Acceptorlike behavior of nitrogen deep traps in GaAs:N

E. A. Stinaff,* D. J. Wolford, K. W. Ver Steeg,† and Tyson D. Hoffmann
Iowa State University, Ames, Iowa 50011, USA

(Received 16 October 2005; revised manuscript received 19 December 2005; published 7 February 2006)

We report the observation of excited states of holes for acceptorlike excitons bound to isolated nitrogen impurities in GaAs:N under high hydrostatic pressures. Appearance of a large absorption resonance (5 K) in optical transmission and photoluminescence excitation spectroscopies leads to the identification of the 2*S* excited hole state associated with the ground-state nitrogen isoelectronic bound exciton—commonly known as the N_X state from earlier GaAs-based alloy studies. Comparison with the well-established effective-mass theory of Baldereschi and Lipari for excited-state *S*-type spectra of acceptors in semiconductors provides good qualitative agreement with our data. We thus deduce at 26.9 kbar the ground-state hole ionization energy as being ~19.2 meV, which in turn leads to a unique electron binding energy of ~10.3 meV for isolated nitrogen traps in GaAs:N at this pressure. These data and accompanying interpretations may provide for further understanding of the deep-level behavior of isoelectronic binding mechanisms in semiconductors.

DOI: 10.1103/PhysRevB.73.075203 PACS number(s): 71.20.Nr, 71.55.Eq, 78.20.−e, 78.55.Cr

I. INTRODUCTION

The unique properties of nitrogen as an isovalent impurity in III-V host semiconducting materials have been the subject of myriad experimental[1–6] and theoretical investigations.[7–14] It has been repeatedly demonstrated that, even in dilute quantities, nitrogen has profound and often counterintuitive effects[15,16] on the electronic properties of the host crystal.[17–23] Although there has recently been considerable interest in the higher-nitrogen-concentration region[24–27]—including the anomalous band-gap-bowing effects observed with atomic-concentration-range nitrogen doping[28,29]—detailed insight into the "deep-level" properties of nitrogen as an isolated impurity has remained an intriguing and largely still unfinished endeavor.[12,13] Crucial to this insight is a clear understanding of the mechanisms of carrier binding at isoelectronic centers. To hopefully further such views, we report the observation of excited states of the exciton bound to isolated nitrogen impurities in GaAs (at 5 K) under the application of high hydrostatic pressures.

II. MATERIALS AND EXPERIMENTAL METHODS

Samples used were high-purity *n*-type GaAs:N prepared by Cl-transport vapor phase epitaxy on *n*-type GaAs substrates, with nitrogen doping achieved by the introduction of NH_3 during the final (~20 μm) of growth.[30,31] Incorporated N concentrations were found to be at the level of $\sim 2\times10^{17}$ cm^{-3}, as determined by secondary-ion mass spectroscopy measurements calibrated by controlled N implantations. It is well known from earlier pressure and alloy work[32,33] that N produces a resonant electron state 150–180 meV above the GaAs Γ_{1c} conduction-band edge at atmospheric pressure [and does not enter the Γ_{1c} direct gap until ~22.5 kbar,[33] or $x>0.2$ in $GaAs_{1-x}P_x$:N (Refs. 32 and 34)]. The application of high and variable hydrostatic pressure is therefore necessary to accomplish observation of the bound exciton recombination due to isolated nitrogen—denoted "N_X" from the earlier $GaAs_{1-x}P_x$:N and $Al_xGa_{1-x}As$:N alloy studies.[34–37]

The samples were mechanically lapped and chemically etched to a thickness of 10–15 μm, photolithographically patterned into 80×80 μm^2 squares, and then loaded together with a small (~10 μm) ruby crystal and a transparent hydrostatic-pressure-transmitting medium into a Be-Cu diamond-anvil pressure cell[38,39] of our own design and considerably more advanced (e.g., allowing for helium 4 loading, maximum operating pressures of >1 Mbar, nonmagnetic environments, etc.) than the traditional Merrill-Bassett cell.[40] Additional samples were also cleaved along the (110) directions into parallelepipeds (cleaved, rather than lithographically patterned) to facilitate future studies of possible lasing mechanisms; these differing geometries (rough-sided squares versus optical cavities) should have no bearing on the comparative results of this study. The well-characterized R_1 line of ruby[38,39] was used to reproducibly determine the pressure at liquid-helium temperatures within the cells.[41]

