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Structural Properties of $SrTiO_3$/GaAs Hetero-interfaces

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The $SrTiO_3$/GaAs hetero-interface is being studied due to the interest of using it in metal-oxide-semiconductor field-effect transistors, where the GaAs substrate would act as the semi-insulating base material and the $SrTiO_3$ would act as the barrier oxide layer between the GaAs and the gate material. Previously, $SrTiO_3$ ultra-thin film deposited on As-terminated GaAs substrate have been studied experimentally [1-3]. SrO termination for $SrTiO_3$ is found to be more stable than TiO_2 at the interface. However, whether Ga- or As-terminated GaAs is more stable at the interface remains unclear. In this work, GaAs thin film layers are grown on $SrTiO_3$ instead of using GaAs as substrate. The $SrTiO_3$/GaAs hetero-interface is characterized using atomic-resolution Z-contrast imaging and energy dispersive spectroscopy (EDS) mapping, along with density functional theory (DFT) calculations.

The sample used in this work is grown using molecular beam epitaxy method. A 10 nm Sr-terminated $SrTiO_3$ thin film is grown on Si (001) substrate with a 4° miscut in the [110] direction and a 2 nm thick SiO_2 buffer layer. Simultaneous Ga and As_2 are exposed to the $SrTiO_3$ surface to form a 1 μm thick epitaxial GaAs layer. The Z-contrast images (Figure 1a and b) are obtained using the aberration-corrected JEOL JEM-ARM200CF scanning transmission electron microscopy (STEM) at 200kV. Figure 1a shows the layered structure of the sample. Step structures are observed at $SrTiO_3$ (001) surface. Figure 1b shows the atomic structure at the $SrTiO_3$/GaAs interface, and can be separated into two areas (Area I and Area II) according to the two steps at $SrTiO_3$ surface. In Area I, we find that the $SrTiO_3$[100] direction is parallel to GaAs[110], and the heterointerface appears sharp with the GaAs dumbbells in perfect registry with the O atoms in the SrO terminating layer. Due to the step of one unit cell of $SrTiO_3$ (3.90 Å), 3/4 unit cell of GaAs (4.24 Å) is missing at the interface in Area II. Therefore, GaAs columns in Area II are not perfectly aligned with $SrTiO_3$ columns due to the lattice mismatch as shown in the image. The sequence of the GaAs dumbbell is determined using the intensity line scan in the Z-contrast image along with atomic-resolution EDS mapping as shown in Figure 2a and b. The intensity profile is consistent with the EDS mapping that the sequence of the GaAs dumbbell in the Z-contrast image is Ga-As, which means, at the interface, the GaAs film is terminated with Ga in Area I while terminated with As in Area II as the structural model insets shown in Figure 1b. According to our DFT calculations [4], the SrO/Ga interface with Ga-O bonding is energetically most favorable among all the proposed configurations, which is in good agreement with the Z-contrast image in Area I. The interfacial structure becomes more interesting when $SrTiO_3$ steps are introduced as shown in Area II. A more detailed study of the step structures using electron energy-loss spectroscopy will be presented where the fine structure of interfacial atoms will be examined. [5]

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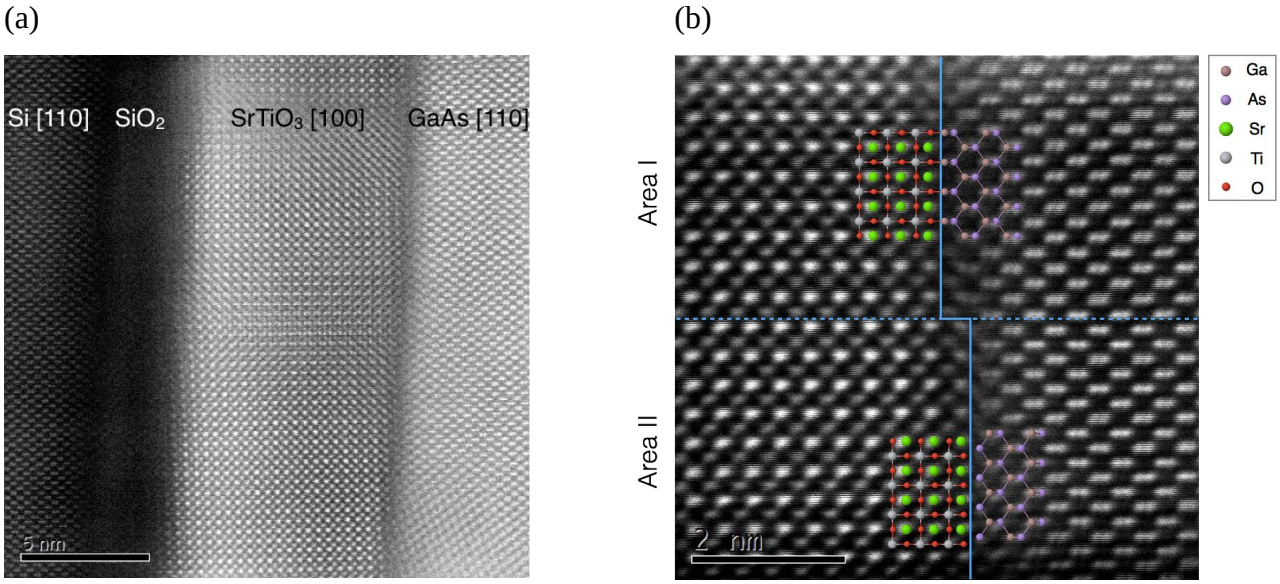

