Oxygen sub-lattice occupancy in thin cuprate films

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Important development and significant advances in scanning transmission electron microscopy (STEM) have exposed intriguing phenomena in many functional complex oxides originating at the atomic scale. With the introduction of the annular bright-field (ABF)-STEM technique [1] new approaches for direct visualisation of light elements have become possible. Combined imaging of light and heavy elements opened up an elegant way for simultaneous acquisition of ABF- and high-angle annular dark-field (HAADF)-STEM images.

In this work, high quality $NdBa_2Cu_3O_7$ (NBCO) thin films have been deposited on TiO_2 terminated $SrTiO_3$ substrate by high-oxygen-pressure diode sputtering [2].The stacking sequence along the crystallographic c-axis in the NBCO layer is as follows: CuO-BaO-CuO_2-Nd-CuO_2-BaO [3]. The perovskite-type structure layers of NBCO are separated by CuO_2 planes with Nd atoms placed in-between the copper-oxygen planes. Chains of CuO extend parallel to the copper-oxygen planes, where barium atoms are placed between the planes and chains. Major changes of its physical properties can appear due to the oxygen content fluctuations in NBCO [3]. For non-stoichiometric $NdBa_2Cu_3O_{7-x}$, x represents the amount of O vacancies present in the CuO chains.

Atomically resolved quantitative STEM imaging was employed to study thin cuprate films with main emphasis to explore the Cu-O bond distortions in NBCO by using an advanced aberration-corrected JEOL JEM-ARM200F microscope equipped with a DCOR probe corrector operated at 200 kV. Using the simultaneously obtained ABF- and HAADF-STEM images (Figure 1 a,b) we were able to quantitatively analyse the local cation and anion sub-lattices. The improvement of the signal-to-noise ratio as well as the reduction of image distortions was achieved by multiple frame acquisition, where short acquisition times and summing up the images after post alignment highly improved the quality. Using ABF-STEM image simulations we could determine the lowest detectable oxygen concentration present in the CuO chains.

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[2] M Salluzzo *et al.* Phys rev B **78** (2008), 054524.

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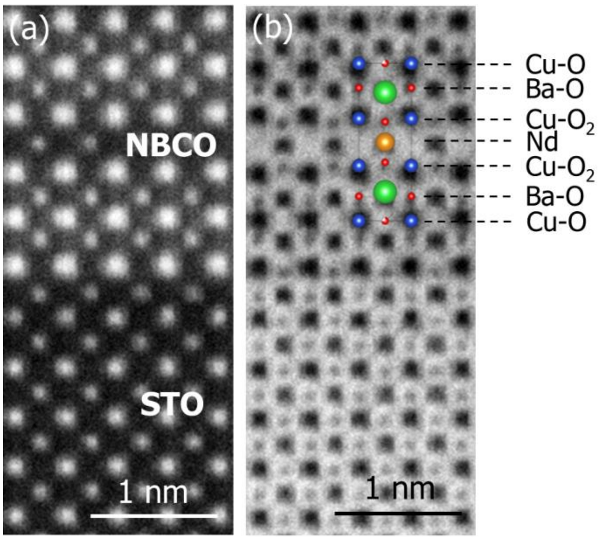

Figure 1: (a) HAADF- and (b) ABF-STEM images of the NBCO/STO interface with an overlay of the NBCO structural model.