

Transmission Electron Microscopic and First-principles Study of SrTiO₃/GaAs Hetero-interfaces

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This SrTiO₃/GaAs interface is primarily being studied due to the interest of using it in metal-oxide-semiconductor field-effect transistors (MOSFETs), where the GaAs substrate would act as the semi-insulating base material and the SrTiO₃ would act as the barrier oxide layer between the GaAs and the gate material. Previously, SrTiO₃ ultra-thin films on As-terminated GaAs substrate have been studied experimentally [1-3]. In this work, various configurations of the SrTiO₃/GaAs interface are considered and characterized using transmission electron microscope (TEM), atomic-resolution Z-contrast imaging and Energy-dispersive X-ray spectroscopy (XEDS), along with first-principles-based density functional theory (DFT) calculations, to study the energetically most favorable configuration and obtain a deep understanding of the structural and electronic properties.

The sample used in this work is grown using molecular beam epitaxy (MBE) method. A 3 nm SrTiO₃ thin film is grown on Si substrate, and covered by a 1 μm thick GaAs layer. The cross-sectional atomic-resolution Z-contrast image (Figure 1) of the SrTiO₃/GaAs interface is obtained using JEOL JEM-3010 TEM at 300 kV. The chemical components are characterized by XEDS. In Figure 1, we can see the typical dumbbell-structure of the GaAs [110] and the SrTiO₃ [100] thin film. A higher resolution Z-contrast image will be obtained from JEOL ARM200CF scanning transmission electron microscopy (STEM) along with XEDS mapping to know the atomic structure and chemical components of the interface in the future work.

First-principles calculations are carried out within the framework of DFT using the projector augmented wave (PAW) method as implemented in the Vienna *Ab initio* Simulation Package (VASP) code with the generalized gradient approximation (GGA) in the scheme proposed by Perdew-Burke-Ernzerhof (PBE). The optimized lattice constant of bulk GaAs (Zinc-blende structure) and SrTiO₃ (perovskite structure) are 5.76 Å and 3.94 Å, respectively. For the thin SrTiO₃ film on GaAs substrate, the lattice constant of SrTiO₃ is set as 4.07 Å to match the GaAs lattice parameters. Double-slab structural model with an 8 Å vacuum in the middle is used to study the SrTiO₃/GaAs hetero-interface (shown in Figure 2). With regard to stoichiometric and non-stoichiometric SrTiO₃ terminated with either SrO or TiO₂ layer in contact with either Ga or As surface, as well as different bonding directions, 32 different configurations of the SrTiO₃/GaAs interface are considered. The formation energy of the interfacial configurations is calculated through the equation

$$E_f = E_{\text{slab}} - n_{\text{Ga}}\mu_{\text{Ga}} - n_{\text{As}}\mu_{\text{As}} - n_{\text{SrO}}\mu_{\text{SrO}} - n_{\text{TiO}_2}\mu_{\text{TiO}_2}.$$

The chemical potential for each component in the equation is constrained by their bulk chemical potentials correspondingly. By comparing the formation energy, non-stoichiometric SrTiO₃ sandwiched by SrO layers are found to be favored in both Ga and As terminated situations. A phase diagram of formation energy comparison for all the interfacial configurations is shown in Figure 3. Non-stoichiometric Ga/SrO interface is found to be energetically most favorable since it occupies the largest area in the phase diagram.

