (annealing in air) the Mn4+ ion concentration increases and excess oxygen will now occupy interstitial positions.

Based on the analysis of the obtained experimental data it is possible to suppose that the reversibility of the phase transitions is possible only when excess oxygen is in interstitial positions in the lattice. If excess oxygen occupies only vacant sites in the lattice, the phase transitions are absent.

The features of the phase formation in the basic undoped compound LaMnO3+δ and in the Ca-doped compound La1-xCaxMn0.98Fe0.02O3+δ are compared.

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