

Thickness-Dependent Defect Evolution in GaAs_{0.92}Sb_{0.08}/GaAs Heterostructures

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GaAs_{1-x}Sb_x/GaAs heterostructures are promising candidates for intermediate-band solar cells (IBSCs). Ternary compounds such as GaAs_{1-x}Sb_x facilitate band-gap tuning by introducing an intermediate band between valence and conduction bands. The efficiency of IBSCs can ideally be as high as 63.7% owing to additional photon absorptions related to electron transitions between valence band to intermediate band and intermediate band to conduction band [1]. A major obstacle to achieving high efficiency is the presence of crystallographic defects which act as non-radiative recombination centers. Understanding defect evolution during crystal growth and subsequently minimizing defects by adjusting growth conditions should improve device performance. Defect-free pseudomorphic growth of mismatched materials enabled by molecular beam epitaxy (MBE) is possible up to some critical thickness as the lattice mismatched epilayer is elastically strained to match the substrate lattice. Beyond the critical thickness the accumulated elastic strain is partially relieved by introduction of misfit dislocations. The nature, distribution and density of heteroepitaxial defects are the result of complex inter-related factors such as growth temperature, lattice mismatch, quality of substrate and thickness of epilayer [2]. This study describes the characterization of defect evolution as a function of epilayer thickness in GaAs_{1-x}Sb_x/GaAs heterostructures grown by MBE using GaAs (001) substrates. The Sb content of the epilayers was measured to be ~8% using high-resolution x-ray diffraction. Cross-sectional TEM samples were prepared using conventional polishing, dimpling and argon ion milling. The milling was carried out at 2.7 keV with samples held at liquid nitrogen temperature in order to minimize any milling damage. A Philips-FEI CM-200 microscope operated at 200 keV was used for imaging. Results are reported for GaAs_{0.92}Sb_{0.08}/GaAs heterostructures with thicknesses in the range of 50 to 4000 nm.

Figure 1(a) shows a schematic cross-sectional view of the investigated GaAs_{0.92}Sb_{0.08}/GaAs heterostructures, while Fig. 1(b) illustrates that the heterostructure with a film thickness of 50 nm showed no defects at the interface, which is as expected since this film thickness is considerably less than the calculated critical thickness of 93 nm given the 0.58% lattice mismatch between the two materials. Figure 2(a) shows the presence of dislocations at the interface in the heterostructure with 100-nm-thick GaAs_{0.92}Sb_{0.08} layer. The contrast modulations observable in Fig. 2(b) for the same sample are indicative of slight compositional inhomogeneities in the film during growth, also observed by photoluminescence [3]. Substantial interfacial defects were present in thicker GaAs_{0.92}Sb_{0.08} layers. For example, the interfaces of 500-nm-thick and 4- μ m-thick GaAs_{0.92}Sb_{0.08} layers with the GaAs buffer layer show the presence of a high density of misfit dislocations, as evident from Fig. 3(a) and (b). Further observations of materials with intermediate thicknesses are ongoing to gain more detailed information about the mechanisms for stress relaxation via interfacial dislocations and threading defects [4].

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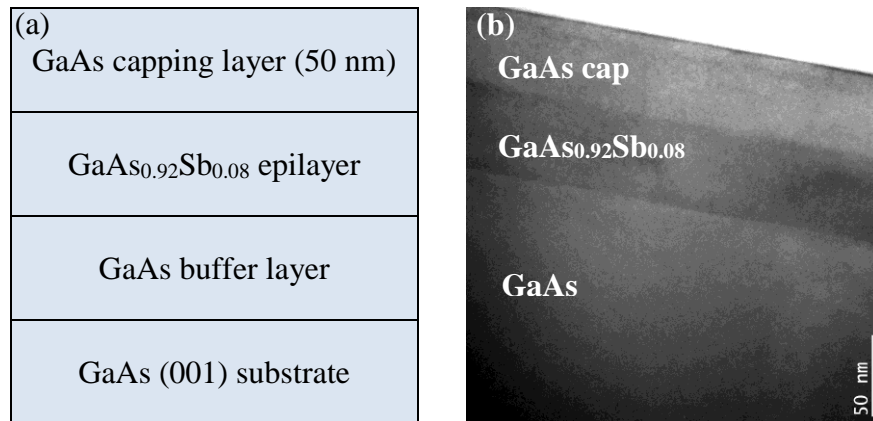


Figure 1. (a) Schematic cross-sectional view of GaAs_{0.92}Sb_{0.08}/GaAs heterostructure, (b) low magnification TEM image of the heterostructure with 50-nm-thick epilayer.

