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Effects of heavy nitrogen doping in III–V semiconductors – How well does the conventional wisdom hold for the dilute nitrogen "III–V-N alloys"?

Yong Zhang[*, 1], **B. Fluegel**[1], **M. C. Hanna**[1], **J. F. Geisz**[1], **L.-W. Wang**[2], and **A. Mascarenhas**[1]

[1] National Renewable Energy Laboratory, 1617 Cole Blvd., Golden, CO 80401, USA
[2] NERSC, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

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Although heavily N doped III–V semiconductors are frequently referred to as dilute nitrogen III–V-nitride alloys in general, it is important to realize that there are some subtle but important differences among them. In the indirect gap semiconductor GaP, since even a single N impurity can have a bound state, as far as the absorption near the band gap is concerned, it is difficult to describe GaP:N as an alloy. The N induced bound states (a hierarchy of impurity complexes) can in fact give rise to rather strong absorption below the indirect band gap, which effectively reduced the energy of the "absorption edge", but the position of the absorption edge cannot be defined in a conventional way. In the direct gap semiconductor GaAs, a single N impurity does not form a bound state but instead has a resonant state above the conduction band edge. In this aspect, GaAs:N is similar to the situation in a conventional alloy, say, GaAs:P, except that the perturbation of N to the host is much stronger than that of P. However, because in reality N incorporation is typically in a random manner and a cluster as small as one N pair can generate bound states, the permissible region for GaAs:N to behave as a regular alloy is in fact rather limited, i.e., only when the N concentration is low enough so that the N pair and cluster states do not significantly interact with the host. In this study, a precise tracking of the evolution of the host and N induced impurity states will be offered for the two prototype systems, GaAs:N and GaP:N, with x varying from as low as $\sim 10^{-5}$ to $\sim 10^{-2}$. Such a study gives valuable insight to the underlying physics of the material evolution, sets up a bench-mark for testing the theoretical modeling of this type of system, and serves to enhance our understanding of the behavior of isoelectronic impurities in semiconductors in general. The dissimilarity between GaP:N and GaAs:N indicates that seeking a unified model for all the isoelectronic doping systems is unrealistic. Our study also indicates that for strongly perturbed systems like GaP:N and GaAs:N, certain materials properties could be less well defined or not uniquely defined, as compared to those in other conventional semiconductor alloys.

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1 Introduction Nitrogen atoms as isoelectronic impurities in III–V semiconductors are known to generate various localized states that can either be bound or resonant with respect to the conduction band minimum [1]. The most studied systems are GaP:N, GaAs:N, and their alloy GaAsP:N. In the last decade, the advances in epitaxial growth has made it possible to incorporate up to a few percent of N into these systems [2, 3], which has led to numerous device applications as well as great interest in the fundamental research of the behaviour of the isoelectronic impurities in semiconductors and the alloy formation of the isoelectronic impurities with the host. Although these materials behave quite differently, especially in the low N doping region, from the conventional alloy, they are still generally referred to as dilute nitride alloys, and described by using the familiar concepts for conventional alloys (e.g., the bow-

* Corresponding author: e-mail: yzhang@nrel.gov, Phone: +01 303 384 6617, Fax: +01 303 384 6655

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ing parameter b) [2]. Despite intensive studies in the recent years, there are yet a few important issues remaining not well understood: (1) What really causes the band gap reduction? (2) How to compare theoretical results with experimental data? (3) How to explain the large discrepancy among different measurements for the "same" properties? (4) How to define the material parameters (e.g., band gap and effective mass) in materials like $GaP_{1-x}N_x$ and $GaAs_{1-x}N_x$? Obviously, before the last question can be properly answered, there will always be some ambiguity when seeking answers for the other questions.

