Growth and oxygenation of infinite-layer $CaCuO_2$ and $SrCuO_2$ thin films

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The discovery of high-T_c superconductivity in cuprates and the central role of the CuO_2 planes for superconductivity in these materials have triggered a large effort in studying the infinite-layer compounds, $ACuO_2$; these systems have a layered structure composed of CuO_2 planes and separated by alkaline metal (A = Ca, Sr, Ba) planes [1].

The infinite-layer compounds are insulating when A is an alkaline metal, but can be doped with electrons or holes, leading to the appearance of superconductivity. Hole doping in these systems is usually associated with the appearance of apical oxygens, both in bulk crystals [2] and in multilayer thin films [3–5]. Controlling the oxygen content in these systems is therefore crucial to determine their properties and eventually induce high-T_c superconductivity. Previous works indicate that the infinite-layer structure is modified in presence of highly oxidising atmosphere, with an expansion of the c-axis parameter [6].

In this work, we study this high c-axis phase and more generally the oxygenation of infinite-layer films of $CaCuO_2$ and $SrCuO_2$ deposited using pulsed laser deposition. Our experimental observations from X-ray diffraction and X-ray absorption spectroscopy indicate that under highly oxidising growth condition, additional oxygens are indeed incorporated in the structure, probably at the apical site of copper, as suggested in [6].

Moreover, we demonstrate that three key parameters should be consider in order to control the oxygen content in these compounds: the size of the A-cation, the oxidising power of the growth atmosphere and the strain state induced by the substrate. A careful choice of these parameters leads to the formation of a doped compounds $ACuO_{2+\delta}$, confirmed by first principle and bond valance sum calculations.

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