Direct identification of antiphase boundaries in GaSb grown on Si with scanning transmission electron microscopy

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State-of-the-art aberration-corrected transmission electron microscopes have marked a new era in the investigation of interfaces and defects. With sub-angstrom electron probes in scanning transmission electron microscopes, it is possible to pinpoint the individual atomic columns at interfaces and defects. Of particular interest is the study of interfaces in III-V compounds grown on Si. Heteroeptaxial growth of GaSb film on Si has the advantage of low cost and less complexity due to the well-established silicon platform. However, GaSb epilayers on Si suffer from high lattice mismatch and sublattice reversal due to the mixed nucleation and/or the surface steps of Si substrates. It has been observed that the formation of an interfacial misfit dislocation array relaxes the lattice mismatch of the system [1]. The mixed domains formation at the interface due to the incongruent nucleation and/or atomic steps a/4 <001> high at the surface of the Si is expected to induce antiphase boundaries (APBs). APBs contain Ga-Ga and Sb-Sb wrong bonds that are electrically active defects which deteriorate the electronic properties. Here, we report observations of the detailed atomic structure of antiphase boundaries in the GaSb/Si samples using an aberration-corrected microscope in order to elucidate the detailed origins of the defects at the interface with Si.

The GaSb films have been grown by molecular beam epitaxy (MBE) on a Si substrate at 600°C using an AlSb buffer layer. The cross-sectional TEM specimens were polished mechanically using Allied High Tech MultiPrep™ System. The polished wedge specimens were then cleaned using a Technoorg Linda Gentle-mill with 300-800 eV Ar ions for approximately 60 min to remove the residues of polishing contamination. The ultrahigh-resolution Z-contrast high-angle annular dark field images were obtained using an FEI Titan 80-300 “cubed” STEM equipped with a high brightness field-emission gun, an electron monochromator, and a CEOS spherical aberration (Cs) corrector of the probe and image forming lenses. The high mechanical and thermal stability of the dedicated environment of the microscope enabled the measurement of the atomic displacement at antiphase boundaries with geometric phase analysis (GPA) [2].

The HAADF-STEM image in Figure 1(a) displays an APB originating from the interface between GaSb and Si. The contrast change between Ga and Sb columns reveals the faceting of the APB from a vertical direction to other crystallographic orientations. The a/4 <001> displacement of the atomic planes along the growth direction [001] is highlighted by Bragg filtering the HAADF images (Fig. 1(b)). In a detailed view of the interface, we observe that the APB originates on a step of double atomic height (Fig. 1 (c, d)). It is anticipated that the atomic layer sequences remain the same on either side of the double step. The arrow on the left side of Figure 1(c) highlights the domain with a Ga-prelayer. Based on the presence of the mixed domain nucleation we conclude that the APB has originated at the intersection of the Ga-prelayer domain with a Sb-prelayer domain. Based on this high-quality image and high stability of the microscope, we have measured the displacement of atomic columns in the proximity of the APB with GPA. The strain field along the y axis (growth direction), ε_{yy}, shows the strain induced by the APB. This strain is attributed to the different bond length of the antiphase bonds compared to in-phase bonds as measured with atomic resolution (Fig. 2(a)). In order to accommodate the strain of the wrong bonds in the APB, the adjacent atomic bonds shrink or stretch and hence cause the lattice rotation (Figure 2(b)).

This contribution shows that HAADF imaging with aberration-corrected STEM can unambiguously unravel the origin of the APBs. This result indicates that the bonding affinity of Ga and Sb to the Si substrate plays an important role in the formation of APBs [3, 4].