Various models or explanations have been proposed in the past few years for explaining the band gap reduction caused by N doping in GaAs and/or GaP [4–12]. Among them, there are three distinctly different ones: two-level repulsion model [4, 5], N impurity band formation [6, 7], and multi-valley coupling [8], which have been applied to both GaAs:N and GaP:N. It appears now for all these three models the subtle but important differences between the two systems have been overlooked. At first glimpse, the GaP:N and GaAs:N are quite similar: isolated N and N pairs form a series of localized impurity states in both systems [13–15], except that in GaAs fewer states are bound. It was speculated that below the host band edge the role of the N bound states should be similar for the two systems [6], which is in fact not true [16]. The indirect band gap in GaP with a large density of states at its X-valley makes a major difference from the direct band gap in GaAs with a small density of states at its Γ-valley, when considering the impurity-host interaction and the relative absorption strength between the impurity-like and host-like states. It is in fact also very important whether or not the isolated N centre generates a bound state. In GaP, since even a single N impurity can have a bound state [13], as far as the absorption near the band gap is concerned, it is difficult to describe GaP:N as an alloy. The N induced bound states (a hierarchy of impurity complexes) can in fact give rise to rather strong absorption below the indirect band gap, which effectively reduced the energy of the "absorption edge" [7, 9], although the position of the absorption edge cannot be defined in a conventional way. In GaAs, a single N impurity does not form a bound state but instead has a resonant state above the conduction band edge [14]. In this aspect, GaAs:N is similar to the situation in a conventional alloy, say, GaAs:P, except that the perturbation of N to the host is much stronger than that of P. Thus, if we were able to incorporate N into GaAs in an ordered array, $GaAs_{1-x}N_x$ would be a well-behaved semiconductor, at least for a limited range of x. However, in reality, N incorporation is more random than ordered, and a cluster as small as one N pair can generate bound states [15]. Therefore, the permissible region for GaAs:N to behave as a regular alloy is in fact rather limited, i.e., only when the N concentration is low enough so that the N pair and cluster states do not significantly interact with the host. Such a region can be estimated as $x < 0.5\%$, using the criterion that the GaAs like band edge excitonic absorption peak is fully smeared out when $x > 0.5\%$ [16]. For higher concentrations, the distortion of N cluster states to the GaAs host-like energy spectrum becomes so severe that this material behaves very differently from a typical alloy (e.g., the line width of the band edge emission being ~100 meV). The dissimilarity between GaP:N and GaAs:N indicates that seeking a unified model for all the isoelectronic doping systems is unrealistic.

Large discrepancies have been found among the experimental studies aimed at obtaining certain key band structure parameters in $GaAs_{1-x}N_x$, e.g., the electron effective mass [6, 17, 18]. One might be tempted to simply attribute the discrepancy to the variation in the accuracy of the experimental data or the nature of the experimental technique being direct or indirect [17]. In fact, the discrepancy is so large that it far exceeds the expected fluctuation if one should apply these different techniques to a typical semiconductor, for instance, GaAs. One cannot help to ask the following questions: Do these different approaches really measure the same property? Are these properties as well or uniquely defined in these new materials as in conventional alloys?

In this paper, we will discuss and attempt to offer some insights to above mentioned issues, although the full answers to all the questions are not yet available. New experimental results for both GaP:N and GaAs:N and new theoretical results for GaAs:N will be presented to facilitate our discussions. In our new experimental studies, a precise tracking of the evolution of the host and N induced impurity states has been achieved for both GaAs:N and GaP:N, with x varying from as low as $\sim 10^{-5}$ to $\sim 10^{-2}$. These results reveal valuable insight to the underlying physics of the material evolution, set up a bench-mark for testing the capability of theoretical modelling techniques, and serve to enhance our understanding of the behaviour of isoelectronic impurities in semiconductors in general. A new effort in the band structure

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calculation of GaAs:N has yielded band gap reductions in best agreement, among all the existing calculations, with the new experimental data, down to the very low doping level of $x \sim 10^{-5}$.

