CRYSTAL STRUCTURE REFINEMENT OF $[M_2Cu_2O_3]_m[CuO_2]_n$ SPIN-LADDER COMPOUNDS IN 4D SPACE

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The compounds investigated here belong to the spin-ladder family of cuprates. The orthorhombic structures of $[M_2Cu_2O_3]_m[CuO_2]_n$ (M = Ca and Sr mainly, m/n = 5/7 or 7/10) can be represented in three-dimensional space by the stacking of three different types of layer: CuO_2, Cu_2O_3 and M, which contain straight and zigzag chains of CuO_4 squares and M cations, respectively. Alternatively the crystal structures can be described in four-dimensional space as composite structures, incommensurate along the direction [001], with two interpenetrating sublattices, $M_2Cu_2O_3$ and CuO_2.

In this work the crystal structures of cuprates were investigated by powder and single-crystal X-ray diffraction. The bulk materials were prepared from oxides and carbonates by solid-state reaction in air. The traveling solvent floating zone method was applied in an image furnace to grow single crystals. Structure refinements in four-dimensional space were carried out using the WinCSD-2008 program.

The composite incommensurate structure of the $(Ca_{0.59}Sr_{0.39}Bi_{0.02})_{10}Cu_{17}O_{29}$ compound, which was previously described by us in a commensurate approximation (m/n = 5/7, space group $F222$, a = 1.1340(2), b = 1.2829(2), c = 1.9441(3) nm [1]) was solved and refined from single-crystal diffraction data in (3+1)-space group $F222(00\gamma)$: a = 1.1340(2), b = 1.2829(2), c_1 = 0.27773(4), c_2 = 0.38882(6) nm, q = 0.7143, R = 0.031 (all reflections), R = 0.029 (main reflections), R = 0.032 (satellite reflections). The experimentally determined modulation vector ($q = c_1/c_2$) coincides with the theoretically calculated value for 5/7 members of the $[M_2Cu_2O_3]_m[CuO_2]_n$ series ($q = m/n = 0.7143$).

A refinement on powder diffraction data of the crystal structure of the spin-ladder compound in the corresponding bulk sample ((3+1)-space group $F222(00\gamma)$, a = 1.1349(1), b = 1.2825(1), c_1 = 0.2755(1), c_2 = 0.39050(5) nm, q = 0.7055) showed the presence of the 7/10 member of $[M_2Cu_2O_3]_m[CuO_2]_n$ series. Consequently, the structure of the spin-ladder compound observed in the single crystal corresponds to a metastable modification of $[M_2Cu_2O_3]_m[CuO_2]_n$ with m/n = 5/7, whereas the ceramics contain the stable modification with m/n = 7/10.

Reference

[1] O. Zaremba, O. Shcherban, R. Gladyshevskii, F. Banfi, E. Giannini. The 5:7 Member of the Spin-Ladder Series in the Bi-Sr-Ca-Cu-O System // (in press).