

E_+ transition in $\text{GaAs}_{1-x}\text{N}_x$ and $\text{GaAs}_{1-x}\text{Bi}_x$ due to isoelectronic-impurity-induced perturbation of the conduction band

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An above-band-gap transition E_+ is experimentally observed in the dilute $\text{GaAs}_{1-x}\text{Bi}_x$ alloy. Precise measurements at very low dilutions are made of the above-band-gap transition E_+ that is observed in $\text{GaAs}_{1-x}\text{N}_x$, making it possible to compare the behavior of the different isoelectronic traps Bi and N in the common host GaAs with respect to their perturbation to the host electronic structure. We suggest that the origin of the E_+ level observed in GaAs is not the isolated isoelectronic impurity level N_x , as is presumed in the band-anticrossing model, but rather the isoelectronic-impurity-induced perturbation of the conduction band L_6^c .

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I. INTRODUCTION

The recent history of nitrogen-doped GaAs has been discussed by several authors,^{1,2} from the direct observation³ of the isolated nitrogen level N_x resonant in the conduction band (CB), through the discovery of the giant band-gap (E_0) bowing,⁴ to the rapid growth of interest in the physical origin and photonic applications of this striking example of band-gap engineering. An explanation of the band-gap bowing in terms of a two level repulsion, termed the band-anticrossing (BAC) model,⁵ gained recognition with the discovery of E_+ , an optical transition induced by nitrogen doping in GaAs.^{1,5} In the low-doping limit at low temperature, E_+ is approximately 290 meV higher than E_0 and increases with increasing nitrogen concentration x . This opposes the decrease in E_0 observed with increasing N concentration. The two effects were qualitatively explained by the BAC model as a repulsion (anticrossing) between the isolated nitrogen level N_x and the conduction-band minimum (CBM) at Γ . In this simple description, N_x , pictured as a dispersionless state, couples with the CBM to form two new states, E_- and E_+ , which diverge from their original noninteracting energies with increasing nitrogen concentration. $E_-(x)$ evolves as the new CBM, resulting in the band-gap reduction, whereas E_+ emerges as another level. The valence band remains practically unchanged.

Fundamentally, the incorporation of nitrogen would cause symmetry breaking and intraband coupling resulting in a level repulsion of the CBM. However, subsequent theories^{6–11} disagreed with the two-band picture of the BAC, arguing for a more complicated interaction involving other Brillouin zone points of the CB as well as the isolated, pair, and cluster states of N impurities. Perhaps the most testable claim of all these theories remained the BAC's contention that in the low-nitrogen limit, E_+ must revert to the isolated nitrogen impurity level N_x . For this reason, the E_+ level became the focus of considerable attention, and several experimental studies undertook careful measurements of $\lim_{x \rightarrow 0} E_+(x)$ and the slope $dE_+(x)/dx$. At 300 K, the assignment of E_+ was inconclusive,¹ appearing to revert either to

N_x or to the very similar energy of L_6^c . The latter presented a challenge to the BAC via an alternative model¹ that proposed a nitrogen-induced splitting of the degenerate CB L states into a singlet state that rises in energy with nitrogen concentration just as E_+ . This was also supported by the results of Francoeur *et al.*¹² that E_+ has the same temperature dependence as L_6^c , which would not be true if it were a transition from the valence-band maximum (VBM) to N_x . Additional studies^{12,13} using contacted electroreflectance were made at temperatures of 80 or 90 K, where the L_6^c conduction band rises at low temperature, slightly relieving the ambiguity caused by the proximity of N_x and L_6^c . However, results at these temperatures still showed E_+ extrapolating to either level, depending on how the x dependence was treated.¹⁴

