Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Atomic Resolution and First Principles Study of the Electronic Structure at $SrTiO_3$/GaAs Hetero-interfaces QIAO QIAO, ROBERT KLIE, SERDAR OGUT, University of Illinois at Chicago, RAVI DROOPAD, ROCIO CONTRERAS-GUERRERO, Texas State University — We examined ultra-thin $SrTiO_3$ films deposited on As-terminated GaAs (001) using molecular beam epitaxy under various O_2 partial pressures. Atomic-resolution Z-contrast images of different $SrTiO_3$ films were obtained using the aberration-corrected JEOL JEM-ARM200CF operated at 80 kV. Using atomic-column resolved EELS, our analysis of the Ti and O near-edge fine structure reveals different bonding configurations at the interface resulting from different growth methods. These results strongly suggest that a Ti pre-layer deposition alleviates the oxidation of the substrate and consequently the Fermi level pinning at the interface, as reported before. We also examined $BaTiO_3$ thin films grown on GaAs (001) with an ultrathin $SrTiO_3$ buffer layer. Interfacial charge distribution related to the polarization of $BaTiO_3$ thin film will be studied using atomic-resolution Z-contrast images, annular bright field images and EELS. Using first-principles DFT calculations, we analyze the formation energies of Ti-related impurity defects in different GaAs surface reconstructions to help interpret the electron microscopy experiments.

Qiao Qiao
University of Illinois at Chicago

Date submitted: 19 Nov 2012 Electronic form version 1.4