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# Direct Observation of Polarization and Charge Transfer at the $BaTiO_3/SrTiO_3/GaAs$ Interfaces

Qiao Qiao[1], Rocio Contreras-Guerrero[2], and Ravi Droopad[2], Robert F Klie[1]

[1.] Department of Physics, University of Illinois at Chicago, Chicago, IL, USA
[2.] Department of Physics, Texas State University, San Marcos, TX, USA

Successful growth of epitaxial oxides on compound semiconductors has been an active goal for several decades now. Because of the structural registration between an oxide and semiconductors in an epitaxial structure, crystalline oxides on III-V semiconductors could potentially provide an interface with lower defect density and better electronic properties than amorphous oxides. While the primary motivation for oxides on GaAs has been the development of a gate dielectric for GaAs-based MOSFETs, heteroepitaxy of crystalline oxides on III–Vs also provides new opportunities for integration of various functional oxides with III–Vs. Perovskite $SrTiO_3$ has been widely used as a substrate for the growth of various functional oxides, such as magnetic, ferroelectric, and piezoelectric oxides; however, $SrTiO_3$ substrates are not available in large sizes and are of poor quality. Currently, $SrTiO_3$ on Si is the most studied epitaxial oxide-semiconductor system[1] and has been used as a means for integrating functional oxides with silicon. Beyond epitaxial oxides grown on Si and Ge, heteroepitaxy of crystalline oxides on III-V semiconductors also suggests new ways for the integration of various functional oxides with high speed electronic and optoelectronic functionalities. Additionally, the deposition of a ferroelectric oxide directly on a high-mobility channel would potentially result in a single-transistor memory element where the polarization state of the ferroelectric layer would determine the state of the transistor.

For the present contribution, 8 nm of $BaTiO_3$ was deposited on 2 unit-cells of $SrTiO_3$ on GaAs (001) using oxide molecular beam epitaxy (MBE), with the overall goal being to characterize the oxide/semiconductor interface using atomic-resolution HAADF/ABF imaging and electron energy loss spectroscopy (EELS). These high-quality $BaTiO_3$ films were achieved using a unique deposition process developed by Droopad[2] using a thin $SrTiO_3$ nucleation layer grown with a ½ ML Ti template layer that allows for commensurate $BaTiO_3$ films to be grown. Because of the close lattice constants between $BaTiO_3$ (with a 45° rotation) and GaAs, it is expected that a thick $BaTiO_3$ layer can be grown which is free from defects and has its *c*-axis oriented in the growth direction leading to out of plane polarization. Recently, it was shown that the $BaTiO_3/SrTiO_3/GaAs$ thin films exhibit ferroelectric polarization[3]. Figure 1 shows atomic-resolution Z-contrast and annular bright field images of $BaTiO_3$[100]/$SrTiO_3$[100]/GaAs[110] and $BaTiO_3$[110]/$SrTiO_3$[110]/GaAs[100] which exhibit atomically sharp interfaces and show no sign of interfacial diffusion or extensive sensitivity to the electron beam. ABF images also show that the first SrO monolayer contacting the GaAs substrate is highly oxygen deficient, and the $SrTiO_3$ buffer layer has an out of plane polarization due to the presence of oxygen vacancies, which can be directly observed by the displacement between Ti and O columns.

A detailed study on the electronic structures at the interface was performed using atomic-resolution EELS and shown in Figure 2. The Ti $L_{2,3}$ edge spectra from the first three Ti columns after the interface show a decreased crystal field splitting compared to bulk $SrTiO_3$, indicating the presence of oxygen vacancies and a distortion of the $TiO_6$ octahedra. The Ti $L_{2,3}$ edge spectrum taken from the $BaTiO_3$ film also suggests that the degeneracy of *3d* $e_g$ orbitals is broken due to the out of plane polarization. O *K* edge spectra show a decreased pre-peak intensity in the $SrTiO_3$ buffer layer, due to the fact that there are

less unoccupied states on the hybrid orbitals between O *2p* and Ti *3d*, which renders screening electrons at the $BaTiO_3/SrTiO_3$ interface.