The “extended” BAC model for $\text{GaAs}_{1-x}\text{N}_x$ has evolved from the original BAC model, from, first, only including the effects of single N impurities, next, to including the effects of N pairs, and finally, to including the effects of N clusters.^{15–20} This approach is based on reformulating the results of tight-binding calculations to express them in the form of a two-band Hamiltonian. This model predicts (a) the emergence of the E_+ level, with a single state with significant Γ character for $x > \sim 0.2\%$ and that this E_+ level is not observable in $\text{GaAs}_{1-x}\text{N}_x$ samples with $x \leq 0.1\%$, and (b) that at low N composition, E_+ forms a sharp resonance in the conduction-band Γ -related density of states, which broadens rapidly at higher N composition when the E_+ level rises in energy to become degenerate with the larger L -related density of states.

The BAC and extended BAC models continue to be used^{21–24} to interpret the band-gap reduction in $\text{GaAs}_{1-x}\text{N}_x$. Very recently, a study²⁵ with improved sensitivity at lower x values has shown that E_+ extrapolates to L_6^c , rekindling the debate on this issue. One of the biggest obstacles to resolving this debate is the proximity in energies of the isolated nitrogen level N_x and L_6^c , this being approximately as small as the experimental uncertainties. The recent emergence^{26,27} of a semiconductor alloy $\text{GaAs}_{1-x}\text{Bi}_x$ now provides an opportunity to alter drastically the energy of the isolated isoelectronic impurity and to observe the resulting changes in elec-

tronic structure. This is analogous to comparative studies¹⁰ between $\text{GaAs}_{1-x}\text{N}_x$ and $\text{GaP}_{1-x}\text{N}_x$, which can be regarded as an attempt to change the host rather than the impurity. Since the differences between these hosts are considerable (e.g., indirect gap vs direct gap), the impurity perturbation to the host conduction bands in these two systems is quite different.^{10,28,29} In contrast, by using $\text{GaAs}_{1-x}\text{Bi}_x$, the host is unchanged and only the energy of the isolated Bi state Bi_x is changed relative to the situation for $\text{GaAs}_{1-x}\text{N}_x$. Although the energy of this isolated impurity state has not been measured, it is predicted to be resonant in the valence band.³⁰ [Reference 30 predicts that measuring Bi_x is not possible using pressure-dependent photoluminescence (PL) studies, unlike $\text{GaAs}_{1-x}\text{N}_x$.] The qualitative application of the BAC model to $\text{GaAs}_{1-x}\text{Bi}_x$ predicts that coupling between the VBM and the isolated Bi level Bi_x forms an upper branch that replaces the VBM and moves upward with bismuth concentration to reduce the band gap, as experimentally observed. The lower branch, moving downward with bismuth concentration, would have a weak dipole coupling to the CBM at Γ , giving an optical transition analogous to E_+ in $\text{GaAs}_{1-x}\text{N}_x$. The behavior that we have observed for E_+ in $\text{GaAs}_{1-x}\text{Bi}_x$, however, is in stark contrast to this prediction.

II. EXPERIMENT

The optical transitions in dilute nitride alloys have been studied^{1,5,12,13,35,36} with modulated reflectance (MR), which is preferred for sharp signals that directly probe the host density of states, both at the fundamental band gap and at higher-energy transitions. This advantage fades for low N concentrations ($<0.1\%$), where the impurity-induced transitions such as E_+ become quite weak. Tan *et al.*²⁵ showed that it was possible to observe the small signals in this dilute regime using microphotoluminescence (micro-PL). Despite the very low PL efficiency from transient hot-carrier populations, PL at, e.g., the spin-orbit transition $E_0 + \Delta_0$ has been seen in isoelectronically³¹ doped semiconductors, and the transition energies found using this method agreed with those obtained using other methods. In micro-PL studies, the high power density with low sample heating enables the observation of E_+ as well as $E_0 + \Delta_0$,²⁵ even in low-concentration samples—assignments that are verified by comparison with the results of MR studies.

