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Direct Observation of Film Polarization and Oxygen Vacancies at the $BaTiO_3/SrTiO_3/GaAs$ Interface QIAO QIAO, Oak Ridge National Laboratory, ROCIO CONTRERAS-GUERRERO, RAVI DROOPAD, Texas State University, STEPHEN PENNYCOOK, Oak Ridge National Laboratory, SOKRATES PANTELIDES, Vanderbilt University, SERDAR OGUT, ROBERT KLIE, University of Illinois at Chicago — We report successful growth of $BaTiO_3$ thin films on GaAs (001) with a $SrTiO_3$ buffer layer using oxide molecular beam epitaxy (MBE), and investigate the oxide/semiconductor interface using atomic-resolution imaging, electron energy loss spectroscopy (EELS) and first principles density functional theory (DFT). Atomic-resolution Z-contrast and annular bright field (ABF) images of $BaTiO_3/SrTiO_3/GaAs$ reveal 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 in contact with 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 the Ti and O columns. The Ti $L_{2,3}$ and O K edge spectra from the $SrTiO_3/GaAs$ interfacial Ti columns indicate the presence of oxygen vacancies and a distortion of the TiO_6 octahedra. DFT calculations show that O vacancies form preferentially at the $SrTiO_3/GaAs$ interface, where they polarize the $SrTiO_3$, and, in turn, inhibit the ferroelectric switching in the $BaTiO_3$.

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