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Low kV Atomic Resolution and First Principles Study of the Structure and Bonding at $SrTiO_3$/GaAs Hetero-interfaces[1] QIAO QIAO, ROBERT KLIE, SERDAR OGUT, University of Illinois at Chicago — Ultrathin transition-meal oxide films on polar substrates have attracted increasing attention in recent years, due to the emergence of novel interfacial phases, not seen in the bulk of either material. In this study, we have combined aberration-corrected atomic-resolution Z-contrast imaging, electron energy loss spectroscopy (EELS) with first-principles density functional theory calculations to examined the atomic and electronic structures of epitaxially grown, ultrathin $SrTiO_3$ (100) films on GaAs (001). We find that the interface is atomically abrupt and no surface reconstruction of the GaAs (001) surface is observed. Using atomic-column resolved EELS, we show that Ti diffuses into the first few monolayers of GaAs and we will present evidence for the formation of As-oxides at the interface depending on the thin film growth conditions. First-principles DFT calculations will be used to analyze the formation energies of Ti-related impurity defects in the bulk and surface regions of GaAs, as well as the stability of any surface reconstruction at the $SrTiO_3$/GaAs interface. These findings are used to explain transport behavior of the $SrTiO_3$ films as a function of deposition conditions.

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