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The high-pressure effect on the crystal structure of cobaltite LaSrCoO4

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Recently studies of complex cobalt oxides have attracted wide scientific interest, due to the large variety of physical properties found in these materials. In contrast to manganites or cuprates, cobaltites have a unique feature - the ability to change the spin state of Co3+ ions with variations in thermodynamic parameters (temperature or pressure). So, depending on the balance of comparable in magnitude intra-atomic exchange energy JH and the splitting energy of the crystal field ⊠CF, nonmagnetic low-spin LS (t2g6, S = 0), magnetic intermediate-spin IS (t2g5eg1, S = 1) and high-spin HS (t2g4eg2, S = 2) states can be realized in cobaltites. It should be noted that the model layered cobaltite LaSrCoO4, which has only trivalent Co3+ cobalt ions, attracts the attention of researchers by a complex mixed spin configuration of low-spin LS and high-spin HS states. Such a model of the ground spin state of cobalt ions is often debated in opposition to the existence of an intermediate spin IS state in this cobaltite.
The effect of high pressure is a direct method for the controlled change in the spin states of cobalt ions due to the variation of interatomic distances and the corresponding valence angles. Studies at high pressures provide a unique opportunity to determine the structural mechanisms of changes in spin states in cobaltites. Detailed studies of the crystal structure of LaSrCoO4 were carried out using neutron diffraction on a DN-6 diffractometer of a pulsed high-flux IBR-2 reactor (FLNP, JINR, Dubna, Russia) using a high-pressure chamber with sapphire anvils in the pressure range up to 5.8 GPa and a temperature range of 7-300 K. The baric and temperature dependences of the unit cell parameters, the volume and the interatomic bond lengths of the LaSrCoO4 compound were obtained.
It has been established that the apical and axial Co-O bond lengths are compressed isotopically but the apex Co-O distance reduces faster than that for the in-plane up to 5.8 GPa, namely the ratio Co-O2/Co-O1 decrease with high pressure from 1.06 to 1.039. The LS state could become the ground state when this ratio is larger than 1.065, so for the LaSrCoO4 was observed the HS ground state due to the decrease of 10Dq and of the eg splitting from the reduction of Co-O2/Co-O1. The ratio of the lattice parameters c/a increase with high pressure, so the octahedra is more symmetrical and the LS state become more stabilized.

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