2 GaP:N In the early study of GaP:N [13], the absorption of N pairs (NN_i lines) has been found to increase in proportion to $[N]^2$, whereas that of the isolated N (A line) to increase in proportion to [N], where [N] is the nitrogen concentration. The absorption of the indirect free exciton at the X point (A_x line) has also been found to be activated because of N doping, but the strength is more than two orders of magnitude smaller than that of the isolated N centre [13, 16]. Within the achievable doping level $<2 \times 10^{19}$ cm^{-3} ($x \sim 0.1$ %) by either LPE or VPE, no appreciable shift has been reported for any one of those N bound states [13]. Into much higher N doping levels of a few percent, Yaguchi et al.'s PLE measurements [9], as well as Zhang et al.'s absorption measurements [7], again have indicated that neither the absorption peak of the A line or A_x line nor those of the NN_i lines show any significant shifts, but the absorption edge apparently extends to the low energy region with increasing N doping level. Despite these then existing results, Shan et al. [5] later still explained the photoreflectance feature observed below the indirect band gap as due to the repulsion between the high-lying Γ point and the A line. The recent band structure calculation of Kent and Zunger [8] instead claims that the band gap reduction is due to a host-like a_1 state with significant L character plunging into the band gap, after crossing two other states with the same a_1 symmetry derived from the A line and X point, as a result of N induced inter-valley coupling. This explanation not only violates the basic "anti-crossing" rule for states with same symmetry, but also disagrees with the experimental facts. According to this calculation, the perturbed L point would have gained significantly more Γ character than the X point, but experimentally the absorption or excitation at the L point has never been observed [9]. Instead, it is the X-point that has been activated even at rather low N doping level [9, 13]. To more closely monitor the evolution of the below band gap absorption and eliminate any possible effect caused by the GaP substrates in previous measurements [7, 9], we have performed low temperature absorption measurements on a set of free standing GaP:N films, with 2 μm nominal thickness, that have been obtained by an epilayer lift-off technique [16]. The results are shown in Fig. 1 [19]. One can see that with increasing [N], the absorption at and between the peaks builds up continuously, without any observable downward moving components either from the A line being repelled down [5] or the host-like state plunging down [8]. In contrast, a continuously downward moving excitonic absorption feature has been seen in GaAs:N [16], which will be further examined in the next section. The absorption between the main absorption peaks in fact comes from either excited states or phonon sidebands for the low [N] samples [20], with added contribution from line broadening effects in the high [N] samples [7, 21]. Effectively, discrete absorption lines in the dilute doping limit merge into a continuum absorption band with increasing N doping, which leads to the red shift of the absorption edge.

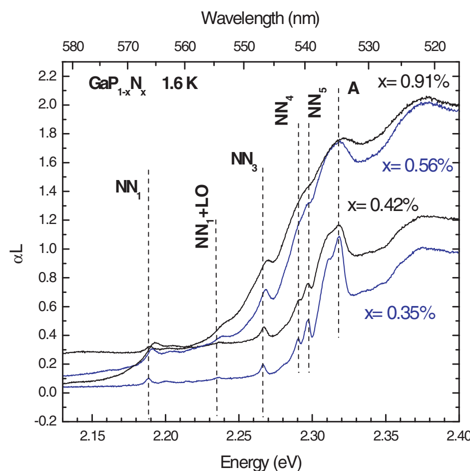

Fig. 1 (online colour at: www.interscience.wiley.com) Low temperature absorption spectra of free-standing GaP:N films.

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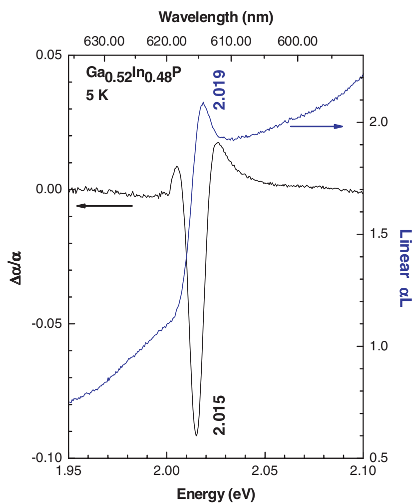

Fig. 2 (online colour at: www.interscience.wiley.com) A comparison between the linear and differential absorption for a conventional alloy GaInP.

