

## Defect Evolution in GaAs-based Low-mismatch Heterostructures

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Epitaxial growth of thin films of ternary semiconductors such as  $\text{In}_{1-x}\text{Ga}_x\text{As}$  on GaAs substrates enables band-gap engineering which is very useful for many device applications such as intermediate-band solar cells, lasers, light-emitting diodes, etc. Due to the difference in lattice parameters between film and substrate, the film/substrate interface is subjected to bi-axial misfit strain leading to the introduction of misfit dislocations which are liable to act as non-radiative recombination centers, that are highly deleterious for device performance. Characterization of interfacial defects in these heterostructures is critical for developing a fundamental understanding of strain relaxation processes and eventually finding a path towards minimizing defect density by optimizing growth conditions, film thickness, etc. In this study, transmission electron microscopy (TEM) was used to investigate defect evolution in molecular beam epitaxy-grown low-mismatch (misfit strain  $\sim 0.6\%$ )  $\text{GaAs}_{0.92}\text{Sb}_{0.08}/\text{GaAs}$  (001) and  $\text{In}_{0.08}\text{Ga}_{0.92}\text{As}/\text{GaAs}$ (001) heterostructures with film thicknesses in the range of 50 to 4000 nm. All samples had a GaAs capping layer of 50-nm thickness. Plan-view and cross-sectional TEM samples were prepared by polishing, dimpling and liquid-nitrogen argon-ion milling. Philips-FEI CM-200 FEG and JEOL ARM-200F microscopes operated at 200 keV were used for bright-field TEM and aberration-corrected scanning transmission electron microscopy (STEM) imaging, respectively.

Figure 1(a) shows a representative plan-view TEM image revealing asymmetric distribution of misfit dislocations along orthogonal  $\langle 110 \rangle$  directions at the film/substrate interface of the heterostructure with 100-nm  $\text{GaAs}_{0.92}\text{Sb}_{0.08}$  layer. **g.b** analysis confirmed that the straight non-periodic misfit dislocations in fig. 1(a) were of  $60^\circ$  type. The asymmetric distribution of  $60^\circ$  misfit dislocations at the initial stage of relaxation is often attributed to different mobility of the two types of  $60^\circ$  dislocations known as  $\alpha$ -dislocations (As-terminated core) and  $\beta$ -dislocations (Ga-terminated core). The asymmetry, however, disappears in thicker films when rapid strain relaxation occurs. Figure 1(b) shows misfit dislocation distribution at the film/substrate interface of the heterostructure with 250-nm-thick  $\text{GaAs}_{0.92}\text{Sb}_{0.08}$  layer, which has undergone rapid relaxation. The asymmetric distribution of  $60^\circ$  dislocations was observed (see fig. 1(c)) at the cap/film interface when the film is sufficiently relaxed to exert sufficient tensile strain to trigger plastic deformation in the capping layer. A simple method was developed to distinguish between the two  $\langle 110 \rangle$  directions in plan-view orientation, which involved crystal polarity determination by matching experimental convergent beam electron diffraction patterns with simulated patterns in  $\langle 110 \rangle$  zone-axis orientation. By measuring dislocation spacing from collage of images recorded from an area of over  $100 \times 100 \mu\text{m}^2$  along the  $\langle 110 \rangle$  directions, it was found that  $\beta$ -dislocation density was higher at the compressively-strained film/substrate interface in both  $\text{InGaAs}/\text{GaAs}$  and  $\text{GaAsSb}/\text{GaAs}$  heterostructures whereas  $\alpha$ -dislocation density was higher at the tensile-strained cap/film interface. Possible mechanisms explaining this kind of asymmetry reversal will be discussed.

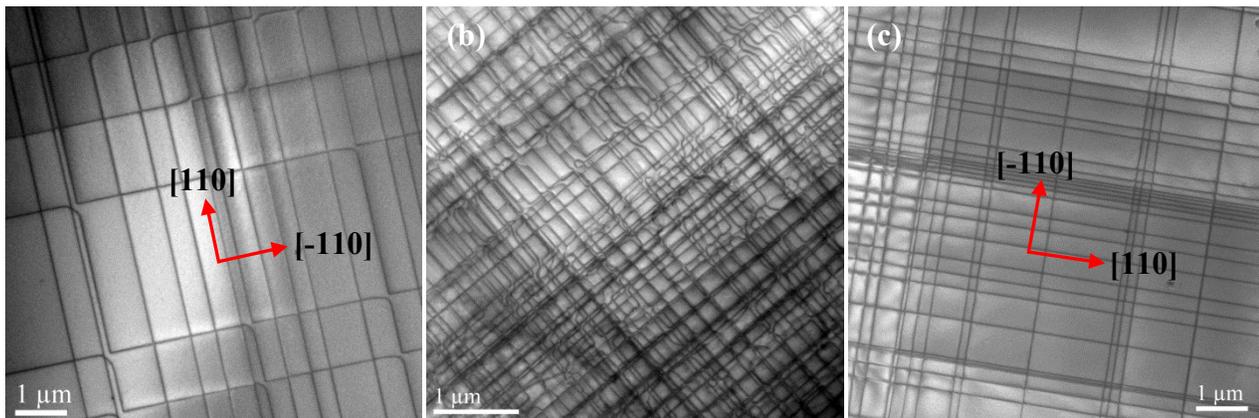
Atomic-resolution high-angle annular-dark-field (HAADF)-STEM imaging was used to obtain information about the atomic arrangement at the defect-cores. All  $60^\circ$  misfit dislocations at both