In short, the epitaxial properties of ferroelectric $BaTiO_3$ grown on GaAs with a $SrTiO_3$ buffer layer have been extensively studied. The $BaTiO_3$ film is free of defects and exhibits an out of plane polarization, while the charge screening effects at both the $BaTiO_3/SrTiO_3$ and $SrTiO_3$/GaAs interfaces have been observed using atomic-resolution HAADF and ABF imaging and EEL spectroscopy. Additionally, the dynamic charge transfer during *in-situ* polarization switching following the application of an electrical bias to the ferroelectric oxide will be discussed.

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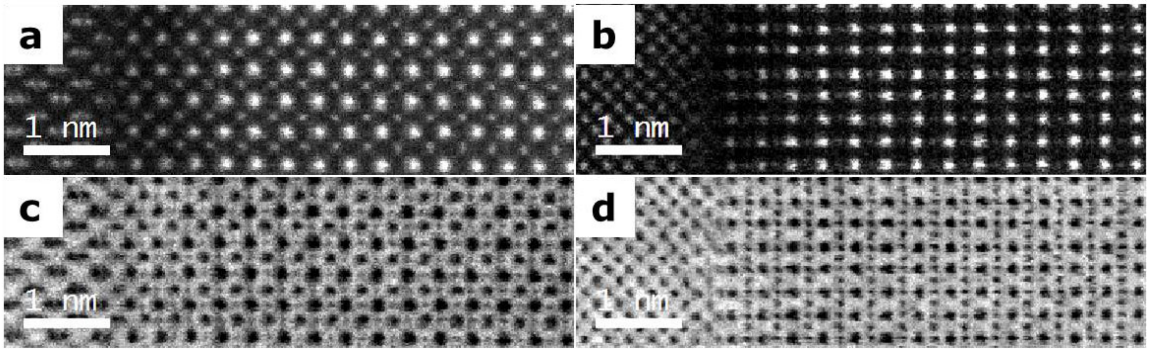


**Figure 1.** Atomic-resolution images exhibit sharp interfaces, oxygen vacancies, and ferroelectric polarization. **a)** HAADF and **c)** ABF images of $BaTiO_3$[100]/$SrTiO_3$[100]/GaAs[110]; **b)** HAADF and **d)** ABF images of $BaTiO_3$[110]/$SrTiO_3$[110]/GaAs[100].

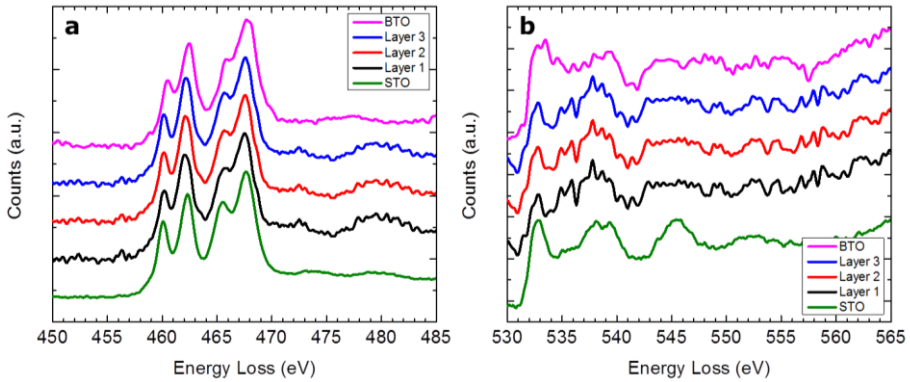


**Figure 2.** EELS of **a)** Ti $L_{2,3}$ edge and **b)** O *K* edge at bulk $SrTiO_3$ (green), 2 unit-cell SrTiO3 buffer layer (black, red and blue) and $BaTiO_3$ film (pink), respectively. The reduced crystal field splitting compared to bulk $SrTiO_3$ reveals the ferroelectric polarization. Charge transfer at the interface can be observed from the decrease of the O *K* edge pre-peak intensity.

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