

Abstract Submitted  
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**Atomic Resolution and First Principles Study of the Structure and Bonding at SrTiO<sub>3</sub>/GaAs Hetero-interfaces**<sup>1</sup> QIAO QIAO, ROBERT KLIE, SERDAR OGUT, University of Illinois at Chicago — Ultrathin metal-oxide films on polar semiconductor surfaces have received much attention in recent years due to occurrence of novel functional properties, including ferroelectricity, superconductivity and the presence of an interfacial 2-dimensional electron gas. In this study, we examine the atomic and electronic structures of epitaxial ultrathin SrTiO<sub>3</sub> (100) films on GaAs (001) using aberration corrected atomic-resolution Z-contrast imaging and electron energy loss spectroscopy (EELS) in combination with first principles calculations to develop a fundamental understanding of the interfacial structure-property relationships. Using atomic-column resolved EELS, we show that Ti diffuses into the first few monolayers of GaAs depending on the thin film growth condition. The effects of Ti diffusion into subsurface GaAs (001) with (4x2)-β2 surface reconstructions will be investigated via first principles calculations. We will also discuss the results for the formation energies of Ti-related impurity defects in the bulk and surface regions of GaAs to help in the interpretation of electron microscopy experiments.

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