For the present study, similar sets of $\text{GaAs}_{1-x}\text{N}_x$ and $\text{GaAs}_{1-x}\text{Bi}_x$ samples were grown by molecular-beam epitaxy (MBE) on GaAs substrates. $\text{GaAs}_{1-x}\text{N}_x$ epilayers of thickness 0.25–1.1 μm were grown by solid-source MBE, similar to those described in Ref. 32. The MBE growth of $\text{GaAs}_{1-x}\text{Bi}_x$ and Bi concentration measurements are described in Ref. 27. All samples were held at 10 K. PL was excited and collected through a 0.6 numerical aperture objective giving a spot size of approximately 1 μm , and then measured with a spectrometer and cooled charge-coupled detector array. The exciting laser had a cw power of 1 mW, either at 647 or 532 nm, which we describe below as resonant and nonresonant excitations, respectively.

III. RESULTS

Figure 1 shows micro-PL spectra for two representative $\text{GaAs}_{1-x}\text{N}_x$ samples under resonant and nonresonant excita-

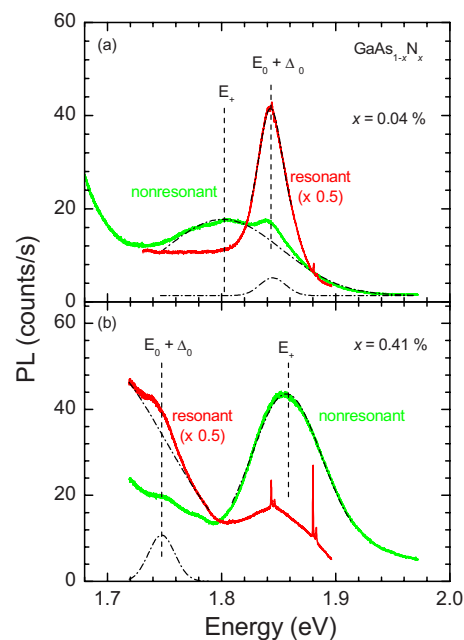


FIG. 1. (Color online) Micro-PL of $\text{GaAs}_{1-x}\text{N}_x$ at 10 K with (a) $x=0.04\%$ and (b) $x=0.41\%$. Spectra for resonant and nonresonant excitations as well as Gaussian fitting curves (dashed lines) are shown for both samples. The spin-orbit transition $E_0 + \Delta_0$ is enhanced under resonant pumping, while the E_+ transition dominates for nonresonant pumping. Sharp lines in the resonant spectra are Raman scattering.

tions. As in Ref. 25, there are two nitrogen-dependent PL peaks whose relative strength varies with excitation wavelength. The wavelengths chosen here yield an improved discrimination between the two spectrally overlapping signals compared to Ref. 25. As in Ref. 25, we identify the sharper signal with the spin-orbit split-off valence-band-to-conduction-band transition, $E_0 + \Delta_0$. This peak is enhanced under near-resonant pumping, and by detuning the laser to 532 nm, it is largely suppressed, revealing the E_+ peak with a minimum of deconvolution required. In this manner, the plot of $E_0 + \Delta_0$ and E_+ as a function of N concentration was generated in Fig. 2. The $x=0$ intercept of the $E_0 + \Delta_0$ curve corresponds to the known low-temperature value of 1.85 eV for the spin-orbit transition in GaAs, confirming its assignment. The broader peaks in Fig. 1 are E_+ , which is confirmed by its N dependence in Fig. 2 and its agreement with MR data.¹² The use of micro-PL makes it possible to extend the measurement of E_+ to lower concentrations, and in fact, to below the crossover of E_+ and $E_0 + \Delta_0$ near 0.1%. This is an important refinement because, as discussed above, the precise energy value of $\lim_{x \rightarrow 0} E_+(x)$ has been the subject of intense scrutiny^{1,12,13,25} in the debate over the origin of E_+ .

