

## Atomic Structure of Extended Defects in GaAs-based Heterostructures

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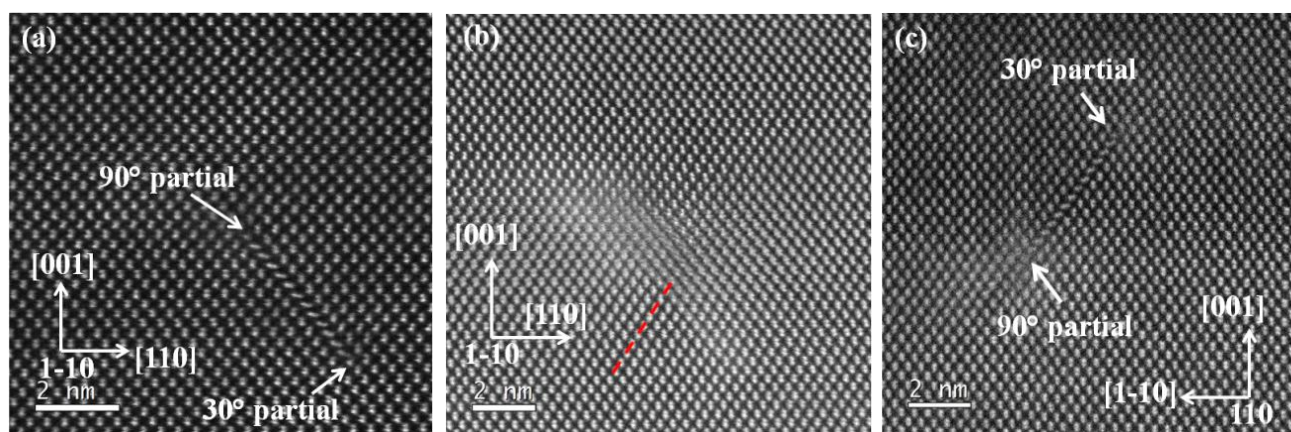
The atomic structure of defects is important to understand since this determines the relaxation kinetics in semiconductor heterostructures as well as electronic properties. Interactions with point defects/impurities, and other line defects, as well as reconstruction of the defect core to locally minimize the distortion field, create numerous possibilities for structural arrangements of the defects. Recent advances in aberration correction for the transmission electron microscope have led to the achievement of sub-angstrom resolution. Thus, atomically-resolved images of defects can be routinely obtained, providing an opportunity to characterize structural defects with greater detail. In this work, extended defects have been investigated using probe-corrected scanning transmission electron microscope (STEM), in a range of GaAs(001)-based epitaxial heterostructures grown by molecular beam epitaxy. The TEM samples were prepared using conventional mechanical polishing, dimpling and argon ion-milling at liquid-nitrogen temperature. A JEOL ARM-200F operated at 200 kV was used for high-angle annular dark-field (HAADF)-STEM imaging. The probe convergence angle was 22 mrad, and the inner and outer angles for HAADF-STEM imaging were 90 and 150 mrad.

Strain relaxation in low-mismatched heterostructures was primarily carried out by dissociated 60° dislocations. Figure 1(a) shows a HAADF-STEM image of a misfit dislocation at the film/substrate interface of an In<sub>0.08</sub>Ga<sub>0.92</sub>As/GaAs heterostructure (misfit strain ~ 0.6%). Burgers circuit analysis identified a dissociated 60° dislocation bounded by 30° and 90° Shockley partials at its two ends. The 30° Shockley partials had a characteristic single atomic column at their core, indicating that these dislocations belonged to glide set. The leading 30° partials of negative dislocations on intersecting glide planes often interacted to form Lomer-Cottrell locks with sessile  $a/6\langle 110 \rangle$  stair-rod dislocations in compressively-strained heterostructures. Hirth locks with  $a/3\langle 001 \rangle$  stair-rod dislocations were not observed as their formation would require a reaction between negative and positive dislocations, whereas only negative dislocations were created to relieve misfit strain in these compressively-strained heterostructures. The density of perfect 60° dislocations was much reduced compared to dissociated 60° dislocations. Figure 1(b) shows a HAADF-STEM image of a perfect 60° dislocation located close to the In<sub>0.08</sub>Ga<sub>0.92</sub>As/GaAs interface. The extra-half plane has been marked by a red dashed line. The majority of the misfit dislocations in tensile-strained GaAs<sub>0.9</sub>P<sub>0.1</sub>/GaAs (misfit strain ~ 0.4%) heterostructures were dissociated 60° dislocations bounded by 90° and 30° partials. Figure 1(c) shows a HAADF-STEM image of a dissociated 60° dislocation at the GaAs<sub>0.9</sub>P<sub>0.1</sub>/GaAs interface. Although formation of  $a/3\langle 110 \rangle$  stair-rod dislocations by the interaction of leading 90° partials of positive misfit dislocations on intersecting {111} glide planes is energetically favorable, such defect configurations were not observed. Figure 2(a) shows a bright-field STEM image of a growth defect extending all the way through the epitaxial film to its top surface. This defect originated at about 142 nm underneath the film/substrate interface in the GaAs buffer layer. Figure 2(b) shows a HAADF-STEM image illustrating that the defect started as an intrinsic stacking fault but transformed into a coherent twin upon operation of Shockley partial dislocations on adjacent {111} planes.

