Atomic and Electronic Structure of SrTiO$_3$/GaAs Hetero-Interfaces

QIAO QIAO, WERONIKA WALKOSZ, SERDAR OGUT, ROBERT KLINIE, University of Illinois at Chicago — Metal-oxide semiconductor interfaces have received much attention in recent years due to their potential applications in metal-oxide-semiconductor field-effect transistors. In this study we examine the atomic and electronic structures of epitaxial SrTiO$_3[100]$ thin films on GaAs[001] using atomic-resolution Z-contrast imaging and electron energy loss spectroscopy in combination with first principles calculations to develop a fundamental understanding of the interfacial structure-property relationships. We will demonstrate that it is energetically favorable for SrO layer of SrTiO$_3$ to be in direct contact with the terminating As layer of GaAs, as opposed to the TiO$_2$ layer. However, the model with the simplest 1x1 surface unit cell is not in agreement with the photoemission data. First principles total energy calculations will be used to consider how different GaAs(001) surface reconstructions are modified in the presence of SrTiO$_3$ to find the low-energy semiconducting interface. Y. Liang et al., Appl. Phys. Lett., 86 (8), 082905 (2005).

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