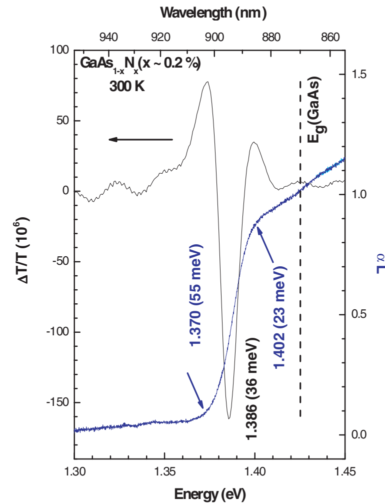

Fig. 3 (online colour at: www.interscience.wiley.com) A comparison between the linear and differential absorption for a GaAsN alloy.

3 GaAs:N The band gap reduction of $GaAs_{1-x}N_x$ was evidenced by the shift of the absorption edge even in the earliest study of this material [2], where the band gap was obtained by fitting the absorption profile to the standard functional form of $(E - E_g)^{1/2}$ that is meant for the free electron inter-band transition. Later, various modulation spectroscopy techniques were used for the purpose of determining the band gap [4, 22, 23]. Although modulation spectroscopy is generally considered as a reliable and accurate way for finding the critical points of the band structure for conventional semiconductors [24], it has been taken for granted that it would work as well for these unusual materials like $GaAs_{1-x}N_x$ and $GaP_{1-x}N_x$. Certainly, the most natural way to define the band gap is to take the energy of the excitonic absorption peak [25], but it is usually assumed that modulation spectroscopy should yield nearly the same value of band gap [26]. Indeed, the discrepancy between the excitonic peak and the differential feature is generally small for typical binaries and conventional alloys, as shown in Fig. 2 for a GaInP alloy. However, the discrepancy becomes significantly larger for the highly mismatched alloy like $GaAs_{1-x}N_x$, as shown in Fig. 3. Therefore, one has to be cautious when making comparisons among different experimental results that might have been obtained using different techniques or criteria, as well as between experimental and theoretical results that do not necessarily represent the same property [16]. Here we use the band gap measurement and calculation for $GaAs_{1-x}N_x$ as an example for illustrating the necessity to exercise such caution.

In an earlier study [27], we noticed that the band gap reduction measured by either electroreflectance (ER) or linear absorption with fitting to $(E - E_g)^{1/2}$ had a scaling component $\alpha \approx 2/3$, when the band gap reduction is given in the form of $\delta E_g(x) = \beta x^{\alpha}$, and the then existing band structure calculations had always yielded a higher value of $\alpha > 0.8$ [28–30]. An explanation has recently been offered by Kent and Zunger [8] who pointed out that the existence of N bound states would slow down the band gap reduction, and adjust the α value to the experimental result of 2/3. We have now realized that the band structure calculation should really be compared to the excitonic absorption peak. Apart from a possible small change in exciton binding energy, the change in the excitonic absorption peak should be closest to the calculated band gap change. Electroreflectance measures, in the simplest situation, the third order derivatives of the dielectric function [24], but it is not clear what is exactly measured in a strongly distorted system like $GaAs_{1-x}N_x$. Figure 4 shows the low temperature absorption data for a set of free-standing GaAs:N samples, with 1 μm nominal thickness [31]. The red shift of the excitonic peak can be clearly tracked with N doping level up to x near 0.5%, so the band gap can be identified unambiguously. Fig. 5 shows the comparison between two sets of experimental data (ER data [27] and the new data of excitonic

