

Molecular beam epitaxy of III-V semiconductors on group-IV (001) substrates: Formation and burying of antiphase domains.

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Abstract — We report on the formation and evolution of antiphase domains (APDs) in III-V layers grown on Si and Ge group-IV substrates. We show that the formation mechanism and morphology of the APDs depends on the material. The in-depth analysis of GaSb growth on both Si and Ge reveals APD burying due to growth rate differences between main and antiphase domains. In contrast, III-As semiconductors show a growth mechanism involving facets.

Keywords— semiconductor, III-V on Si, heteroepitaxy, monolithic integration, antiphase domain

The hyperconnectivity revolution opens the door to new technological opportunities, such as the IoT although it raises challenges. To keep improving performances, integrating III-V optoelectronic devices with Silicon photonic integrated circuits (PICs) is considered a promising option.

The monolithic integration, or direct epitaxy, of III-V semiconductors on Si platforms translates into the formation of a large density of defects compared to the growth on native substrates. Lattice mismatch, thermal expansion coefficient mismatch, and polarity mismatch are respectively responsible for dislocations, cracks, and antiphase domains (APDs) and boundaries (APBs). A mechanism of formation and burying of the antiphase domains for III-V layers grown on Si was recently proposed by Cornet *et al.* [¹]. According to this model, when the main domain and the APDs are populated by parallel steps, *i.e.* by steps of different compositions, the main domain grows faster than the APDs because the incorporation rate at the steps is different, and the APDs get progressively buried. This model was later demonstrated to be valid for the case of the growth of GaSb on Silicon (001) substrates [²].

Recently, we conducted similar studies with other combinations of III-V materials (GaSb, GaAs, InAs) and group-IV substrates (Si, Ge) to check the universality of the model. We combined reflection high-energy electron diffraction (RHEED), X-Ray diffraction (XRD), and atomic force microscopy (AFM) to analyze the structure and the surface properties of the layers grown on the various substrates. Different APD morphologies were obtained (Figure 1 top), which we relate to the nature of the material being grown as well as to the growth conditions. Emerging-APB-free GaAs and InAs layers were also successfully grown (Figure 1 bottom). The analysis of the different atomic step distribution at the surface, and of the overgrowth mechanisms for GaAs and InAs is in progress and will be discussed in detail at the conference.

Our work thus provides detailed insights into the formation and burying of APDs during the growth of a variety of III-V materials on group-IV substrates.

¹ “Zinc-blende group III-V/group IV epitaxy: Importance of the miscut”, C. Cornet *et al.* Phys. Rev. Mat.4, **053401** (2020), DOI:10.1103/PhysRevMaterials.4.053401

² “Crystal Phase Control during Epitaxial Hybridization of III-V Semiconductors with Silicon”, Marta Rio Calvo *et al.* Adv. Electron. Mater, **8**, **2100777** (2022), DOI: 10.1002/aelm.202100777

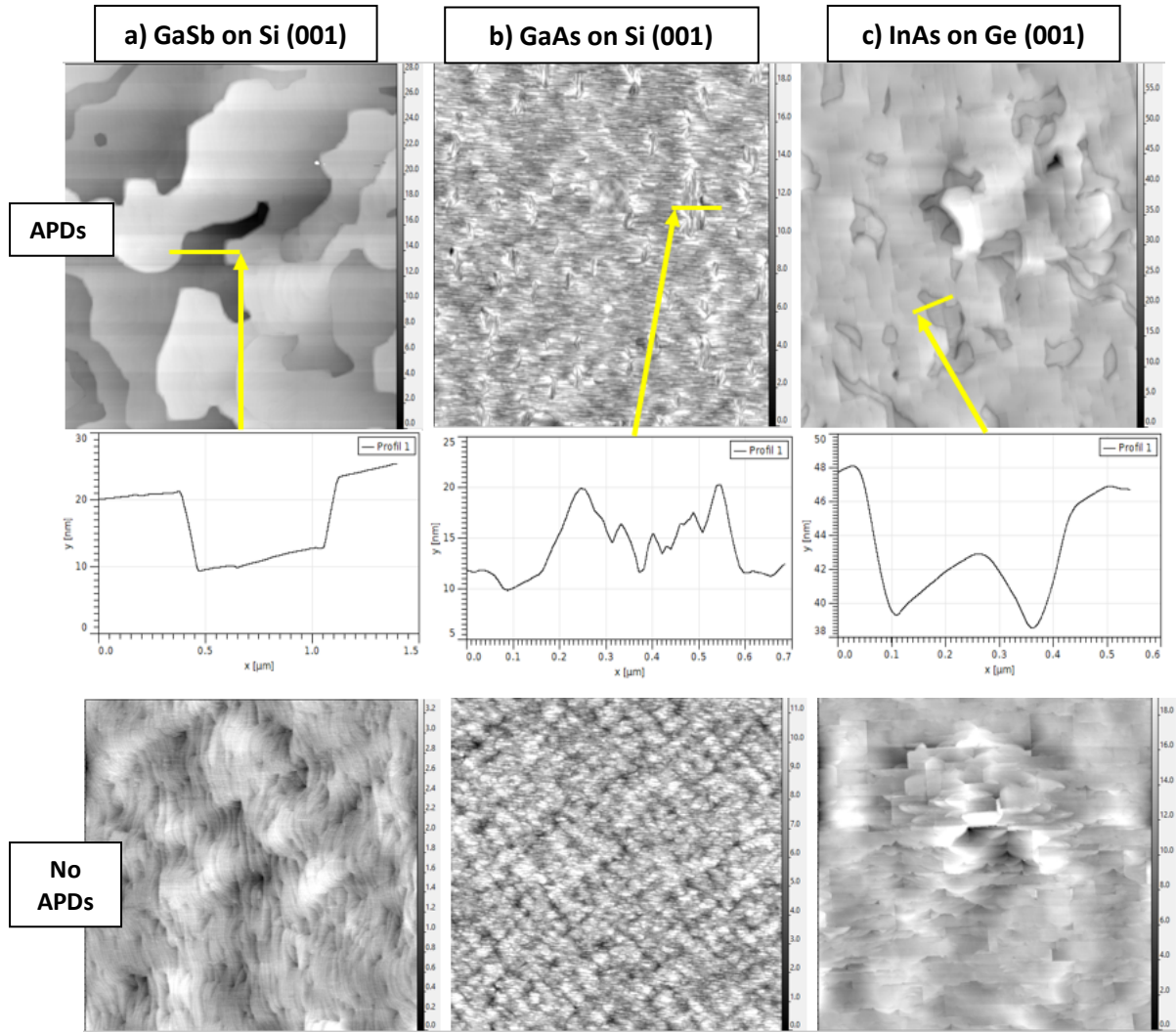


Figure 1: 5 μm x 5 μm AFM image of **a)** GaSb on Si (001), **b)** GaAs on Si (001), **c)** InAs on Ge (001) layers with (top panel) and without (bottom panel) APDs. The AFM profiles of the layers with APDs are displayed in the middle panel. Two different plateaus corresponding to the main and antiphase domain (MPD and APD) are clearly identified for GaSb. In contrast, facets are visible for both GaAs and InAs. After APD burying, the GaSb surface exhibits a nicely stepped morphology, which is less clear on III-As layers.