# Hydrogen Cleaning Induced Surface Modifications of GaAs(110)

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Zincblende III/V nanowires typically exhibit non-polar (110) surfaces as side facets [1]. Since characterization is mostly performed in a different (UHV)-chamber than growth, such nanowires are commonly exposed to the atmosphere. For the nanoscopic analysis of such III/V nanowire (110) growth surfaces, hydrogen cleaning is a commonly used procedure to remove residual adsorbates, such as e.g., oxygen. While hydrogen cleaning is reported to be destruction free [2] and to achieve clean, atomically flat surfaces with well-defined electronic properties—as they are expected directly after growth—the actual processes and dynamics during cleaning are rarely examined. However, a detailed understanding of these issues is crucial for the interpretation of electronic surface properties, of the growth of nanowires, as well as the incorporation and distribution of dopant atoms.

Here, we investigate the modifications of *n*-type GaAs(110) surfaces as a model system upon controlled atomic hydrogen exposure at room temperature and under commonly used cleaning conditions at the atomic level. For depiction and measurement at the atomic scale, we used scanning tunneling microscopy and spectroscopy under UHV conditions. Using these methods, we study the geometric arrangement of the adsorbed atoms, the newly introduced defects, as well as additional electronic (defect) states and Fermi level pinning. First, we confirm the debuckling and roughening of the (110) surfaces by hydrogen adsorption at the atomic level. This was predicted by Ref. [3] from methods showing only integral information, but without atomic resolution. We see both effects in images with atomic resolution: Hydrogen adsorption debuckles the surface while the roughening is in fact related to the formation of very specific defects derived from arsenic vacancies. Further, we link the structural changes to changes in electronic properties and confirm our STS results by tunnel current simulations. Second, the effects of hydrogen cleaning itself are shown in images with atomic resolution. Two effects are observed: The formation of native defects as well as the (re)creation of atomically flat surfaces. Again, electronic properties are evaluated from tunneling spectra and confirmed by tunnel current simulations. These findings lead to a comprehensive picture of the processes involved in the hydrogen cleaning procedure of III/V semiconductor surfaces.

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[2] Webb et al., Nano Lett. **15**, 4865-4875 (2015)
[3] M'Hamedi et al., Semicond Sci Technol **2**, 418 (1987)

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# Suplementary Pages

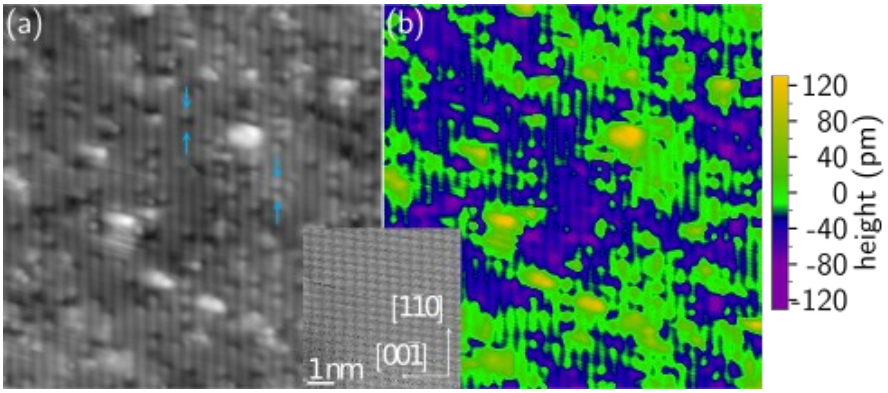


**Figure 1**: (a) STM image of the hydrogen exposed surface. A surface roughening by additional defects (blue arrows) is observed. (b) false color image of (a): Surface areas coded blue are debuckled by hydrogen adsorption while surface areas coded green are not. Inset: Clean, as-cleaved surface for comparison: Atomic rows are visible through all images, while the clean as-cleaved surface does neither show additional adsorbates or defects nor a variation in surface relaxation.

