

Abstract Submitted  
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**Energetic stability of SrTiO<sub>3</sub> on GaAs(001) interfaces**<sup>1</sup> JOELSON COTT, ROCIO CONTRERAS-GUERRERO, RAVI DROOPAD, BYOUNGHAK LEE, Texas State Univ-San Marcos — The successful growth of epitaxial SrTiO<sub>3</sub> (STO) film on Si substrate using Molecular Beam Epitaxy (MBE) has proved that it is feasible to monolithically integrate the functional oxides with high mobility compound semiconductors [1,2]. While STO has been also deposited on GaAs without amorphous interfacial layers, the exact interface structure has been controversial; while Scanning Transmission Electron Microscopy (STEM) analysis indicates As/Sr interface layers, X-ray diffraction (XRD) measurement shows signs of Ga/SrO interface. Using ab initio calculations, we demonstrate that forming a fully oxidized layer directly on top of GaAs substrate is thermodynamically unstable. Instead, an oxygen-depleted Sr metal layer stabilizes the SrTiO<sub>3</sub>/GaAs interface, in accordance with STEM measurement. We also show that the interface structure observed by XRD is possible under oxygen-rich conditions. The identification of different interface structures and the corresponding growth conditions can be useful for development of growth processes of oxide/semiconductor heterostructures.

[1] R. Contreras-Guerrero et al, J. Cryst. Growth 378, 238 (2013)

[2] R. F. Klie et al, Appl. Phys. Lett. 87, 143106 (2005).

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