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Effects of heavy nitrogen doping on the host band structure of GaP B. FLUEGEL, YONG ZHANG, J.F. GEISZ, A. MASCARENHAS, National Renewable Energy Laboratory — A recently observed excitation peak in photoluminescence excitation (PLE) spectra of $GaP_{1-x}N_x$ epilayers, that remains pinned ***below*** the Γ point of the $GaP_{1-x}N_x$ with N concentration, is attributed to a transition from the valence band edge to either the $t_2(X_3)$ or $t_2(L)$ conduction bands by Buyanova et al. [PRB 69, 201303(R), 2004]. A theoretical study based on an empirical pseudopotential band structure calculation offers an alternative explanation for the pinned peak claiming that it is produced by high energy N-cluster states, despite the fact that the calculated pinned peak is ***above*** the Γ point [Duidy et al., PRB 70, 161304(R), 2004]. Using absorption and PLE studies on free-standing samples, we show that this pinned peak is merely an artifact that arises from the GaP buffer layer and is not associated with the GaP:N epilayers. Also, we directly probe the host conduction band minimum (CBM) near X_{1C} using absorption, which shows that a weak CBM absorption peak remains stationary up to nitrogen composition x = 0.1 % before it is smeared out by the inhomogeneous broadening. This result further supports the conclusion that the absorption below the host CBM in heavily N doped GaP is primarily due to the formation of an impurity band consisting of broadened states of N pairs and clusters (Zhang et al, PRB 62, 4493, 2000).

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