Sample emission was detected using a GaAs photomultiplier tube, coupled to a Spex 0.85 m double-grating monochromator (with a typical resolution of 0.4 Å), while all experiments were performed at ~5 K in a helium gas exchange optical cryostat. Photoluminescence (PL) was excited using the 4579 Å line of an Ar^+ laser, with the excitation beam focused to a nominal beam waist of ~5 μm upon the sample surface, with power densities being held at $\sim10^3$ W/cm^2, while all emissions were collected in conventional "backscattering" geometry. In complementary fashion, photoluminescence excitation (PLE) was also sequentially measured using a tunable dye laser (R6G or DCM) as the excitation source, wherein the wavelength of the dye source output was continuously monitored using a Burleigh wavemeter (with a typical resolution of 0.4 Å, or ~0.1 meV), while its variable power output was stabilized to within ~1% using an acoustic-optic modulator. Hence, in all of the experiments both PL and PLE were routinely performed together upon the *same sample surface area*, both with equivalent and high spectral resolution. For all PLE excitation spectra taken, the resolving monochromator was set to monitor the $N_X(B)$ zero-phonon line as the characteristic signature of N-trap-related

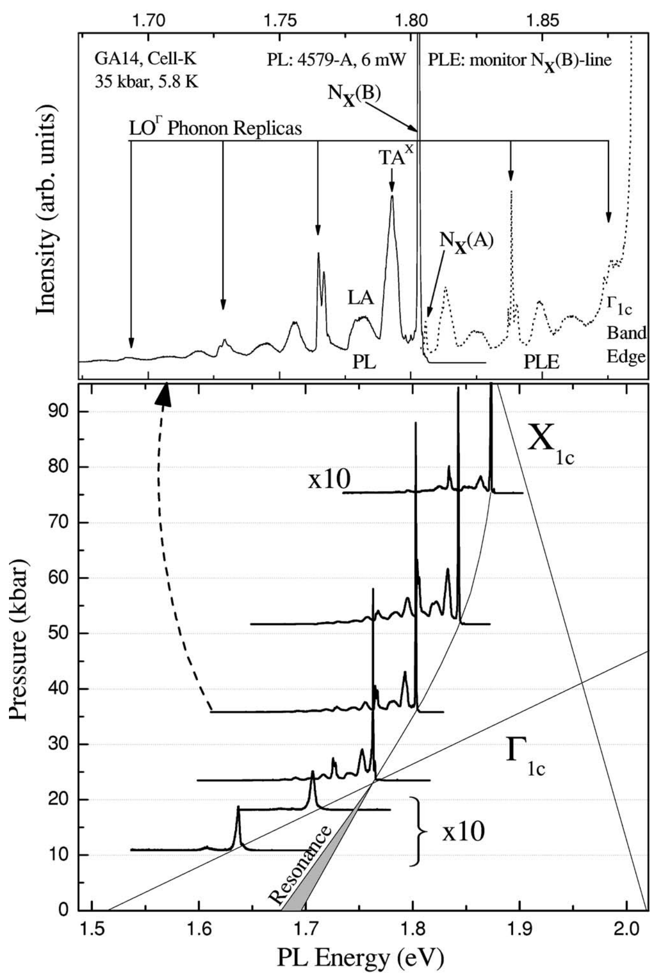


FIG. 1. Bottom panel shows stacked PL spectra of GaAs:N as function of pressure. The Γ_{1c} and X_{1c} band edges are also displayed for clarity. In the top panel is plotted a comparison between PL and PLE for a given pressure showing the characteristic optical (LO^{Γ}) and acoustic (TA^{X}, LA) phonon replicas.

