doi:10.1017/S1431927613009677
Microsc. Microanal. 19 (Suppl 2), 2013

Characterization of Oxide Films Grown on $SrTiO_3$-Buffered Si (001) Substrates

Ajit Dhamdhere[1], Martin D. McDaniel[2], Kristy J. Kormondy[3], Agham Posadas[3], Thong Q. Ngo[2], John G. Ekerdt[2], Alexander Demkov[3] and David J. Smith[1]

[1] Department of Physics, Arizona State University, Tempe, AZ 85287
[2] Department of Chemical Engineering, University of Texas, Austin, TX 78712
[3] Department of Physics, University of Texas, Austin, TX 78712

Epitaxial oxide films and heterostructures integrated with silicon offer great opportunities for the next generation of electronic devices based on novel physical phenomena occurring in thin oxide films. Potential device applications demand very high quality oxide thin films with atomically flat interfaces [1]. Pulsed Laser Deposition (PLD) has historically been the preferred method used for epitaxial oxide film growth. However, the atomic-layer deposition (ALD) method is a potentially attractive alternative since it permits growth at lower temperatures than PLD. In this study, epitaxial films of anatase titanium dioxide and strontium titanate (STO) have been grown by ALD on Si (001) substrates buffered with thin STO layers grown by MBE [2,3]. Four unit cells of STO grown by MBE typically served as the template for the ALD growth. In addition, vicinal substrates in which periodic stepped surfaces are created by cutting single crystal substrates at miscut angles show unique electronic properties such as periodic surface potentials and complete surface reconstruction [4]. Thus, films grown on vicinal STO-buffered Si substrates with original miscut angles of 4° were also examined. Cross-section transmission electron microscopy (TEM) samples were prepared using conventional mechanical and dimple polishing followed by argon-ion-milling to achieve electron transparency. High-resolution TEM images were recorded with a JEM-4000EX operated at 400 keV, with a structural resolution of ~1.7Å, and high-angle annular-dark-field (HAADF) images were recorded with a JEM-2010F STEM operated at 200 keV, with probe size ~2Å.

Observations of the anatase/STO/Si samples revealed that the anatase layer was highly crystalline and well oriented with the substrate, as shown in Fig. 1. A thin layer of amorphous SiO_x (~0.5 nm) was observed at the STO/Si interface of the as-grown sample, but the oxide layer thickness increased significantly (~2.2nm) for samples annealed at temperatures of greater than 250°C, which was attributed to oxygen from the TiO_2 layer oxidizing the silicon substrate. Figure 2 shows that thick layers of ALD-deposited STO are again highly crystalline, with well-separated grain boundaries. No clear interface is visible between the ALD-grown STO and the MBE-grown STO, although a partially amorphized (oxide) layer of ~0.5 nm is visible at places along the STO/Si interface. Figure 3 reveals that MBE-grown STO films deposited on vicinal Si substrates generally follow the topography of the substrate quite well but not always, and the STO is observed to be of excellent crystallinity with some occasional grain boundaries. A partially amorphous layer is sometimes visible in the vicinity of the vicinal steps. The HAADF image in Fig. 4 clearly shows vicinal step heights of 1 or 2 unit cells. Further work to be reported at the meeting will include atomistic modeling of the STO/Si offcut interface and aberration-corrected imaging and spectroscopy.

References:

[1] J. Mannhart, et al., MRS Bulletin 33 (2008) 1027-1034.
[2] M. D. McDaniel, et al., J. Vac. Sci. Technol. B 30 (2012) 04E111.
[3] M. D. McDaniel, et al., J. Vac. Sci. Technol. A 31 (2013) 01A136.
[4] F. Leroy, et al., Phys. Rev. B 76 (2007) 045402.
[5] This work was partly supported by NSF DMR-1006725, ONR N000-14-10-1-0489 and AFOSR. The authors acknowledge use of facilities in the John M. Cowley Center for High Resolution Electron Microscopy at Arizona State University.