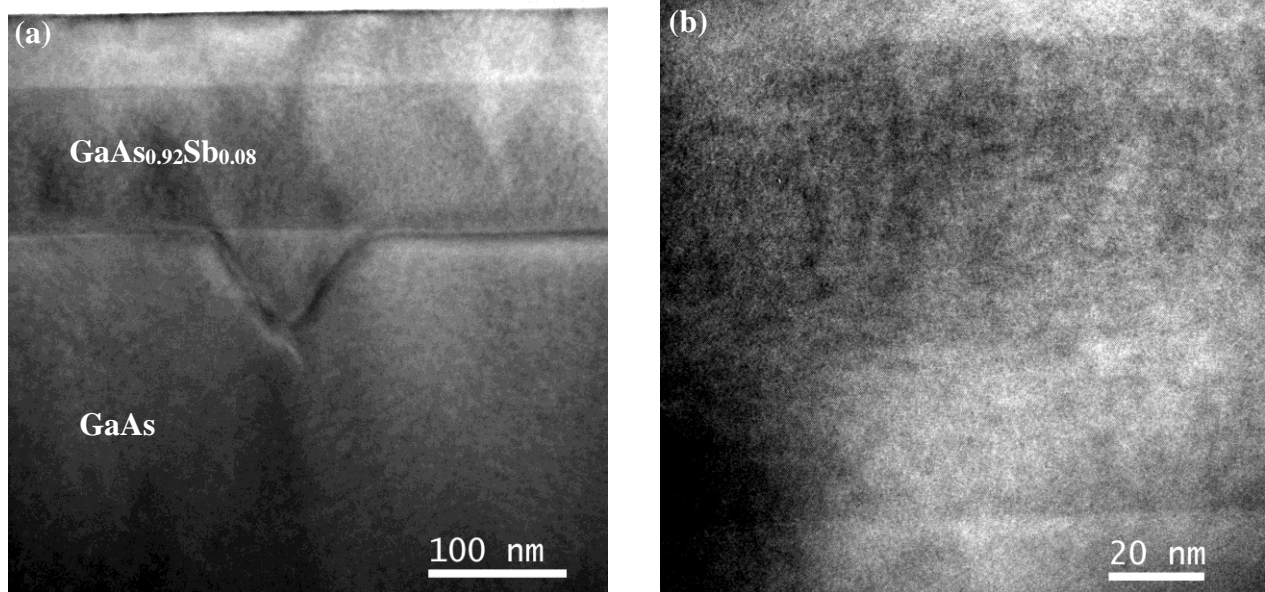


Figure 2. (a) Cross-sectional TEM image of the heterostructure with 100-nm-thick epilayer showing presence of interfacial defect, (b) Contrast modulation across the epilayer in the same heterostructure indicates slight compositional inhomogeneity.

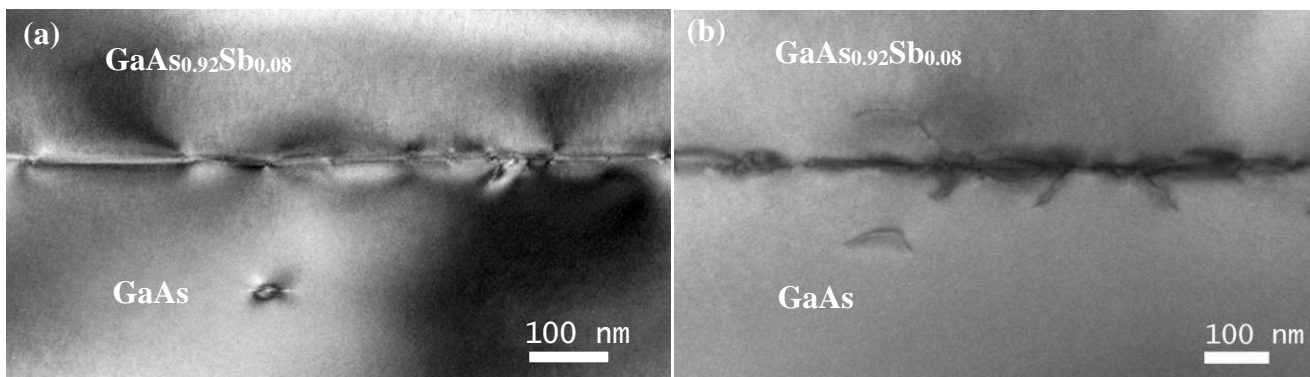


Figure 3. TEM images of the heterostructures with (a) 500 nm, and (b) 4 μm, epilayers showing misfit dislocations at GaAs_{0.92}Sb_{0.08}/GaAs interface.