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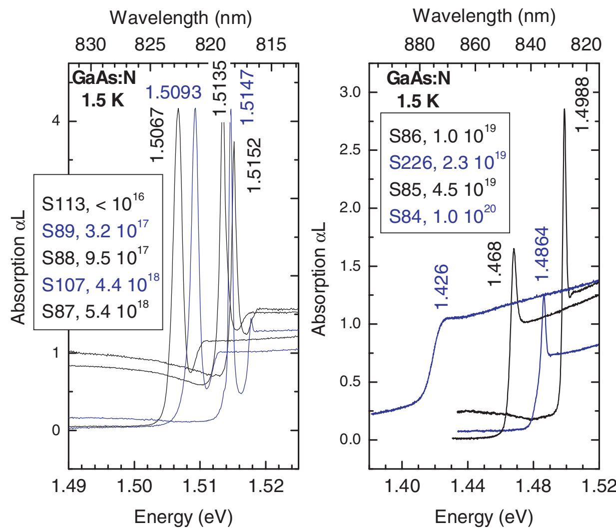

Fig. 4 (online colour at: www.interscience.wiley.com) Low temperature absorption spectra of free-standing GaAs:N films.

peaks), which clearly reveals the significant difference of the two techniques. In fact, the scaling component obtained from the low x region is found to be rather close to 1 ($\alpha = 0.96$). Therefore, the perfect match between the ER data [27] and the improved calculation [8] is unfortunately not for the right reason. The continuous red shift of the excitonic absorption peak indeed collaborates with the conclusion of various band structure calculations that the GaAs-like band edge moves down as a result of N doping [8, 10, 11, 28–30, 32]. However, instead of attempting to dismiss the impurity band formation in $GaAs_{1-x}N_x$ [8], one should really recognize the subtle difference between GaAs and GaP, thus, the interplay between the two effects in affecting the band edge absorption. It is worth emphasizing that N induced bound states in GaAs:N do form an impurity band but their density of states is too low to lead to a significant absorption compared to that of the host-like states. Nevertheless, they are sufficiently abundant to cause a significant reduction in the carrier lifetime and diffusion length, and unusual electronic properties near the absorption tail of the alloy [33].

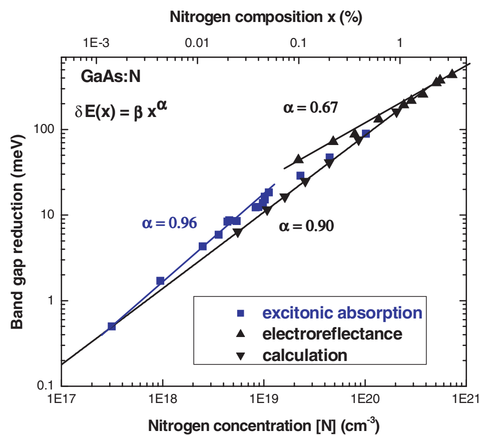

Fig. 5 (online colour at: www.interscience.wiley.com) Band gap reductions for GaAs:N obtained from fitting electroreflectance spectra, excitonic absorption peaks, and our band structure calculations.

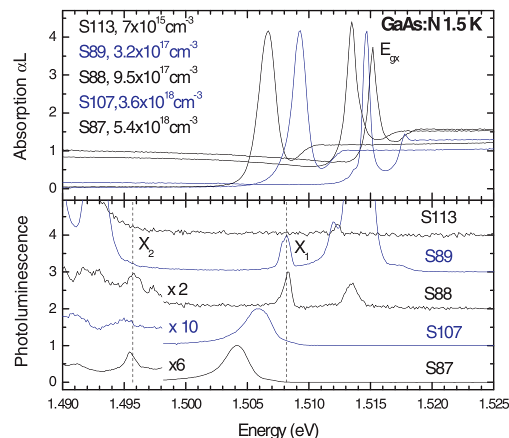

Fig. 6 (online colour at: www.interscience.wiley.com) Low temperature absorption and PL spectra for GaAs:N samples with varying N concentration. All PL spectra are scaled to the intensity of the X_1 line.

