Evolution of III-V Nitride Alloy Electronic Structure: The Localized to Delocalized Transition

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move down in energy into the fundamental band gap, and overtake the CS one by one. (ii) Once the CS are swept by the PHS, the ensuing "amalgamation of states" forming the conduction band-edge exhibits , as its low-energy tail is dominated by the just swept-in CS, whereas its higher-energy end consists of the more extended PHS. This localized-delocalized duality in the band edge leads to exciton localization in the tail states, Stokes shift between absorption (into PHS) and emission (from CS), blueshift of low-temperature photoluminescence (PL) with increasing temperature (due to thermal transfer of carriers from CS to PHS), and anomalous pressure dependence of the band gap (due to the weak pressure dependence of the CS, at the band edge, compared to the bulk). (iii) As the impurity concentration increases further, the amalgamated band-edge state broadens, the states delocalize, and the system turns into a conventional alloy with smoothly varying physical properties. These nitride systems thus illustrate a novel class of alloy behavior, which

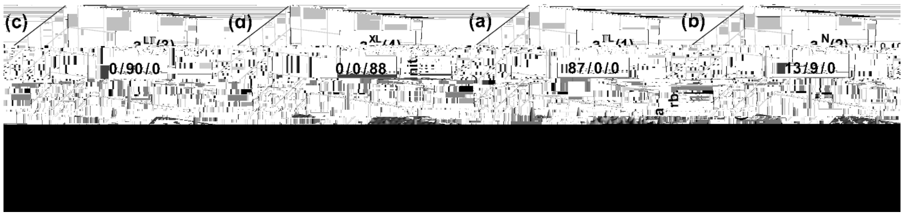

FIG. 2. Wave functions of the lowest energy a_1 conduction states of Ga<u>As</u>:N ($x_N \sim 0.05\%$). The x and y axes lie in the [100] and [010] directions, respectively.

high-order cluster states, spread throughout the upper part of the band gap hardly absorb light, but can be efficiently populated by tunneling from the higher-energy mobile PHS occupied optically. Thus CS are seen in PL, even though their concentration is low. This creates a Stokes shift between absorption and emission [11]. Furthermore, deeper CS appear in PL as the temperature is raised [10], when these levels are fed by cascading from the thermally populated higher-energy mobile states. The calculated pressure dependence of the pairs and cluster states in GaAs is $a_p = 20\text{–}60$ meV/GPa, while for the isolated N level $a_p = 40$ meV/GPa. These values are much reduced relative to the Γ_{1c} bulk value of 100 meV/GPa due to mixing of X_{1c} and L_{1c} character with much reduced a_p.

Calculations for GaP:N show similar behavior when compared to GaAs:N (Fig. 1), except that in the ultradilute limit (a) the $a_1(N)$ level is already inside the band gap at $E_c - 30$ meV, compared with the measured [6,9,13,14] E_c