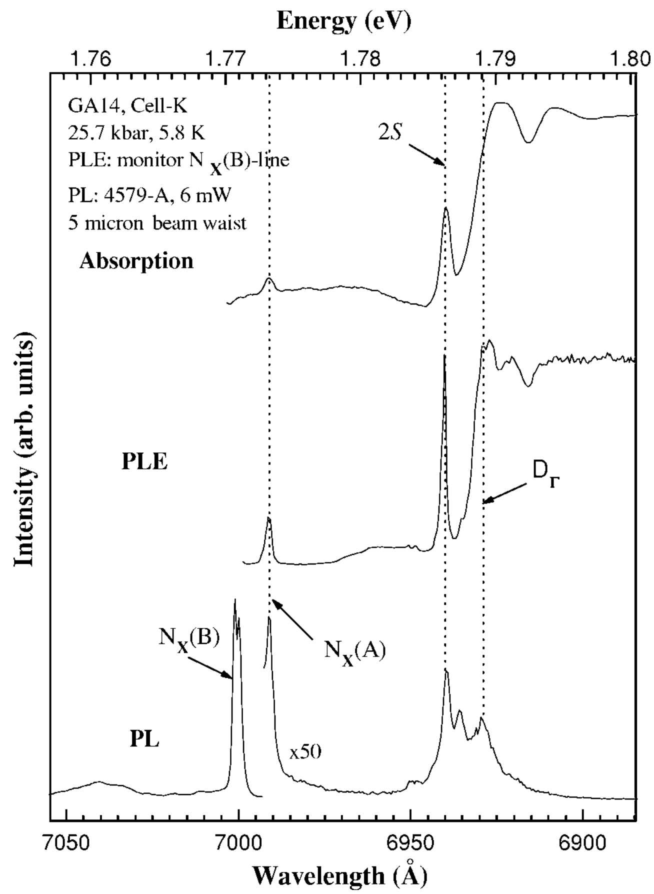


FIG. 2. Stacked PL, PLE, and absorption spectra of GaAs:N showing the strong absorption into the 2*S* excited state of the hole bound to N_X.

absorption processes. For complementary transmission measurements a broadband tungsten lamp was focused upon the rear surface of the sample, whereby a spectral-calibration determination of the lamp (absent the sample) was used to "normalize" the transmission spectra from through the sample.

III. RESULTS AND DISCUSSION

A. Nitrogen deep-level behavior

We begin in Fig. 1 with a discussion of the general PL characteristics over a broad pressure range, all at 5.8 K, and encompassing the extremes under which the isolated-N-impurity-bound exciton—N_X—lies within the host GaAs energy band gap versus pressure.[33,42] For convenience, the spectra have been rendered into a quasi-three-dimensional display accommodating the positions at each pressure of the Γ_{1c} and X_{1c} conduction-band edges.[42] As a deep defect[9,43] the N_X impurity level follows no particular nearby band edge,[44] but instead varies in energy with a relatively small pressure coefficient of $\sim$2.63 meV/kbar irrespective of the band structure,[44] until high pressures (>80 kbar) whereupon the level mimics the dependence of the indirect X_{1c} edge, passing out of the X_{1c} gap as a resonance above $\sim$87 kbar.[45] At the low-pressure opposite extreme it is represented as an electron resonance with the Γ_{1c} conduction band. Such pressure behaviors have been predicted for N (A_1 symmetric) deep traps by tight-binding theory[9,43] and those results agree quite nicely with the data presented here. To represent and clarify these behaviors Fig. 1 shows the superimposed band structure which indicates a Γ_{1c}-X_{1c} crossing at 41.5 kbar,[42] and a N_X electron resonant state at *atmospheric pressure* of $\sim$1.68 eV, or $\sim$160 meV above the Γ_{1c} conduction-band edge.[32,33]

To illustrate the rich spectrum of the isolated N center a single PL spectrum and its corresponding PLE spectrum at a pressure of 35 kbar have been plotted in the top panel of Fig. 1, wherein the germane optic ($LO^{\Gamma}\sim$34.2 meV, $X\sim$34.5 meV) and acoustic ($TA^{X}\sim$10 meV, LA$\sim$22 meV) phonon sidebands have been accented for clarity. The first and most prominent feature to note is that the PL spectrum is dominated by the otherwise forbidden $N_X(B)$ line, while the allowed $N_X(A)$ is only predominantly observed in the excitation process of PLE.[33] These lines are due, respectively, to N-bound excitons carrying total angular momentum of $J=2$

and $J=1$ (B and A levels, respectively, as in GaP:N) of the "ground" $1S$ state of the N_X level of the isolated nitrogen impurity, and are found in all of our GaAs:N samples to be split by the noted unusually large pressure-dependent correlation and exchange (jj coupling).[1,3,46] This splitting is clearly identifiable in the PL spectra shown in Fig. 2 where the $N_X(A)$ and $N_X(B)$ zero-phonon lines (1.7732 and 1.7710 eV) are found to be split by ~2.2 meV. This extreme splitting, compared to the relatively small and virtually invariant-in-magnitude (in the absence of stress and/or magnetic fields) A-B splitting of 0.8 meV found characteristically in GaP:N,[2] is suggestive of enhanced electron-hole spatial overlap[46] found in GaAs:N as compared to the isolated center in GaP:N.[2] There is also presumably mixing of the $J=1$ and 2 states, for example, due to possible additional lowered symmetry surrounding the isolated N center that may be characteristic of N in alloys and GaAs.[32,33,46] These two effects together, splitting and mixing, lead to thermal depopulation (at 5 K) of the usually overwhelmingly dominant $N_X(A)$ line in favor of the ordinarily forbidden $N_X(B)$ line.[2,46]