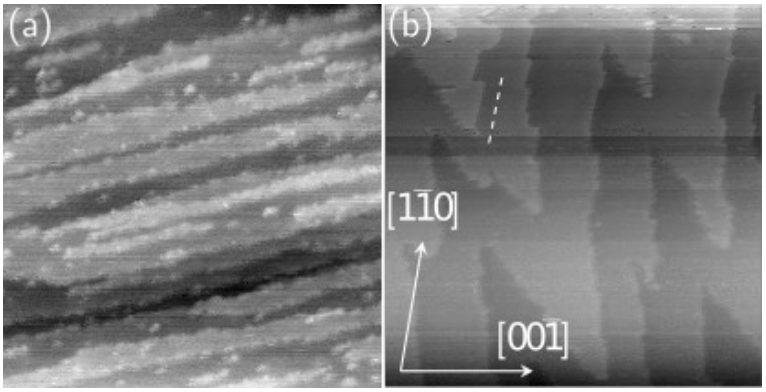


**Figure 2**: (a) STM image of the clean as-cleaved surface with additional strain. A high density of steps along [112] direction is visible. Additionally, there is a high amount of adsorbates preferably adsorbed at the step edges. Only small areas of flat surfaces are visible. (b) STM image of the hydrogen cleaned surfaces. Step edges now align along the atomic rows in [110] direction (indicated by white dashed line). Step density is lowered and flat surface areas are bigger than before hydrogen cleaning. Step edges now show electronic contrast (brighter edges from additional dangling bonds). No further adsorbates are visible.

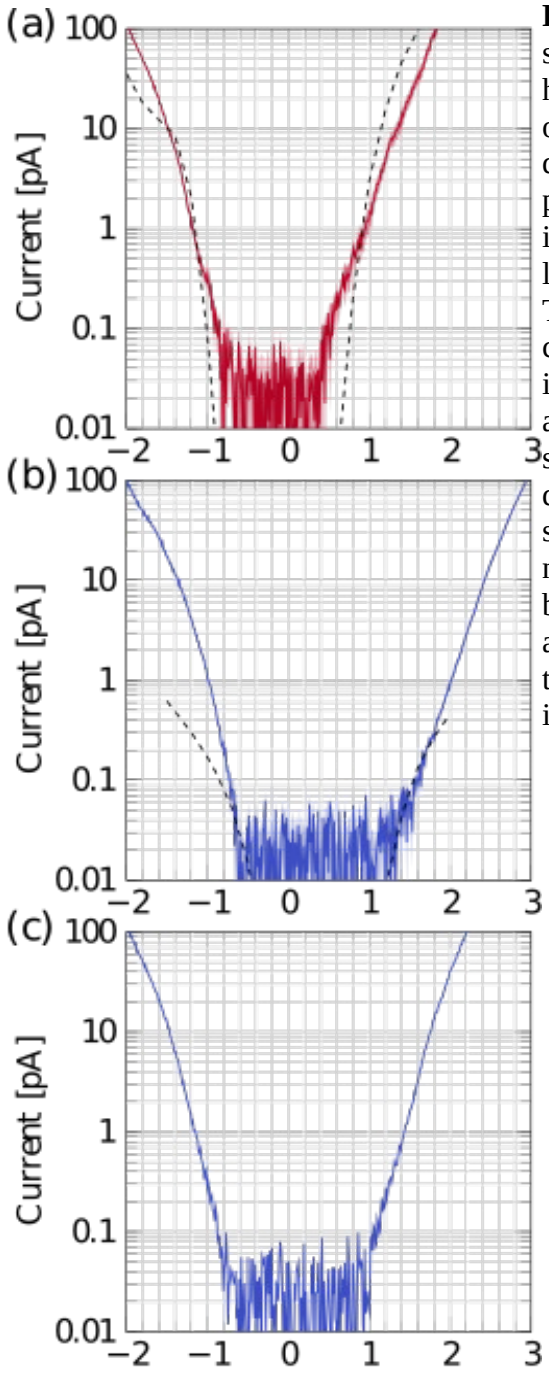


**Figure 3**: ST spectra of the (a) clean, as-cleaved surface, (b) hydrogen exposed surface, and (c) hydrogen cleaned surface. (a) Since there are only very few defects at the clean surface directly after cleavage, there is no surface pinning observable. The band structure therefore is susceptible for tip induced band banding leading to a comparable small apparent band gap. The Fermi level is located close to the conduction band as expected for *n*-type material in general. (b) Due to the high concentration of additionally introduced defects, the band structure is pinned at the Fermi level. Since the defects themselves introduce additional defect states within the band gap, the apparent band gap now appears too wide and shifted towards higher biases indicating *p*-type behavior. (c) The apparent band gap fits the fundamental one while the Fermi level is positioned in the center, indicating intrinsic behavior.