In-plane, commensurate GaN/AlN junctions: single-layer composite structures, multiple quantum wells and quantum dots

ENGIN DURGUN, ABDULLATIF ONEN, DENIZ KECIK, SALIM CIRACI, Bilkent University - UNAM — In-plane composite structures constructed of the stripes or core/shells of single-layer GaN and AlN, which are joined commensurately display diversity of electronic properties, that can be tuned by the size of their constituents. In heterostructures, the dimensionality of electrons change from 2D to 1D upon their confinements in wide constituent stripes leading to the type-I band alignment and hence multiple quantum well structure in the direct space. The δ-doping of one wide stripe by other narrow stripe results in local narrowing or widening of the band gap. The direct-indirect transition of the fundamental band gap of composite structures can be attained depending on the odd or even values of formula unit in the armchair edged heterojunction. In a patterned array of GaN/AlN core/shells, the dimensionality of the electronic states are reduced from 2D to 0D forming multiple quantum dots in large GaN-cores, while 2D electrons propagate in multiply connected AlN shell as if they are in a supercrystal. These predictions are obtained from first-principles calculations based on density functional theory on single-layer GaN and AlN compound semiconductors which were synthesized recently.

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