Turning now to $\text{GaAs}_{1-x}\text{Bi}_x$, Fig. 3 shows micro-PL from three $\text{GaAs}_{1-x}\text{Bi}_x$ samples measured using 647 nm excitation. The spectral region studied (PL was measured in the region demarcated by horizontal arrows in Fig. 4) lies between the dominating high-energy tail of the band-gap PL and the strong PL from the weakly x -dependent $E_0 + \Delta_0$ at 1.82–1.86 eV. The latter is resonantly enhanced, just as in $\text{GaAs}_{1-x}\text{N}_x$. Between these regions, E_+ can be observed,

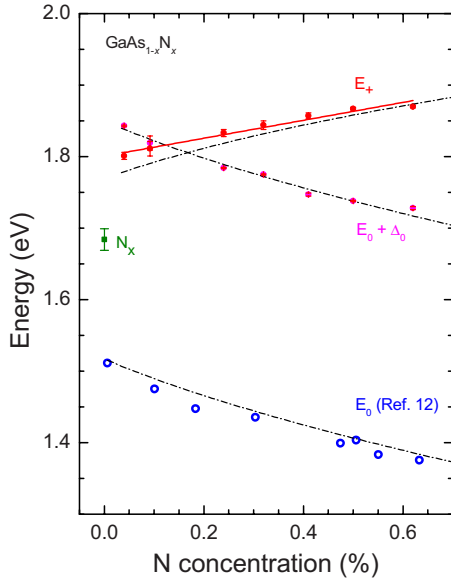


FIG. 2. (Color online) Peak transition energies E_+ and $E_0 + \Delta_0$ extracted from PL spectra similar to Fig. 1 (solid points with error bars represent fitting uncertainty). Also plotted are 80 K E_0 data from Ref. 12 shifted by +11 meV appropriate for 10 K (open points). The single data point N_x is the measured energy of the nitrogen impurity level (Refs. 3 and 38). Dashed curved lines are a fit of the BAC model (Ref. 35) to the combined E_+ data of the present work ($0.04\% \leq x \leq 0.6\%$) and Ref. 12 ($0.3\% \leq x \leq 2.1\%$) and the E_0 data of Ref. 12 ($0\% \leq x \leq 2.1\%$). The noninteracting levels were determined to be $N_x = 1.770$ eV and $\text{CBM} = 1.517$ eV - 45 meV/%N, and the interaction matrix element $= 2.5x^{1/2}$ eV. The solid straight line is a linear fit to the E_+ data of the present work.

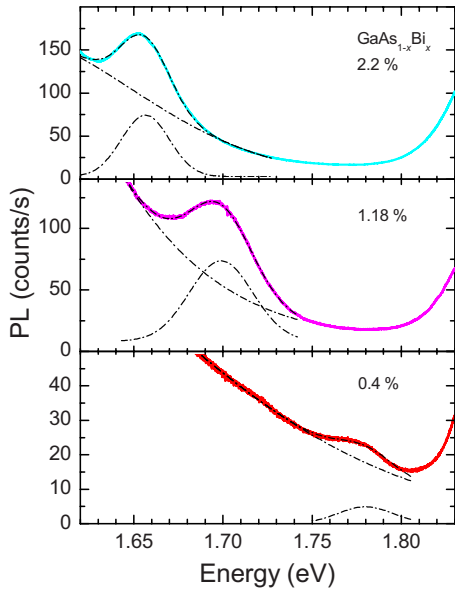


FIG. 3. (Color online) Micro-PL of 10 K $\text{GaAs}_{1-x}\text{Bi}_x$ for three bismuth concentrations. E_+ energies were identified by Gaussian fits (dashed lines).

