LAYERED RARE EARTH MANGANITES UNDER EXTREME CONDITIONS

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Due to the strong interaction between different degrees of freedom (spin, charge, orbital, and phonon subsystems), layered manganites have attracted much attention last decades. Under external conditions (temperature, pressure, mechanical stress, electric and magnetic fields), strong correlated materials exhibit unusual optical, electronic, and magnetic properties. A-site ordering in layered $LnBaMn_2O_6$ manganites leads to a significant change in the phase state: materials with large lanthanide ions Ln = La, Pr exhibit ferromagnetic behavior above $T_C > 300$ K, while oxides with small elements Ln = Y – Sm are charge- and/or orbital-ordered insulators with a transition temperature to the "bad metal" state above 350 K. The size of the ion also determines the sequence and type of structural transitions. In particular, for $SmBaMn_2O_6$, the structure is orthorhombic, space group *Cmmm*, $2a_p \times 2b_p \times 2c_p$, where $a_p \sim c_p$ denotes to simple cubic perovskite. Propagation vector $\mathbf{k_1}$ (00½) is connected with the ordering of the simple perovskite cells of $LnMnO_3$ and $BaMnO_3$, while $\mathbf{k_2}$ (½½0) is caused by the tilting of the MnO_6 octahedra. The metal-insulator transition (T_{MI}) is caused by charge ordering ($T_{CO1} = T_{MI} \sim 380$ K) of Mn^{3+} and Mn^{4+} ions, which leads to a new superstructure of $2\sqrt{2}a_p \times 2\sqrt{2}b_p \times 4c_p$ (space group *Pnam*) [1]. In this case manganese ions are ordered in an AABB-type manner along the c-axis, resulting in a 4-fold period along the c-axis. A further cooling leads to a change in the type of charge ordering from AABB to AAAA at $T_{CO2} \sim 200$ K, respectively, and a 4-fold increase in the parameter along the c-axis disappears. Below T_{CO2}, the structure is described as $2\sqrt{2}a_p \times 2\sqrt{2}b_p \times 2c_p$, space group $P2_1am$. In the case of $LaBaMn_2O_6$, there is almost no distortion of the MnO_6 octahedra at low temperatures, so the structure remains tetragonal, $a_p \times a_p \times 2c_p$, space group *P4/mmm*. The result of the competition of different phases and, as a consequence, structural states under the influence of external pressure and temperature of layered manganites is quite unpredictable [2]. Thus, for La- and Nd-based oxides, we have discovered for the first time superstructure reflexes with d ~ 23 Å, which indicates new phase and structural states of oxides under extreme conditions.

[1] Morikawa D., Tsuda K., Maeda Y., Yamada S., Arima T. Charge and Orbital Order Patterns in an *A*-Site Ordered Perovskite-Type Manganite $SmBaMn_2O_6$ Determined by Convergent-Beam Electron Diffraction // J. Phys. Soc. Jpn., 2012, V. 81, P. 09360
[2] S. Titova, E. Sterkhov, V. Sidorov, N. Chtchelkatchev, F. Alabarse, High pressure - low temperature study on $NdBaMn_2O_6$ double manganites, Journal of Alloys and Compounds, 2025, P. 183151.

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