References

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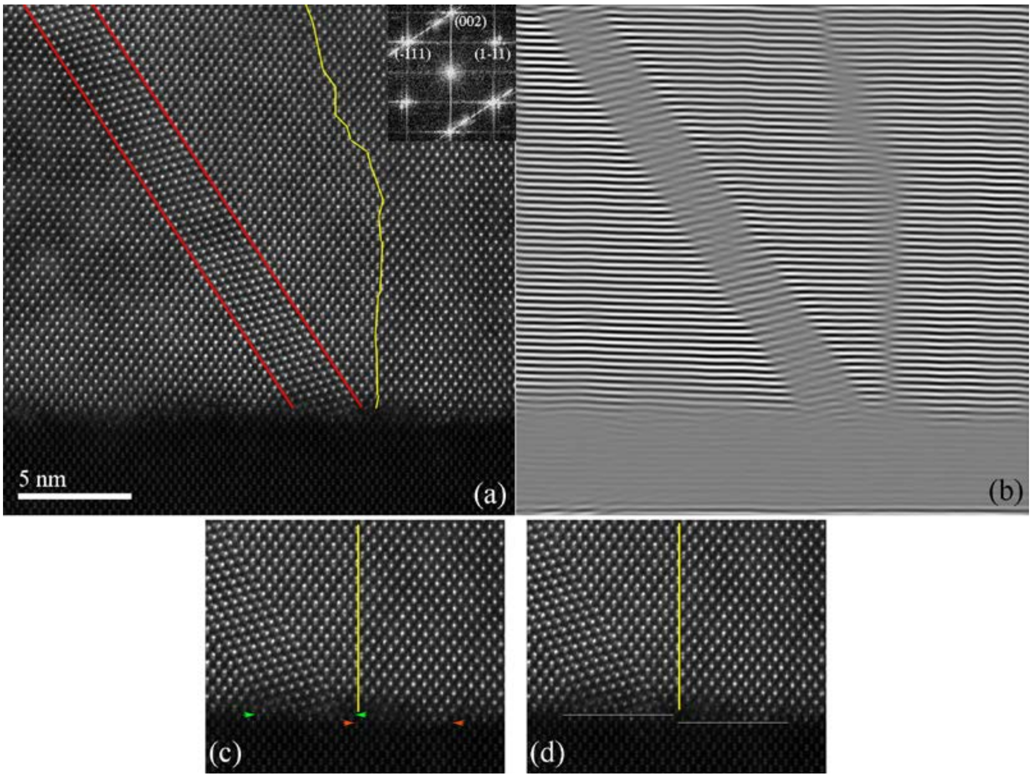

Figure 1. *(a) HAADF-STEM image of GaSb-Si interface with an APB (outlined with the yellow line) with its Fourier transform in the inset, (b) The Fourier filtered image of (a) using the (002) reflection. (c) The magnified image of the interface at the origin of the APB in (a) with arrows displaying the last atomic plane of Si. (d) The white lines highlight the last atomic plane of Si on either side of the boundary.*

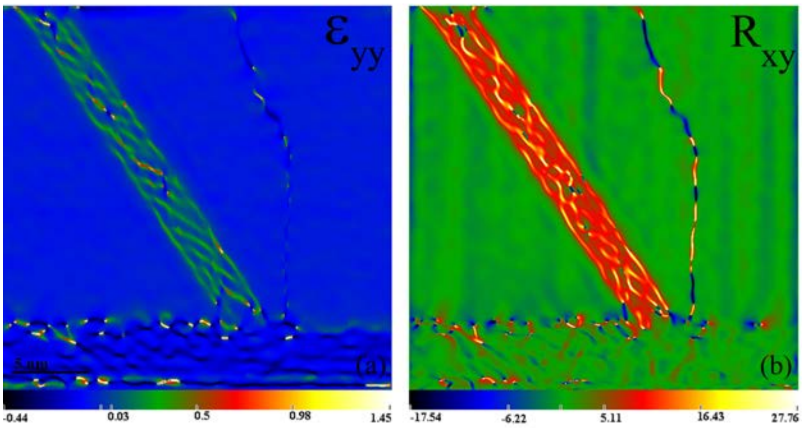

Figure 2. *The strain map (a) perpendicular (ε_{yy}) to the interface and (b) the rotation matrix (R_{xy}).*