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A new approach, a self-consistent pseudopotential-based change-patching method, has recently been developed by Wang [34] for calculating the electronic structure of $GaAs_{1-x}N_x$ alike. We have used this new method to calculate the band structure of $GaAs_{1-x}N_x$. As an approximation, we consider an ordered array with one N atom per supercell, instead of the random structure in a real sample. The supercell is a cubic box with a multiplication factor n along three directions of the basic zinc-blende cubic cell, with n varying from 3 to 10. In previous calculations [10, 29, 30], n has been restricted to even number, so the L to Γ folding always occurred in the supercell calculation. Because the relative large L component was found in the conduction band edge state, the L–Γ coupling induced by N doping was attributed to be the dominant effect of the band gap reduction. However, there is no physical reason to limit n being even. In this calculation, we allow n also to be odd so that the L to Γ folding will not happen and the hypothesis of the L–Γ coupling can be tested. The results of our calculations are included in Fig. 5. One can see that all the calculated data points, for n both even and odd, fall on a single smooth curve, which clearly indicates that the explanation of the L–Γ coupling (repulsion) is misleading. Our calculation is found to excellently agree with the experimental data in the low doping limit, when the effect of the randomness in the real sample is expected to be insignificant.

The major deficiency of the approach of having the impurity incorporation in an ordered array is that the formation of pairs and triplets statistically in a random sample is excluded. In responding to this criticism [7, 27, 33], an attempt has been made to realistically simulate the randomly doped structure with the use of large supercell in the empirical pseudopotential approach [8]. One of the major results derived from the new effort is the prediction of how the N-induced bound states respond to the change in N doping level: *As the nitrogen concentration increases, the conduction band minimum moves down rapidly to lower energies. At the same time, the energies of the bound states are pinned and remain fixed. The downward moving band edge sweeps the discrete bound states into the conduction band one by one.* For the first time, in a recent careful study [31], we are able to simultaneously track the band edge excitonic absorption peak and the N bound states with varying N doping level. The results are shown in Fig. 6. The two N pair bound states [15], X_1 and X_2, are found to also red shift, as the decreasing band gap approaches them, but the impurity-host interaction depends strongly on the binding energy. Contrary to the prediction of Kent and Zunger [8], the nitrogen bound states do not remain fixed to be passively swept past by the downward moving band edge. The contradiction can easily been understood by noting that the calculated bound states have much larger binding energies (~100 meV) than those for X_1 and X_2 (<20 meV) due to the inadequate accuracy of the impurity potential in the empirical pseudopotential approach. A recent magneto-PL study [35] of $GaAs_{1-x}N_x$ with $x > 0.1$ % also indicates that the nitrogen induced bound states may have different degrees of localization, depending on how close energetically each bound state is to the host-like band gap.

4 Discussions

4.1 The alloy of GaAs and GaN and the bowing parameter The conventional understanding of an alloy A_xB_{1-x} is that when A and B are mixed homogeneously, the properties of the new material will evolve continuously from one end point to the other. It is highly unlikely that such an evolution can ever occur for the highly mismatched compounds like GaAs and GaN or GaP and GaN. However, one may relax the requirement of the full range tunablility, and instead examine the possibility of a continuous modification to the property of the host in a limited doping region, as for example, the band gap change in a few percent N doping range in GaAs. In such a situation, the attempt to describe the new material in a traditional manner, e.g., using a strongly x dependent bowing parameter $b(x)$ for $GaAs_{1-x}N_x$, might not be appropriate or necessary. Especially, in some cases, one of the end points might not even exist in nature (e.g., $GaAs_{1-x}Bi_x$ [36, 37]). Therefore, it is more convenient to just view these systems as heavily doped semiconductors rather than alloys. In fact, the results of our calculations, shown in Fig. 5, can be fit very well to the simple form $\delta E_g(x) = \beta x^{\alpha}$, with $\beta = 10.853$ eV and $\alpha = 0.897$, through out the region of x considered. If we force $E_g(x)$ to the standard formula $E_g(x) = E_g(0) + x(E_g(1) - E_g(0)) - bx\,(1 - x)$, we will have a bowling parameter b strongly depending on x: $b = 30$ eV, 24 eV, and 20 eV for $x = 0.01\%$, 0.1% and 1%, respectively.

