Interface-Driven Faceted Epitaxy of GaAs on Si(331) with Self-Organized Nanocorrugation and Anisotropic Emission (Supplementary Material)

R. Méndez-Camacho[1], E. Cruz-Hernández[2],* J. Alanis[2], E. H. Sánchez-Martínez[2], M. A. Zambrano-Serrano[1], E. A. Cerda-Méndez[3], M. A. Vidal[2], and M. López-López[1]
[1] *Physics Department, CINVESTAV.* [2] *CIACYT-UASLP.* [3] *IICO-UASLP.*
(Dated: August 12, 2025)

A. RHEED and Surface Evolution at the Initial stages

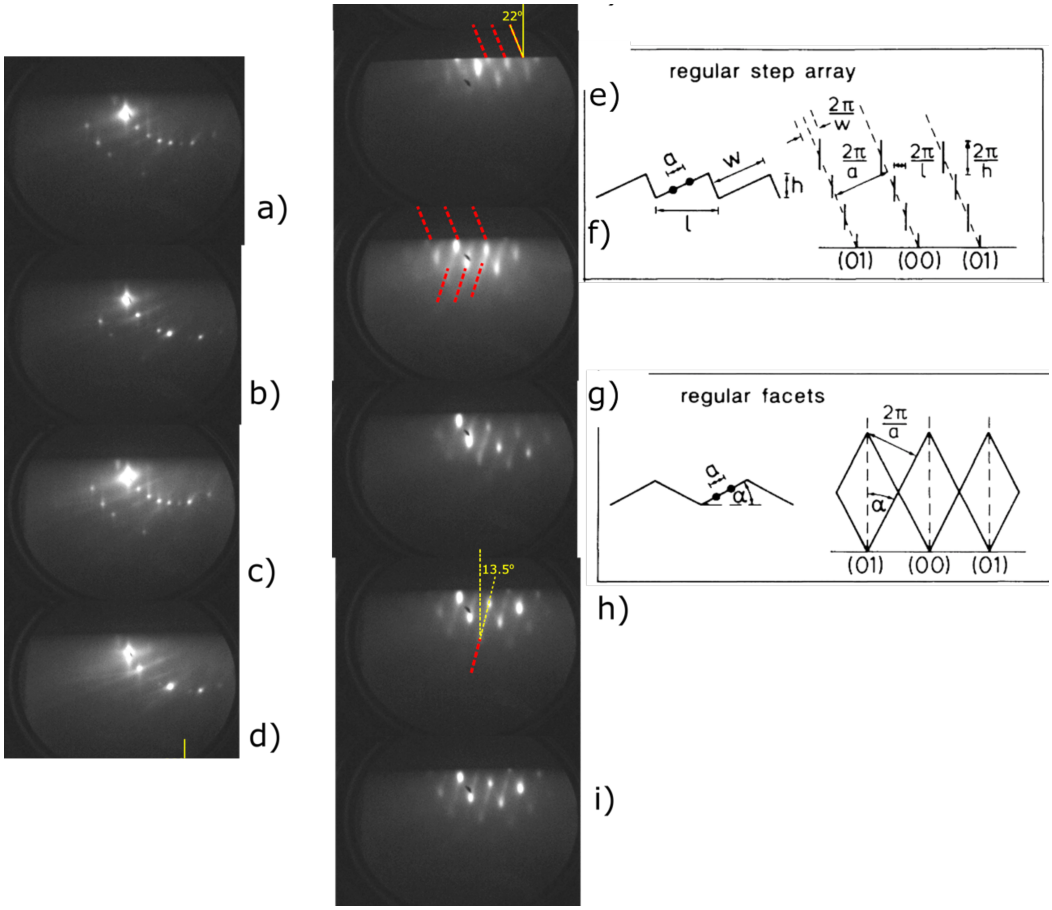

Figure 1s: RHEED patterns recorded during the initial stages of Ga monolayer deposition and GaAs growth on a Si(331) substrate. Images were acquired along the [$\bar{1}$10] azimuth at a substrate temperature of 450 °C. Growth sequence: (a) Clean Si(331) surface following oxide desorption. (b) Immediately after Ga monolayer deposition: the RHEED pattern exhibits minor modifications. (c) After a few seconds, the pattern returns nearly to its original state. (d) As the As flux slowly reaches the surface, evident changes in the diffraction pattern emerge. (e) The appearance of a pattern characteristic of a regular step array is observed; a schematic illustration of this type of surface is shown on the right (adapted from [1]). The 22° inclination corresponds to (111) atomic steps. (f–g) Progressive evolution of the surface towards a regular faceted structure is observed as Ga and As continue to be deposited at low rates. The schematic in (g) illustrates this faceting behavior, where the measured 13.5° angle corresponds to the (110) crystallographic planes.