References:

- [1] R. F. Klie *et al*, *Appl. Phys. Lett.* **87** (2005) 143106.
 [2] Q. Qiao *et al*, *Phys. Rev. B.* **85** (2012) 165406.
 [3] Y. Liang *et al*, *Appl. Phys. Lett.* **85** (2004) 1217.
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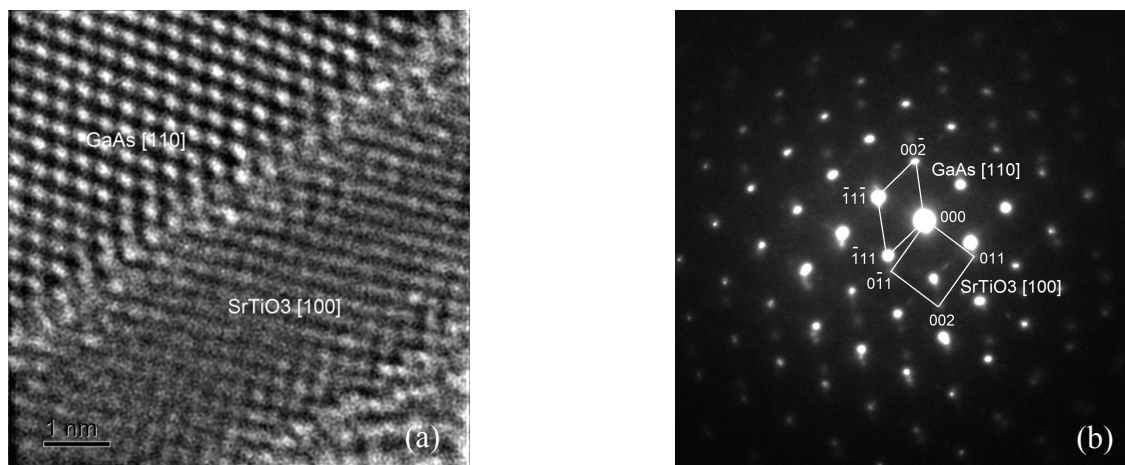


Figure 1 (a) Atomic-resolution Z-contrast image of the SrTiO₃/GaAs hetero-interface. The GaAs is seen in [110] projection while SrTiO₃ is in [100] projection. (b) Diffraction pattern on this condition.

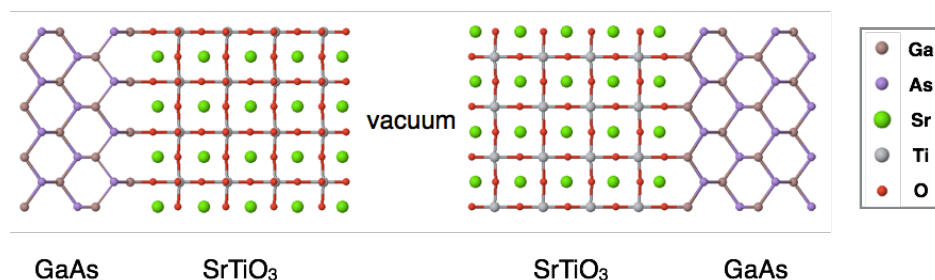


Figure 2 Double-slab structural model used in the DFT calculations. A non-stoichiometric SrTiO₃ terminated with SrO monolayer on the Ga-terminated GaAs substrate is shown in the figure.

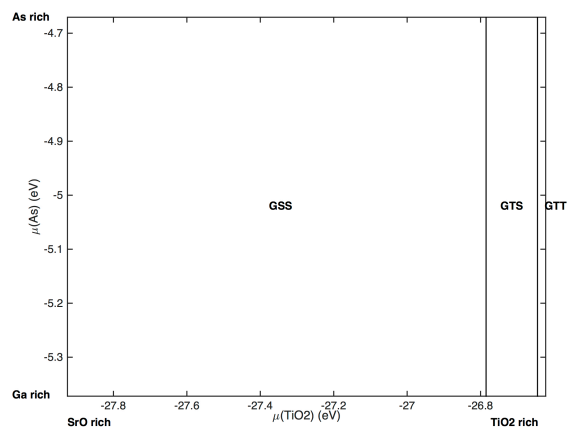


Figure 3 Phase diagram of the formation energy for the interfacial configurations. GSS, GTS, GTT represent the non-stoichiometric Ga/SrO, stoichiometric Ga/TiO₂ and non-stoichiometric Ga/TiO₂ interfaces, respectively.