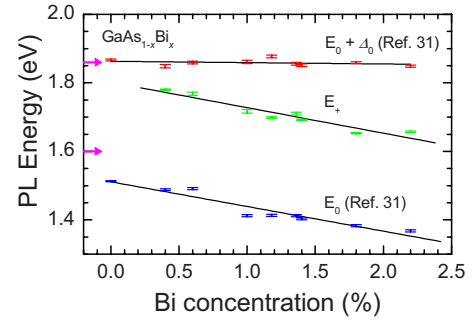


FIG. 4. (Color online) E_+ energies of Fig. 3 plotted as a function of bismuth concentration. $E_+(0)$ extrapolates to 1.802 ± 0.030 eV. The same analysis as a function of band-gap reduction (Ref. 1) eliminates the effect of possible errors in Bi concentration and gives a statistically identical result of 1.801 ± 0.025 eV. Also plotted are 150 K E_0 and $E_0 + \Delta_0$ energies of the same samples measured in Ref. 31, shifted by +33 meV for comparison at 10 K. Solid lines are linear fits. Arrows demarcate the energy region searched for E_+ .

ranging from a small peak in the dilute samples to a very distinct peak at higher concentrations. The signal is smaller than that for E_+ in $\text{GaAs}_{1-x}\text{N}_x$ at an equivalent N concentration. The peak energies from the entire sample set are plotted in Fig. 4, revealing that in $\text{GaAs}_{1-x}\text{Bi}_x$ E_+ decreases with increasing Bi concentration. Also plotted are E_0 and $E_0 + \Delta_0$ measured at 150 K on the same samples in Ref. 31 and shifted by 33 meV (Ref. 33) for comparison with the 10 K data. The use of this GaAs temperature correction was established in Ref. 34, where the $\text{GaAs}_{1-x}\text{Bi}_x$ band gap was shown to track that of GaAs from 80 to 300 K. The correction is further confirmed by the $x=0$ intercept of the E_0 curve in Fig. 4, which corresponds to the accepted GaAs band-gap value of 10 K.

IV. DISCUSSION

The $\text{GaAs}_{1-x}\text{N}_xE_0 + \Delta_0$ transition plotted in Fig. 2 closely parallels the measured band-gap data from Ref. 12. As previously discussed,^{1,5,12} this is consistent with the picture of N causing only a minimal perturbation to the valence band (VB). Nitrogen's effects on the CB are much more pronounced, as seen in the very different relative x dependences of E_0 and E_+ . With the E_+ data for the very-low- x regime, this allows a detailed analysis of the functional shape of $E_+(x)$ for the very dilute alloy. In the high- x regime, the micro-PL data points in Fig. 2 overlap the MR data from Ref. 12 within experimental uncertainty; however, the slope of the micro-PL data, concentrated at the low- x region, is higher than that of the MR data from Ref. 12, which covers a larger- x region. This indicates nonzero curvature in $E_+(x)$, a possibility that was suggested in Ref. 12 and which is of relevance to the formulation of the BAC model. In the simplest form of this model, the nitrogen-induced shifts of E_0 and E_+ are exactly equal and opposite;⁵ however, MR data^{1,12,13} showed that the slope of E_+ versus x (at $x > 1\%$) is much flatter than that of E_0 . This conflict was addressed via a phenomenological modification of the BAC that included in the noninteract-

ing CBM an additional term linear in x .³⁵ With appropriate choices of this term, the isolated nitrogen energy, and the BAC coupling matrix element, the model could be made to fit closely both E_0 and E_+ , including their different slopes and the measured curvature^{12,36} of E_0 near $x=0$. Whether an equal and opposite curvature occurs in the E_+ data,^{35,36} as would be required by the model, has been unknown due to the difficulty of measuring E_+ at low concentrations. Using micro-PL measurements, in the present work, we have measured E_+ for nitrogen concentrations as low as 0.04%, revealing that the curvature of E_+ is significantly less than what is seen for E_0 . In Fig. 2, the dashed curves show a simultaneous fit of the BAC model to the combined E_0 and E_+ data of the present work and that of Ref. 12. The interaction matrix element obtained in this way underestimates the curvature of E_0 while overestimating the curvature in E_+ , and the BAC model thus provides no better a fit to E_+ than would a simple line.