* esteban.cruz@uaslp.mx

B. Comparison with high-resolution STEM images

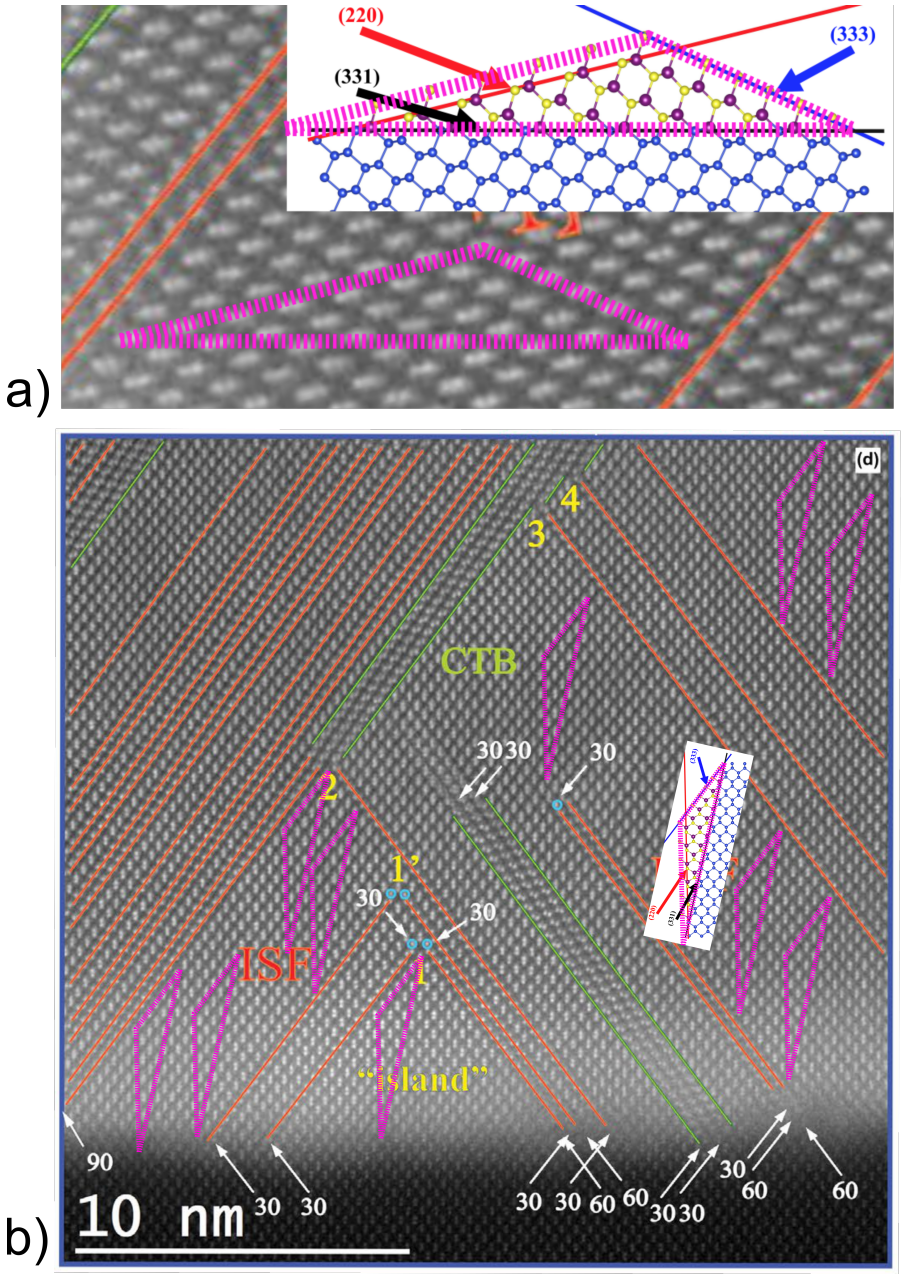

Figure 2s: High-resolution scanning transmission electron microscopy (STEM) image of GaAs grown on Si(100) substrates, reproduced (pending permission) from Ref. [2]. Ref. [2] provides a detailed analysis of the different types of crystalline defects commonly observed in this kind of epitaxial growth. In the image, orange and green lines, along with light blue circles, highlight various types of defects. Regions lacking these markings are considered defect-free. (a) A magenta triangle highlights a single unit of a facet, characteristic of GaAs growth on Si(331), and illustrates how it fits within the STEM structure. This unit facet is composed of 7 atomic planes along the (111) direction, 8 along the (110), and 13 along the (331). (b) Zoomed-out view of the STEM image showing an extended region with defect-free domains, arranged in a way that enables the formation of such unitary facets. Notably, the region labeled "island" has a GaAs thickness that matches exactly the height of one such facet unit.

[1] Nötzel, R., Däweritz, L. & Ploog, K. Topography of high-and low-index GaAs surfaces. Phys. Rev. B 46, 4736–4743 (1992).
[2] Kozak, R. et al. Strain relaxation in epitaxial GaAs/Si (0 0 1) nanostructures. Philos. Mag. 97, 2845–2857 (2017).