HREM characterization of BST-MgO interface

O.M. Zhigalina[1], A.N. Kuskova[1], A.L. Chuvilin[2], V.M. Mukhortov[3], Yu.I. Golovko[3] and U. Kaiser[2]

1. Institute of Crystallography, Russian Academy of Sciences, 119333, Moscow, Russia
2. University of Ulm, Albert-Einstein-Alee 11, 89069, Ulm, Germany
3. South Scientific Centre, Russian Academy of Sciences, 344006, Rostov-on-Don, Russia

zhigal@ns.crys.ras.ru
Keywords: films, ferroelectric, interface

It is known the properties of thin ferroelectric films can be different from bulk materials, that is concerned with an influence of mechanical stress (up to several GPa) at the film – substrate interface [1]. The stress can be partially (or fully) relaxed by means of misfit dislocation formation. So it is necessary to investigate both thin films and heterostucture interfaces at the atomic level to understand relationships between the microstructure and the electrical properties.

High resolution electron microscopy (HREM) is a powerful method for the study of the film – substrate interface at the nanometer scale. Combined with geometric phase analysis, useful information can be obtained concerning local strains, variations in lattice parameters in the region of the film – substrate interface. Image analysis was carried out using especially written scripts for Digital Micrograph 3.5 (Gatan) [2].

For TEM and HREM investigations cross sections were prepared by both ion milling in Gatan PIPs 691 and focussed ion beam (FIB) technique in Quanta 200 3D (SMA Company). All samples were characterized in a Tecnai G^2 30ST and a FEI Titan 80-300 at accelerating voltage of 300kV, using imaging, electron diffraction and high-angle-annular dark-field (HAADF) STEM detector.

$(Ba_{0.8}Sr_{0.2})TiO3$ (BST) thin epitaxial films were deposited on [001]-oriented MgO substrate by rf sputtering. Recently it has been shown [3] the degree of stress in the epitaxialy grown thin films is a function of the film thickness. The method of geometric phase analysis was used to visualize local strains and extrinsic dislocations in the BST-MgO interface for films with different thickness (5 – 1000 nm).

BST thin films revealed a monocrystalline structure with low-angle blocks boundaries ($\theta < 2^0$) (Figure 1). The main reason of the block structure was a surface geometry (holes and hills) of MgO substrate.

Digital analysis of cross sections HREM images (Figure 2) allowed us to visualize and compare misfit dislocations and displacement fields around their cores at the heterostructure interface for films with different thickness.

It has been shown by Z-contrast STEM images and image simulation there are two possible ways of film-substrate atomic bonds at the BST-MgO interface: titan-oxygen or barium-oxygen. Analysis of dark field high resolution STEM images has indicated both variants of bonds can be observed.

S. Richter, A. Schwedt (Eds.): EMC 2008, Vol. 2: Materials Science, pp. 381–382,
DOI: 10.1007/978-3-540-85226-1_191,

1. Y.S. Kim, D.H. Kim, J.D. Kim, et. al., Appl. Phys. Lett., **86** (2005), p.102907
2. A.K. Gutakovskii, A.L. Chuvilin, Se Ahn Song, Izvestiya RAS, ser. phys., **71** (2007) p.1464
3. P.-E. Janolin, Bo-Kuai Lai, Y.I. Yuzuk et. al., Book of abstracts EMF-2007 Bled, Slovenia p.74
4. The work was supported by RFBR grant № 07-02-12259-ofi and the State Program for Support of Leading Scientific schools, project № NSh-1955.2008.2. We kindly acknowledge SMA Company for the help in sample preparation.

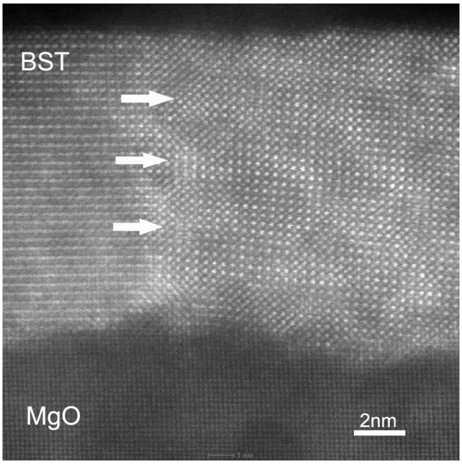

Figure 1. High-resolution dark field image of the block boundary (white arrows) in BST thin film. Cross-section.

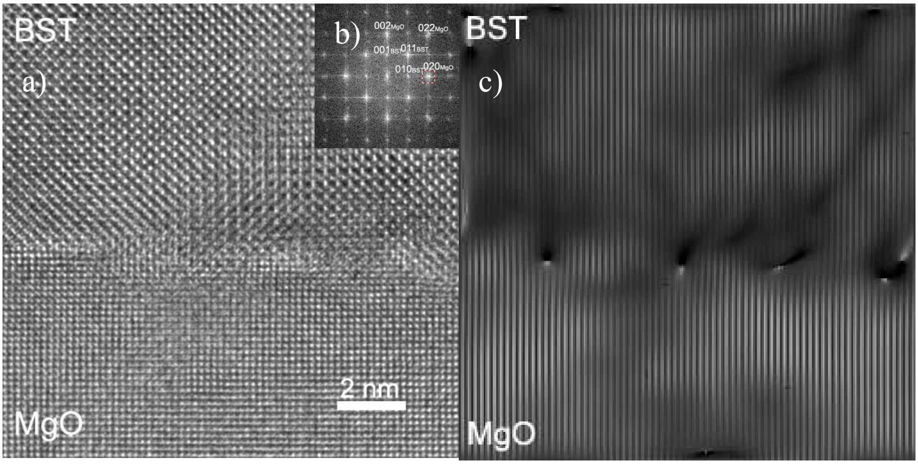

Figure 2. a) HREM image of BST-MgO interface; b) corresponding FFT; c) maps of variations of lattice parameters combined with (020) – filtered image displaying the (020) planes ending the interfacial dislocations.