B. N_X excited states

An additional line is clearly observed in the comparison of PL, PLE, and transmission (plotted as "relative" absorption) shown in Fig. 2 for a temperature of 5.8 K and a pressure of 25.7 kbar. This feature, found to lie ~13 meV above the $N_X(A)$ line, displays uncommonly large intensities in both absorption and PLE. Although this absorption and emission falls within the energy range of the TA phonon replica of the $N_X(B)$ zero-phonon line, the fact that it is observed at the same energy in PL (together with an extremely narrow spectral linewidth of ~0.2 meV in PLE and ~1.2 meV in absorption) precludes the possibility that this emission may be due, for example, to additional unidentified phonon participations involving the N_X state. Also seen is the familiar and commonly observed emission from the shallow-donor-bound exciton—denoted D_Γ—associated with the Γ_{1c} conduction-band-edge donor excitons.[32,42] The D_Γ state lies ~6 meV below the Γ_{1c} edge, and is found to rigidly track the direct conduction-band edge with pressure (and as such may be used as a convenient check on the ruby-pressure measurements as the Γ_{1c} edge shifts linearly with pressure at a rate of 10.8 meV/kbar up to $\leqslant$50 kbar).[42]

Due to the close proximity (~9 meV) of this additional line to both D_Γ and the Γ_{1c} direct band edge an alternative explanation for this emission and absorption might conceivably be an additional unexpected shallow-donor-bound exciton, or an acceptor exciton state—and not the isolated N trap. Tracking the emission with varying pressure will establish the association of the composite spectral lines and reveal whether they arise from processes identifiable with the N_X or D_Γ-states. To this end, Fig. 3 shows versus pressure just such a dependence of what we shall hereafter refer to as the "$2S$ excited hole state" of the N_X deep trap. As the pressure is increased, it becomes evident that this additional line ($2S$) does not shift in energy with the band edge D_Γ emission, but rather rigidly tracks with respect to pressure both the N_X emission and absorption. This is characteristic of "excited-state features" associated with deep-trapping levels, and lends further credence to the identification of these lines as being associated with a previously unobserved "excited state" of the N_X exciton. This is consistent with its unusually intense absorption and PLE signal strengths (exceedingly large oscillator strength). For both strong absorption and PLE to occur together, not only must an efficient absorption channel be opened, but also an efficient relaxation channel into the final state must exist—as, for example, the prominent corresponding peak found in PL at the same energy in Fig. 2.

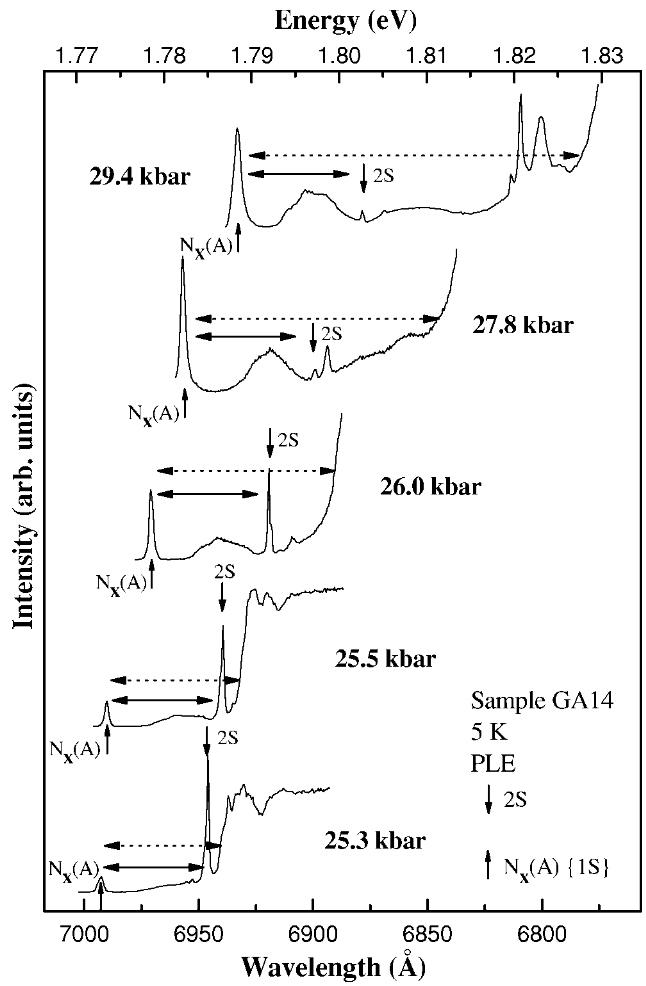


FIG. 3. Stacked PLE spectra of the $2S$ excited state of N_X showing the correlation to the deep-level behavior of the N_X exciton. The relatively constant separation between $N_X(A)$ and the first ($2S$) excited state is indicated with solid horizontal arrows. Horizontal dashed arrows indicate the increasing separation between $N_X(A)$ and the GaAs band edge.

