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Cross-sectional scanning tunneling microscopy of GaN and InN epitaxial layers: defects, surface states, and Fermi-level pinning

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Group III-nitride semiconductors are the material system of choice for highly efficient light emitters, as they possess excellent optoelectronic properties within the spectral range from ultraviolet to green. However, the main drawback of group III-nitride semiconductors is the lack of large bulk material substrates for the growth of optoelectronic devices. Therefore, most epitaxial layers have to be deposited on lattice-mismatched and thermal-mismatched substrates or on pseudo substrates. In both cases, the defect density is rather high, influencing the optoelectronic properties of the epitaxial layers. Therefore, it is of critical to identify simultaneously the defects present and the electronic properties of the materials as well as of growth surfaces.

This issue is addressed by investigating the geometric and electronic structure of different III-N epitaxial layers by cross-sectional scanning tunneling microscopy (X-STM) and spectroscopy (X-STS). The buried structure of the epitaxial layers is accessed through cross-sectional m-plane cleavage surfaces. A variety of defects are observed in the STM images of GaN and InN epitaxial layers, of which dislocations and (for GaN) v-shaped defects are the most prominent ones. We identify the electronic properties of the different types of defects. Furthermore, we illustrate that the strain fields of the dislocations allow to track quantitatively the subsurface path of the dislocations. On this basis we map the dislocation density including the projected line directions of the dislocations. The dislocations are found to be bent away from the inclined semipolar facets of v-shaped defects, due to a strain-induced repulsive interaction. The dislocation distribution itself is characterized by agglomerations and intersecting bundles of dislocations with parallel projected line directions, suggesting many body effects in the repulsive strain interactions.

The electronic properties of the m-plane GaN cleavage surface are governed by a “hidden” empty Ga-derived surface state, with a small extension of the density of states into the vacuum at its minimum in the band gap. STS shows that this intrinsic surface state within the band gap pins the Fermi energy only at positive voltages, but not at negative ones. This polarity-dependent Fermi level pinning is attributed to the limited electron transfer from the conduction band to the surface state due to quantum mechanically prohibited direct transitions. Thus, a chargeable intrinsic surface state in the band gap may not pin the Fermi level or only at one polarity, depending on the band to surface state transition rates.

Finally, InN cleavage surfaces exhibit a Fermi level within the band gap at the surface and hence no electron accumulation layer. The intrinsic properties of high quality InN are thus similar to other III-V semiconductors and the previously reported intriguing properties are rather related to low material quality and surface decomposition/contamination.