Determination of interface structure of YBCO/LCMO by a spherical aberration- corrected HRTEM

Z.L. Zhang[1], U. Kaiser[1], S. Soltan[2] and H.-U. Habermeier[2]

1. Materials Science Electron Microscopy, University of Ulm, 89069 Ulm, Germany
2. Max-Planck-Institut für Metallforschung, D-70569, Stuttgart, Germany

zaoli.zhang@uni-ulm.de
Keywords: Cs-corrector, HRTEM, interface

Heterostructure interface plays an important role in modern microelectronics, which could be effectively used to control various electronic and magnetic properties by tuning the atomic structure and chemical composition of the interfaces. The interface also creates new and unexpected phenomena produced by the strong interaction among the electrons. Heterostructure interfaces consisting of superconducting and ferromagnetic manganese oxide attract much attention recently [1-3]. Generally, a chemically pure and atomically sharp interface is needed for achieving particular properties. However, to visualize the atomic structure of interface consisting of light and strong scatters with high precision in detail is only possible by applying spherical-aberration correction techniques [4-5].

Figure 1 is an representative HRTEM image of one interface of a bi-layer heterostructure YBCO($YBa_2Cu_3O_{7-\delta}$)-LCMO($La_{2/3}Ca_{1/3}MnO_3$)-YBCO, which was acquired by an objective-lens Cs-corrected Titan FEI 80-300 microscope under a C_S of -1.0 µm and small over-focus. The image indicates a perfect epitaxial relationship along the *c*-axis due to extreme low mismatch. The orientation relationships in between are: YBCO [001] //LCMO [001] and YBCO [100]//LCMO [110]. Under this condition atoms in the adjacent two layers and the interface are clearly visible and imaged as white atoms, which enable to readily determine the atom types combined with atomic model. Further analysis reveals that the interface is composed of CuO plane and –LaCaO plane. Oxygen atom column contrast is clearer and stronger in the LCMO layer than in YBCO layer. Oxygen contrast is not pronounced in CuO2 chain (but, detectable by line-profile) whereas it is remarkable in BaO chains. Using multislice method [6], simulated HRTEM images based on the atomic model are inserted, which demonstrates reasonable fitting with experimental contrast under similar experimental condition, therefore, corroborating the experimental contrast observed and atom configurations at the interface.

Figure 2 shows the variations of plane spacing over a rectangular area about 3.0 nm by 1.5nm from position A to B. Closely examination on the spacing reveals that the interface spacing (denoted by arrow 1 and 2) is larger, 0.227nm, than the averaged value (denoted by arrow 5 and 6), 0.192 nm, in LCMO layer. Atom planes at the interface slightly expand compared to the adjacent atom planes.

Further HRTEM study, combined with exit wave reconstruction, the whole three layer recorded in one image, reveals that such heterostructure usually exhibits two dis-

S. Richter, A. Schwedt (Eds.): EMC 2008, Vol. 2: Materials Science, pp. 379–380,
DOI: 10.1007/978-3-540-85226-1_190,

tinct interfaces, which are either CuO-LaCaO (as shown in Fig.1.) or BaO-MnO termination layers, one on each side of the LCMO layer.

1 J. Chakhalian, et al, Science **318**(2007)1114.
2 M. Varela, A.R. Lupini, S.J. Pennycook, et al, Solid-State Electronic. **47** (2003) 2245.
3 T. Holden, H.-U. Habermeier, et al , Phy.Rev.B **69**(2004)064505.
4 M. A. O'Keefe, Ultramicroscopy **108** (2008) 196.
5 L. Houben, A. Thust, K. Urban, Ultramicroscopy **106** (2006) 200.
6 A. Chuvilin and U.Kaiser, Ultramicroscopy **104** (2005) 73.

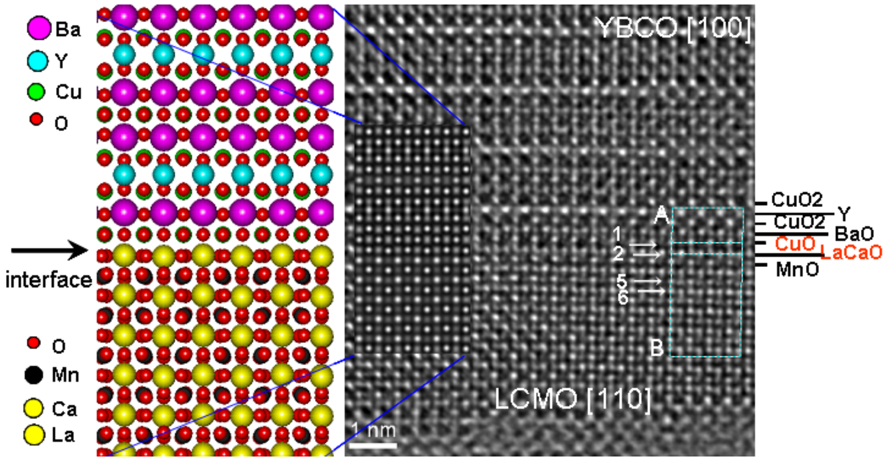

Figure 1 (a) High-resolution image of the interface of YBCO/LCMO recorded under a negative C_S (-1.0 µm) and defocus, where the LCMO terminates in a LaCa-O plane while YBCO terminates in CuO plane. The simulated image based on the atomic model (left) is inserted. Note that oxygen atom column contrast in CuO plane is weak.

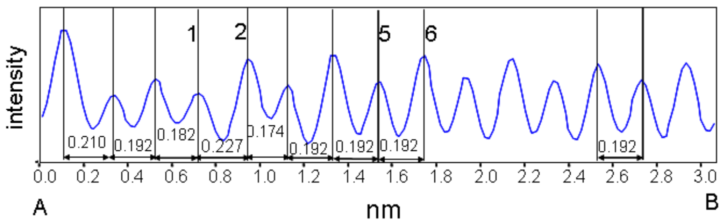

Figure 2. Intensity traces across the interface over a rectangular areas (in Fig.1) illustrating the variation of plane spacing. It is clearly seen that a large spacing exist in the interface, i.e. 0.237 nm. The first neighbor atom planes both in YBCO and LCMO are somehow compressed, which reflect a smaller spacing relative to the averaged values.