Having established the association of the observed composite excitation with the N_X deep trap, the next step is to analyze detailed spectra to decide whether still further higher n-excited states might also be discovered, and from what their electronic origin might derive. To this end, Fig. 4 presents a PLE spectrum taken at 5.8 K and 26.9 kbar, wherein just such a succession of higher-lying excitations "tied" to the N_X state may be clearly made out. These same excitation energies are recorded in Table I, together with theoretically

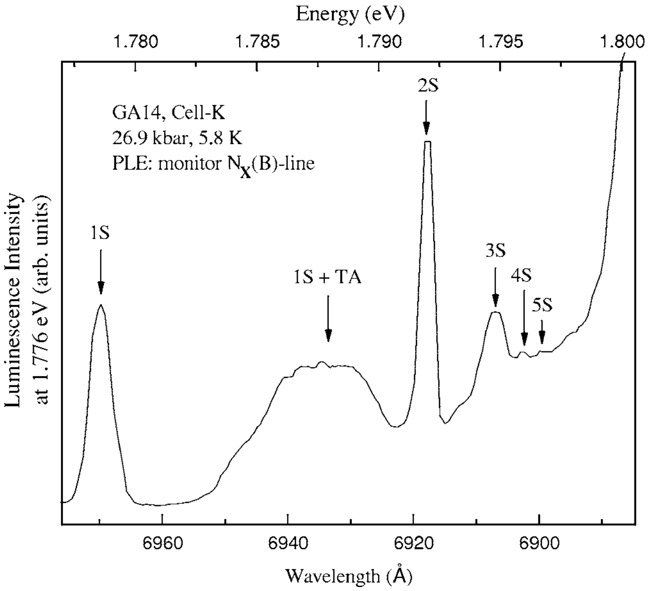
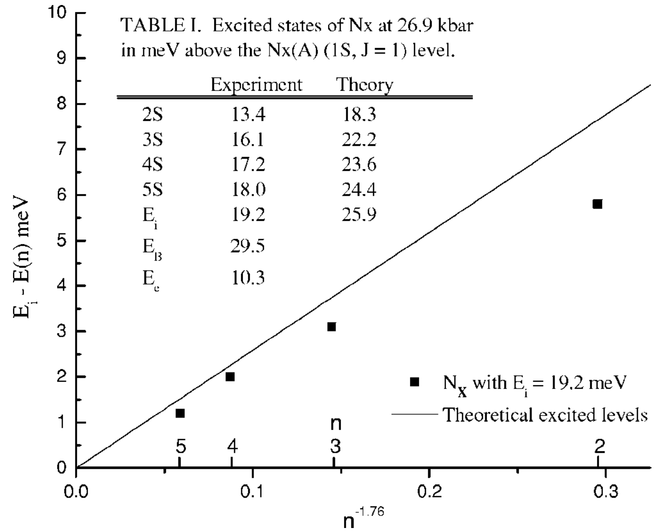


FIG. 4. Excitation spectra at 5.8 K monitoring the $N_X(B)$ $(J=2)$ emission. Labeled are the nS excited states of the hole bound within the N_X exciton. Also observed is the broad TA replica of the zero-phonon line.



	Experiment	Theory
2S	13.4	18.3
3S	16.1	22.2
4S	17.2	23.6
5S	18.0	24.4
E_i	19.2	25.9
E_B	29.5	
E_e	10.3	

FIG. 5. Comparison of the observed excited states to the EM theoretical values (solid line). The ionization energy of the hole, E_i, was found by taking the series limit.

predicted effective-mass (EM) energies for excited states of a hole bound to an "ideal acceptor" in GaAs, as will be discussed below.