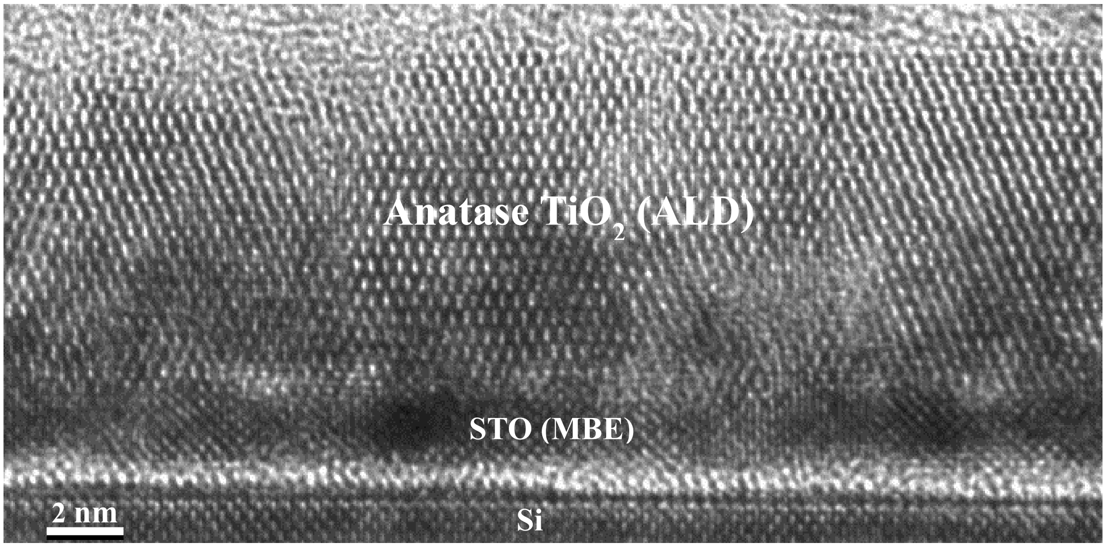

Figure 1: Cross-sectional TEM micrograph of TiO_2 (~10 nm) / STO (~1.5 nm) / Si (001).

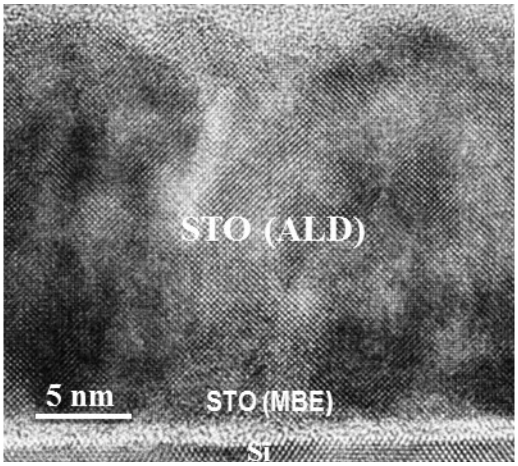

Figure 2: Cross-sectional TEM micrograph of STO (ALD) (~22.5 nm) / STO (MBE) (~1.5 nm) / Si (001).

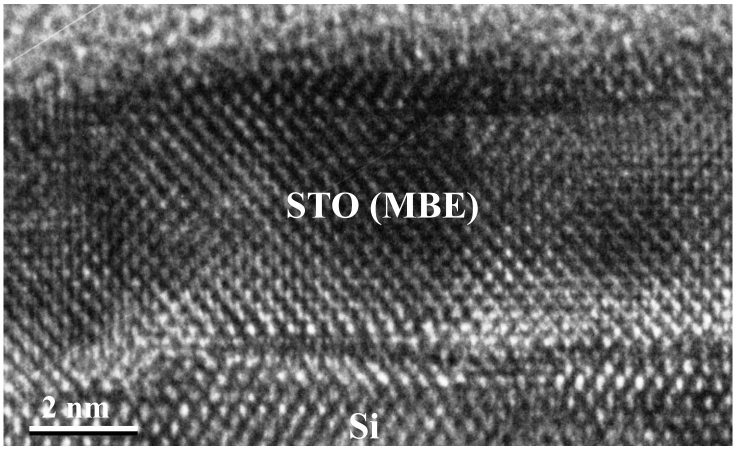

Figure 3: Cross-sectional TEM micrograph of STO (MBE) (~4.7 nm) grown on vicinal silicon (001) substrate.

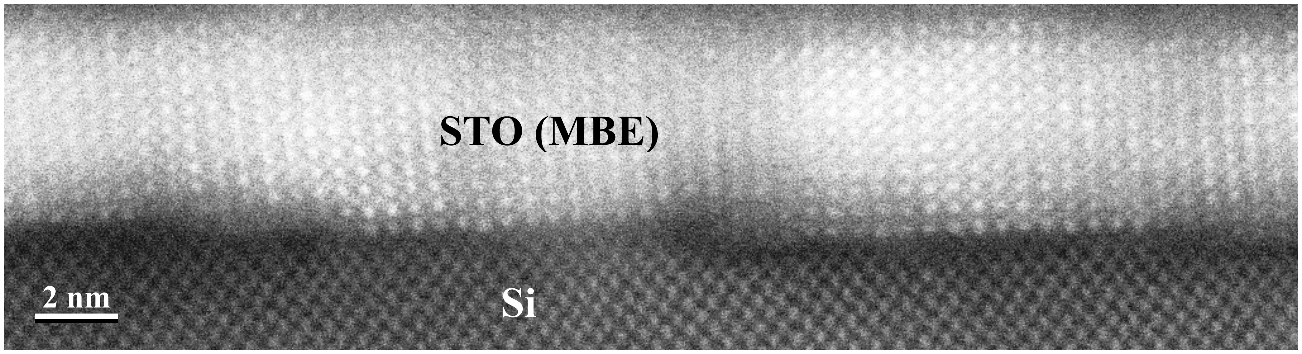

Figure 4: Cross-sectional HAADF image of STO (~4.7 nm) as grown by MBE on vicinal silicon (001) substrate.