film/substrate and cap/film interface were found to be dissociated. Figure 2(a) shows atomic-resolution HAADF-STEM image of an intrinsic stacking fault (ISF) located at the film/substrate interface of the heterostructure with 1000-nm-thick GaAs<sub>0.92</sub>Sb<sub>0.08</sub> layer. Burgers circuit analysis showed that this ISF was created by dissociation of a perfect 60° dislocation with  $\mathbf{b} = a/2[0\bar{1}1]$  and bounded by 90° partial dislocation with  $\mathbf{b} = a/6[11\bar{2}]$  and 30° partial dislocation with  $\mathbf{b} = a/2[1\bar{2}1]$  at its two ends. The core of the 30° partial dislocations in most cases was comprised of an unpaired atomic column. Comparison with structural models (shown in fig. 2(b)) proposed by previous authors [1] led to the conclusion that 60° misfit dislocations in these systems were predominantly of glide character. In addition to ISFs, atomic-resolution images of Lomer edge dislocations and stair-rod dislocations were also obtained. Atomic structure of these dislocation-cores will be discussed in detail. [2]

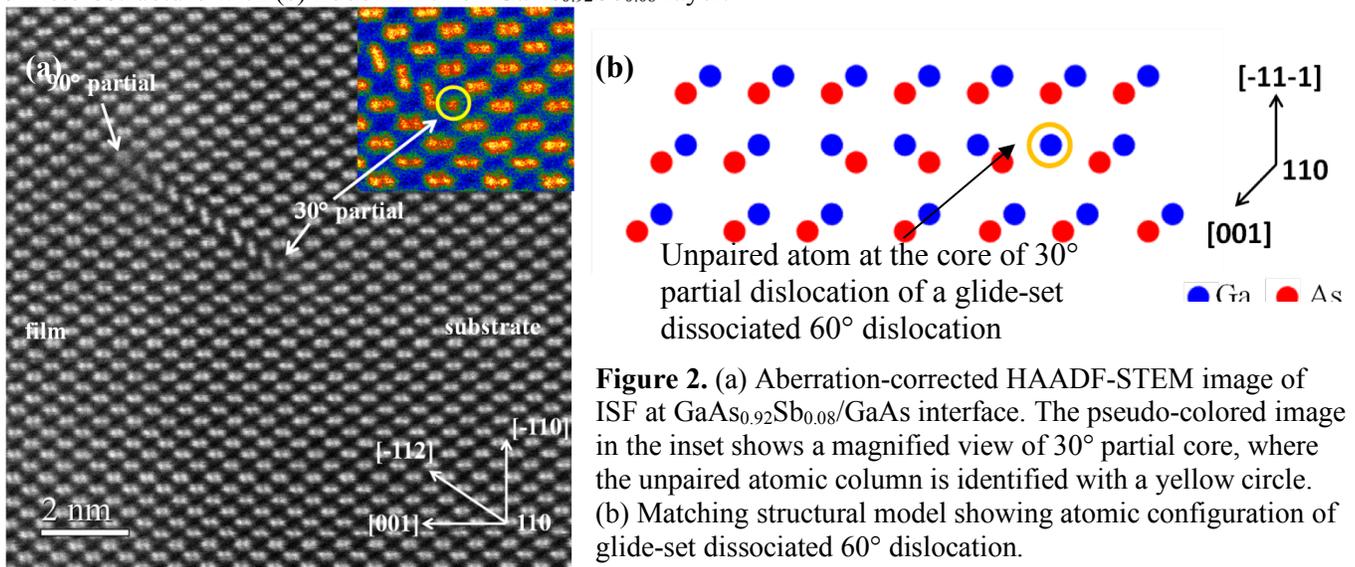
References:

[1] J. P. Hirth and J. Lothe, Theory of Dislocations, 2nd ed. (Wiley, New York) 1982.

[2] This work was supported by the National Science Foundation and the Department of Energy under NSF CA No. EEC-1041895. The authors acknowledge the use of facilities within the John M. Cowley Center for High Resolution Electron Microscopy at Arizona State University.



**Figure 1.** Plan-view <001> TEM images showing distribution of misfit dislocations at the film/substrate interface of heterostructures with (a) 100-nm-thick, and (b) 250-nm-thick GaAs<sub>0.92</sub>Sb<sub>0.08</sub> layer, and at the cap/film interface of heterostructure with (c) 2000-nm-thick GaAs<sub>0.92</sub>Sb<sub>0.08</sub> layer.



**Figure 2.** (a) Aberration-corrected HAADF-STEM image of ISF at GaAs<sub>0.92</sub>Sb<sub>0.08</sub>/GaAs interface. The pseudo-colored image in the inset shows a magnified view of 30° partial core, where the unpaired atomic column is identified with a yellow circle. (b) Matching structural model showing atomic configuration of glide-set dissociated 60° dislocation.