C. Comparison to EM model

The microscopic model first proposed by Hopfield, Thomas, and Lynch[1,3] (HTL) to explain anomalous exciton binding to neutral impurities has now solidly stood for some four decades as a cogent starting point for an intuitive understanding of the binding of an exciton to any isoelectronic substituent. Within this model, the large difference in electronegativity[47,48] (central-cell potential or the chemical shift) between first-row impurities and the anion of the host crystal provides an attractive potential for an electron to be trapped at an "isoelectronic acceptor."[2,3] Once the electron is confined, it induces a long-ranged Coulomb field which may in turn bind a free hole, thus forming an isoelectronic bound exciton, described for N traps as "acceptorlike" impurities. This is the situation for nitrogen doping in GaP and GaAs- and GaP-based alloys, and our current GaAs:N example under pressure. The binding potential for the electron is short ranged and, therefore, leads to a relatively spatially compact electron charge distribution surrounding the N impurity site.[7–10,43] It then becomes reasonable to make the comparison of the N_X-bound exciton to that in GaP:N (A and B lines), GaAs:N, and their related alloys of a neutral acceptor of S symmetry. Following just such an approach, Cohen and Sturge[4,49] were able to find in GaP:N surprising agreement between the excited nS hole state energies bound to deep NN_i $(i \leq 6)$ pairs in GaP and the effective-mass theory for shallow acceptor states, as formally developed earlier and quite generally for a wide range of semiconductors by Baldereschi and Lipari.[50,51] Shallower NN_i $(i \geq 7)$ pair-binding energies, however, were found to be consistently smaller than predicted theoretical interpretations based solely upon ideal shallow-acceptor core potentials. Despite this minor shortcoming it is instructive to compare the EM-calculated energies from Refs. 50 and 51 to those observed in experiment for our current example of GaAs:N.

Starting with the results of Baldereschi and Lipari,[50,51] the following EM parameters were used (in units of m_0) for GaAs: $\gamma_1=6.98$, $\gamma_2=2.06$, and $\gamma_3=2.93$ for the hole, $m_e^*=0.067$ for the electron,[52] and a static dielectric constant of $\epsilon_0=12.53$.[53] These parameters were used to deduce the N_X acceptor energy levels from the tabulated results in Refs. 50 and 51. Just as Cohen and Sturge found for GaP:N,[4,49] these energies may be fitted to the following semiempirical expression:

$$E_i - E(nS) = E_0 n^{-1.76},$$

wherein E_i represents the ionization energy in the $1S$ hole ground state, E_0 equals the acceptor ground-state binding energy of 25.9 meV characteristic of GaAs (in the absence of central-cell corrections), and n represents the enumeration of the nth excited hole state. To this end, Fig. 5 presents a comparison of our first four experimentally derived excited-state energies of the N_X exciton hole to their corresponding theoretical EM excited hole states.The hole ionization energy E_i is deduced by taking the series limit of the high-lying excited states—a value found in the present GaAs:N case to be 19.2 meV. This comparison clearly demonstrates the discrepancies that may accompany direct comparison between purely EM calculations and actual experiments on nonideal acceptors, such as isolated nitrogen traps.[4,49] Nevertheless, this is not unexpected, as N as an isoelectronic acceptor in GaAs might differ from rigorous EM theory[4,49–51] in two crucial respects. First, nitrogen's atomic core in the HTL model[1] is attractive to electrons, and, therefore, repulsive to holes (although this repulsive core effect should have minimal influence as the N central-cell potential is particularly short ranged).[7] Second, and considerably more important, is the fact that the electron charge distribution cannot be fully localized upon the impurity site (as it would be in an ideal acceptor),[50,51] thus having the net effect of reducing the overall long-ranged Coulomb potential strength for holes. Further, since the N_X level within the band gap varies widely with respect to nearby band structure with pressure (Fig. 1), the N_X exciton localization will without doubt be a strong and sensitive function of this electron binding energy E_e. Such is reflected in the widely varying phonon coupling types and strengths we find versus pressure in GaAs:N, a result which has been more directly dealt with elsewhere in relation to N traps in alloys,[46] and we find mirrored in the details of the phonon coupling strengths versus pressure in GaAs:N in these studies.[37]

D. Binding energies

From knowledge of the GaAs band-edge luminescence (D_Γ or D_X^0 neutral donor-bound exciton) the total exciton binding energy may clearly be determined at any given pressure.[42] As an example, the total N_X exciton binding energy is found in Fig. 3 to be 29.5 meV. From this result, the electron binding-energy portion E_e of the total exciton energy (E_i+E_e) for N trapping in GaAs may be arrived at as being ~10.3 meV (for 26.9 kbar) from direct subtraction of the exciton energy from that of the Γ_{1c} band edge. Nevertheless, it should be stated that such an assumption should be taken in the context of the N trap being a *bona fide* deep level in GaAs.[9,43] Hence, it still possesses electronic composition derived from a full multiband view of the host band structure making up the bound N_X electron charge distribution in its electron wave function—including, for example, even distant *s*-derived symmetry states from deep within the valence band and high up in the conduction bands.[9,12–14,43]