Other authors have explained^{2,9,11,12,25} E_+ as a transition from the VBM to the split-off singlet state L_6^c . In GaAs, L_6^c is located at 1.815 ± 0.031 eV above the VBM,³⁷ matching closely the 1.801 eV value extrapolated at $x=0$ from the linear fit in Fig. 2. The large discrepancy^{12,25} presented in Fig. 2 between $\lim_{x \rightarrow 0} E_+(x)$ and the measured value of the isolated nitrogen impurity level N_x energy [1.67–1.70 eV (Refs. 3 and 38)] continues to persist in this present work, and the data presented in Fig. 2 at small x leave little room for any model that would allow E_+ to come from N_x .

We now turn to the $\text{GaAs}_{1-x}\text{Bi}_x$ data and examine the effect of replacing the resonant isolated impurity state in the CB with one in the VB. As mentioned earlier, the spin-orbit coupling is strongly affected by Bi incorporation, and $E_0 + \Delta_0$ no longer parallels E_0 .^{30,31} As shown in Fig. 4, rather than increasing with Bi doping as would be expected from the BAC model, E_+ now decreases, closely following E_0 with a constant separation of 290 meV. As in the case for the $x \rightarrow 0$ limit for nitrogen doping, this separation between E_+ and E_0 is close to the Γ - L splitting of GaAs. Thus, in both dilute isoelectronic alloys, we find that E_+ extrapolates to nearly the same energy for $x=0$, and that this is the Γ - L transition energy of the host. This behavior occurs in both dilute isoelectronic alloys despite the vast difference between their isoelectronic impurity atoms, i.e., Bi resonant in the VB or N resonant in the CB. The indifference of the value of $\lim_{x \rightarrow 0} E_+(x)$ to the location of the impurity atom's energy

level indicates that in $\text{GaAs}_{1-x}\text{N}_x$, E_+ does not represent a transition to the isolated isoelectronic impurity level N_x , contrary to the premise of the BAC model for this alloy.

From this we conclude that, as with N, the loss of lattice translational symmetry due to the addition of Bi to GaAs results in the Γ - L transition E_+ . Here, the perturbation to L_6^c and to the CB, in general, is weaker than in the case of $\text{GaAs}_{1-x}\text{N}_x$ due to the larger energy separation of L_6^c from the isolated Bi impurity level. The CB energies at Γ and L remain largely unchanged, and E_+ therefore follows the reduction in E_0 that results from the rising of the VBM with increasing Bi content. This offers a consistent picture of the two isoelectronic alloys, in which their differences are a result of the isolated impurity state being in either the CB or the VB. It also supports the similarity of the E_+ temperature dependence to that of the conduction band at L (Ref. 12). The band-gap reduction in GaAs caused by the introduction of N or Bi can be understood only through calculations involving all of the energetically nearby states,^{8,9,30} not simply as a repulsion of the VBM or CBM that results from the impurity level acting alone. The BAC model proposed for GaAsN is fundamentally a two-band interaction model. It assumes that one of these bands (E_-) evolves from the CBM at Γ , whereas the other (E_+) evolves from N_x . The present study shows the latter assumption to be untrue, and if the premise on which the BAC model is formulated is false, then the model is invalid. In contrast to the predictions of the extended BAC model,^{15–20} we are able to observe E_+ down to $x=0.04\%$, and at ultradilute N concentrations, we observe E_+ to converge to L_6^c .

Our results are fully consistent with the *ab initio* molecular-dynamics-based predictions of Ref. 9 that $a_1(L_{1c})$ gives rise to the E_+ transition, as well as with the more recent local-density-approximation calculations combined with ellipsometry-based results of Ref. 11 concluding that E_+ is mostly formed by transitions from the valence band to the L_{1c} -derived singlet state, occurring near the center of the Brillouin zone.

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