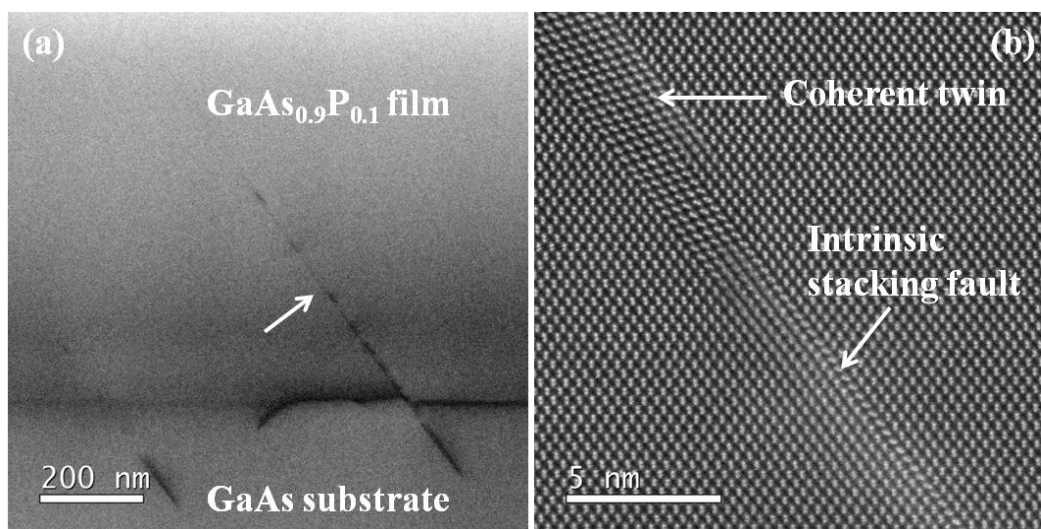
Strain in high-mismatched heterostructures can be spontaneously released by the formation of an array of  $90^\circ$  Lomer dislocations at the film/substrate interface. The atomic configuration of these dislocation cores in technologically important systems such as GaSb/GaAs(001) (misfit strain  $\sim 7.8\%$ ) is not well-understood. Further investigations are ongoing to unravel the core structure of Lomer dislocations at GaSb/GaAs hetero-interfaces. [1]

#### References:

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**Figure 1.** Aberration-corrected HAADF-STEM images: (a) Interfacial dissociated  $60^\circ$  dislocation in  $\text{In}_{0.08}\text{Ga}_{0.92}\text{As}/\text{GaAs}(001)$  heterostructure; (b) Perfect  $60^\circ$  dislocation in  $\text{In}_{0.08}\text{Ga}_{0.92}\text{As}/\text{GaAs}(001)$  heterostructure; and (c) Interfacial dissociated  $60^\circ$  dislocation in  $\text{GaAs}_{0.9}\text{P}_{0.1}/\text{GaAs}(001)$  heterostructure.



**Figure 2.** (a) Bright-field STEM image showing defect (indicated by white arrow) that extends through the entire film of  $\text{GaAs}_{0.9}\text{P}_{0.1}/\text{GaAs}$  heterostructure; (b) Atomic-resolution HAADF-STEM image reveals that the defect nucleates as intrinsic stacking fault, but transforms into a twin fault.