Interestingly, we also find in our experiments that there appears to be a clear pressure dependence of the details of the hole excited state spectra of Fig. 4. Thus, although PLE intensities (oscillator strengths) of the *nS* excited hole states are found to decrease rapidly with increasing pressure above 26.9 kbar (for this observation we provide no theoretical offering), it is still possible to make out a clear and definitive, but modest increase at higher pressures of ~0.5 meV/kbar for the 1*S*-to-2*S* hole energy separation. This behavior is qualitatively consistent with both the EM theory for shallow acceptors and the deep-level behavior of the nitrogen trap, as it indicates that the dramatic increase in the binding energy of the N_X exciton with increasing pressure manifests itself as an increasingly bound, and, therefore, more spatially compact N_X electron charge distribution. This additional electron localization will necessarily lead to a correspondingly larger hole-binding energy, which would more closely resemble the energies derived from EM theory. Such a hole bound state was demonstrably found to be revealed among the widely varying exciton binding energies Cohen and Sturge[4,49] reported across the NN_i series in GaP:N. Further, unlike our above results, they found no hole bound-state spectra for the isolated N center in GaP. Theoretical refinements to the EM model have been developed which more carefully take into account the less-than-fully-localized electron bound to N in GaP.[10,54] For example, Zhang[10] found that due to the compact but incompletely localized electron charge distribution, a theoretical hole binding energy for isolated N arose in GaP of 27.2 meV, accompanied by a remaining derived E_e equal to ~5.8 meV. Extensions of such approaches may lead to a more complete understanding of our refined observations for GaAs:N, as we are clearly beginning with a finite multivalley representation of (at least) E_e for N_X in GaAs:N.

Based upon the above-noted pressure dependence of the 1*S*-to-2*S* hole excitation energy we may make an additional conclusion, short of a detailed calculation. The directly deduced hole binding energy (Fig. 4) of 19.2 meV at 26.9 kbar along with the observed binding energy pressure dependence of ~0.5 meV/kbar allows us to extrapolate the hole ground-state binding at 41.5 kbar to a value of 26.5 meV. This is in comparison with an EM hole ground-state binding energy of 25.9 meV from the work of Baldereschi and Lipari[50,51] in absence of the central cell.[47,48] This conclusion is consistent with the behavior of the N_X level with increasing pressure. The N_X level varies continuously in binding energy with respect to the nearby direct and indirect edges as pressure is varied, as is clearly displayed in Fig. 1. Indeed, it begins as a conduction-band resonance some 160 meV above the Γ_{1c} band edge in GaAs at atmospheric pressure and evolves through the Γ_{1c} band as pressure is raised. It then emerges from the band at ~22 kbar as a discrete bound state (with significant phonon coupling) and then progressively deepens within the Γ_{1c} gap as pressure is increased, until the Γ_{1c}-X_{1c} band crossing which sets in at ~41.5 kbar. It is here at band crossing that the N_X level reaches its deepest value of ~140 meV within the band gap. From here, toward higher pressures, N_X becomes increasingly shallower within the X_{1c} gap, until the level departs from the indirect gap, again as a conduction-band resonance above ~87 kbar.[45] (Interestingly, this general binding energy dependence mirrors much of that for N in $GaAs_{1-x}P_x$ and $Al_xGa_{1-x}As$ versus alloy composition.[32,34,37]) Therefore at 41.5 kbar, where the N_X level has its deepest binding energy, the hole binding closely resembles that of an ideal acceptor. This implies that at its deepest binding the N iselectronic trap in GaAs is behaving as a virtually ideal HTL trap, with the bound electron fully localized just as Cohen and Sturge found for nearer-neighbor NN_i pairs (of considerably larger exciton binding energies) in GaP.[2,49] We also note that although isolated N is of "dubious electron binding" in GaP, in GaAs under pressure it may be decidedly regarded as a *bona fide* multiband deep electron trap.[9,12,13,43]

IV. CONCLUSION

In conclusion, we have presented evidence of excited *acceptorlike* states of the exciton bound to nitrogen (the N_X level) in GaAs:N with the application of hydrostatic pressure. These states qualitatively follow the broadly and firmly established EM theory of Baldereschi and Lipari for acceptors with *S*-type symmetry in semiconductors. The substantial quantitative deviation we find from that of an ideal acceptor in GaAs, however, is indicative of the expected less-than-fully-localized spatial extent taken by the N_X bound electron. Analysis of the data reveals an estimated ground-state hole ionization energy of 19.2 meV (at 26.9 kbar), which may be directly compared with the EM theory yielding a minimum ground-state hole binding energy of ~25.9 meV for ideal holes in GaAs (absent the central cell). This, together with detailed knowledge of the Γ_{1c} band edge in GaAs, results at this pressure in an electron localization energy for the isolated N trap of ~10.3 meV. We also find in experiment there to be a pressure dependence of this hole binding energy of 0.5 meV/kbar, which extrapolates to a derived maximum hole binding energy of ~26.5 meV at the Γ_{1c}-X_{1c} band crossing—a value consistent with N in GaAs under pressure being both an ideal HTL isoelectronic center and a *bona fide* multiband deep electron trap. It should be noted that this value of 26.5 meV agrees unaccountably well with the computed hydrogenic acceptor value (absent the central cell) for GaAs as described by Baldereschi and Lipari. The results related herein should therefore allow for further refinements to the theoretical descriptions of the isolated nitrogen trap in GaAs and their possible relevance to the scientifically and technologically important dilute nitrogen $GaAs_{1-x}N_x$-related alloys.