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4.2 Electron effective mass in $GaAs_{1-x}N_x$ As discussed above, the band gap, perhaps the most fundament parameter for a semiconductor, becomes not so trivially defined in $GaAs_{1-x}N_x$ alloy. No wonder that the determination of the electron effective mass for this and related materials is even more controversial, as been discussed in a recent review article [38]. Magneto-PL has frequently been used for extracting the electron effective mass or reduced mass. In $GaAs_{1-x}N_x$, quite different results have been obtained in the most recent studies [35, 39]. It appears that the PL peak, even under very high field (e.g., $B > 30$ T), might not actually originate from the band gap transition [35, 40], due to the energy relaxation and the existence of various N related bound states. The results of using various other techniques, quantum confinement [6], ODCR on quantum well samples [17] and thermo-magnetic transport [18], are all subjected to further investigation as to what has really been measured. A brief discussion on the case of quantum confinement may be given here to shed some light on the complexity of the issue. N doping not only lowers the GaAs band edge but also introduced a series of states of varying degree of localization at the vicinity of the band edge. The states within this complex energy spectrum are expected to respond differently when the quantum confinement is applied to the $GaAs_{1-x}N_x$ layer, which results in a modification to the internal structure of the spectrum. Obviously, the host-like states are likely to be pushed up more than those impurity-like states, which leaves the impurity-like states more susceptible to the modulation probe. This consideration might explain why the effective mass obtained from the electroreflectance measurements on $GaAs_{1-x}N_x$/GaAs QWs [6] are significantly larger than those from other techniques [17, 18]. Another issue which should be mentioned is the effect of the incorporation of Indium into $GaAs_{1-x}N_x$. One trivial effect is that an appropriate amount of In may help to compensate the lattice mismatch caused by N doping in GaAs, and thus, reduce structural defects in the material. Another less trivial but probably more important effect, physically, is that the incorporation of In lowers the conduction band edge, thus, reduces the number of N related bound states. Therefore, as found experimentally, $Ga_{1-y}In_yAs_{1-x}N_x$ behaves more like conventional alloys than $GaAs_{1-x}N_x$, and the experimental results for $Ga_{1-y}In_yAs_{1-x}N_x$ are indeed less of controversy [41]. Because of this effect, one should not simply assume that the theory for $GaAs_{1-x}N_x$ is equally applicable for $Ga_{1-y}In_yAs_{1-x}N_x$ by merely making an adjustment in band gap.

5 Conclusions It is an unrealistic wish to develop a unified model or theory that equally applies to all the dilute nitrogen III–V-nitride materials. Many familiar physical properties in conventional semiconductors have been shown to be either less well defined or not uniquely defined, which prompts us to be vigilant when making comparison between different experimental results and between experiment and theory. In GaP:N, the red shift of the absorption edge is primarily due to the impurity band formation of nitrogen bound states [7]. None of the nitrogen bound states has been found to be repelled down by the proposed repulsive interaction with the Γ conduction band edge [5], and there is no experimental evidence for the assertion that N doping induces the L-like host state to plunge into the band gap [8]. In GaAs:N, the primary reason for the band gap reduction is the downward shift of the GaAs band edge [32, 28]. Nevertheless, contrary to the theoretical prediction [8], nitrogen bound states interact strongly with the host, and shift with the movement of the band edge [31].

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