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Direct Visualization and Image Simulations of Oxygen Sublattice Occupancy in Thin Cuprate Films

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Functional complex oxides display fascinating phenomena arising at the atomic scale that have been discovered due to considerable progress in scanning transmission electron microscopy (STEM). Significant improvements in technical and methodological development have paved the way to new possibilities for direct visualization of light elements with introduction of the annular bright-field (ABF)-STEM technique [1]. Simultaneous acquisition of ABF- and high-angle annular dark-field (HAADF)-STEM images has enabled concurrent imaging of materials consisting of light and heavy elements.

In the present study, high quality $NdBa_2Cu_3O_7$ (NBCO) thin films have been deposited on TiO_2 terminated $SrTiO_3$ (STO) substrates by high oxygen pressure diode sputtering [2]. The stacking sequence of NBCO layers along the crystallographic c-axis 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 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. The oxygen content fluctuations in NBCO can cause major changes of its physical properties [2]. In non-stoichiometric $NdBa_2Cu_3O_{7-x}$, x means the amount of O vacancies present in the CuO chains. High dependency of Tc on the charge balance between the copper-oxygen planes and copper-oxygen chains has been previously reported [4].

We have used atomically resolved quantitative STEM imaging to explore thin cuprate films with special emphasis on 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. Low magnification HAADF-STEM image of the NBCO thin films are in shown in Figure 1a. Atomic resolution HAADF- and ABF-STEM images of the NBCO/STO interface are shown in Figures 1b,c together with an overlay of the structural model of NBCO. The simultaneously acquired HAADF- and ABF-STEM images enabled us to quantitatively analyze the local cation and anion sublattices and their distortions. In order to improve the signal-to-noise ratio and to reduce image distortions through scanning distortions, HAADF- and ABF-STEM images were acquired as series of frames using a short acquisition time and were post aligned and added to improve counting statistics. In addition, we have employed extensive STEM image simulations (Figure 2). The lowest detectable oxygen concentration present in the CuO chains (as visible in ABF-STEM images) and its relationship to the sample thickness will be discussed.

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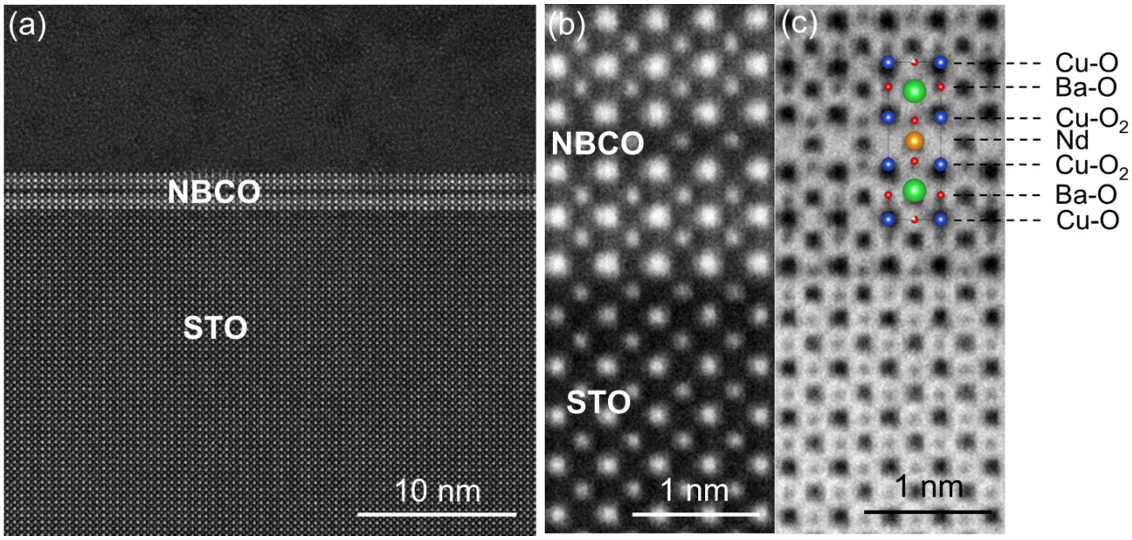

Figure 1. (a) Low magnification HAADF-STEM image of a NBCO thin film grown on a STO substrate. (b) HAADF- and (c) ABF-STEM images of the NBCO/STO interface with an overlay of the NBCO structural model.

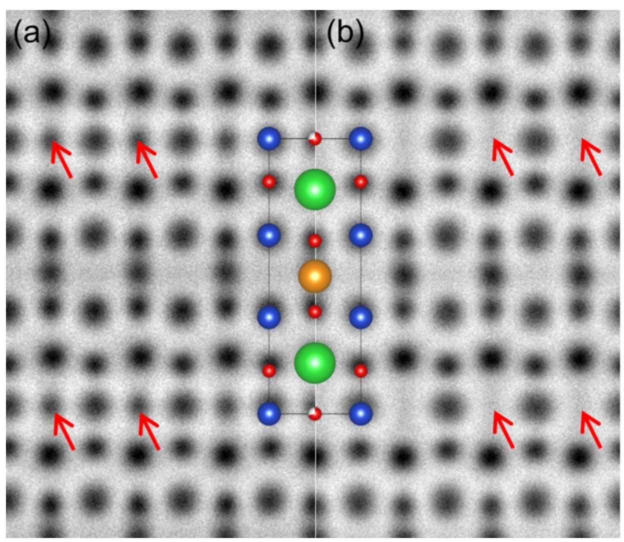

Figure 2. (a,b) Simulated ABF-STEM images at different oxygen occupancies, (a) 0.72 and (b) 0.05. Positions of oxygen atoms in the CuO chains are marked with red arrows indicating the presence/absence of oxygen based on the oxygen occupancy.

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