Figure 1 (a) Cross-sectional Z-contrast STEM image of the layered structure of the sample used in this work. (b) (Color online) Atomic-resolution Z-contrast STEM image of the $SrTiO_3$/GaAs hetero-interface. The proposed structural models of the atomic arrangement at the interface are shown as insets. The step structure of the interface is marked by blue solid line. Area I and II are separated by blue dashed line. Radial Wiener Filter within Gatan Digital Micrograph is used to reduce noise in the Z-contrast images.

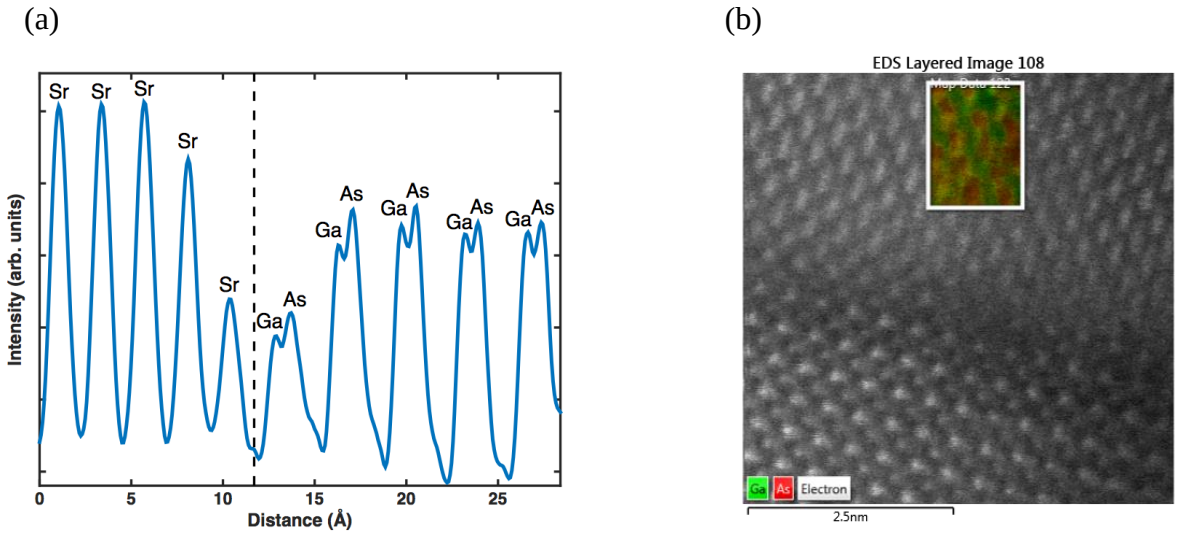

Figure 2 (a) Intensity scan of the Sr/GaAs atomic column in the Z-contrast image in Figure 1b. The dashed line denotes the interface. The intensity is averaged for the eight Sr/GaAs atomic columns in Area I and is smoothed using Gaussian function. Since the intensity is proportional to Z^2, where Z is the atomic number, the intensity of Ga atoms is slightly lower than that of As atoms. (b) (Color online) Atomic-resolution EDS mapping of GaAs near the interface. Ga (As) atoms locate at the lower (upper) positions in the dumbbells.

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