*Corresponding author. Present address: Naval Research Laboratory, Washington, DC 20375, USA. Electronic address: stinaff@bloch.nrl.navy.mil

†Present address: Centennial Medical Center, Nashville, TN 37203, USA.

[1] J. J. Hopfield, D. G. Thomas, and R. T. Lynch, Phys. Rev. Lett. **17**, 312 (1966).

[2] D. G. Thomas and J. J. Hopfield, Phys. Rev. **150**, 680 (1966).

[3] W. Czaja, in *Festkorperprobleme*, edited H. J. Queisser (Pergamon-Vieweg, Braunschweig, 1981), Vol. 11, p. 65.

[4] E. Cohen and M. D. Sturge, Phys. Rev. B **15**, 1039 (1977).

[5] Y. Zhang, A. Mascarenhas, J. F. Geisz, H. P. Xin, and C. W. Tu, Phys. Rev. B **63**, 085205 (2001).

[6] S. Francoeur, M. J. Seong, M. C. Hanna, J. F. Geisz, A. Mascarenhas, H. P. Xin, and C. W. Tu, Phys. Rev. B **68**, 075207 (2003).

[7] R. A. Faulkner, Phys. Rev. **175**, 991 (1968).

[8] W. Y. Hsu, J. D. Dow, D. J. Wolford, and B. G. Streetman, Phys. Rev. B **16**, 1597 (1977).

[9] H. P. Hjalmarson, P. Vogl, D. J. Wolford, and J. D. Dow, Phys. Rev. Lett. **44**, 810 (1980).

[10] Y. Zhang, Phys. Rev. B **45**, 9025 (1992).

[11] Y. Zhang and A. Mascarenhas, Phys. Rev. B **61**, 15562 (2000).

[12] L. W. Wang, Appl. Phys. Lett. **78**, 1565 (2001).

[13] P. R. C. Kent and A. Zunger, Phys. Rev. B **64**, 115208 (2001).

[14] P. R. C. Kent and A. Zunger, Phys. Rev. Lett. **86**, 2613 (2001).

[15] H. M. Cheong, Y. Zhang, A. Mascarenhas, and J. F. Geisz, Phys. Rev. B **61**, 13687 (2000).

[16] M. J. Seong, H. M. Cheong, S. Yoon, J. F. Geisz, and A. Mascarenhas, Phys. Rev. B **67**, 153301 (2003).

[17] T. Shima, Y. Makita, S. Kimura, H. Sanpei, Y. Fukuzawa, A. Sandhu, and Y. Nakamura, Appl. Phys. Lett. **74**, 2675 (1999).

[18] J. D. Perkins, A. Mascarenhas, Y. Zhang, J. F. Geisz, D. J. Friedman, J. M. Olson, and S. R. Kurtz, Phys. Rev. Lett. **82**, 3312 (1999).

[19] W. Shan, W. Walukiewicz, J. W. Ager III, E. E. Haller, J. F. Geisz, D. J. Friedman, J. M. Olson, and S. R. Kurtz, Phys. Rev. Lett. **82**, 1221 (1999).

[20] Y. Zhang, A. Mascarenhas, H. P. Xin, and C. W. Tu, Phys. Rev. B **63**, 161303(R) (2001).

[21] F. Masia, A. Polimeni, G. B. H. von Hogersthal, M. Bissiri, M. Capizzi, P. J. Klar, and W. Stolz, Appl. Phys. Lett. **82**, 4474 (2003).

[22] R. Intartaglia, T. Taliercio, P. Valvin, B. Gil, T. Bretagnon, P. Lefebvre, M.-A. Pinault, and E. Tournié, Phys. Rev. B **68**, 235202 (2003).

[23] S. Francoeur, J. F. Klem, and A. Mascarenhas, Phys. Rev. Lett. **93**, 067403 (2004).

[24] M. Weyers, M. Sato, and H. Ando, Jpn. J. Appl. Phys., Part 2 **31**, L853 (1992).

[25] M. Weyers and M. Sato, Appl. Phys. Lett. **62**, 1396 (1993).

[26] T. Makimoto, H. Saito, T. Nishida, and N. Kobayashi, Appl. Phys. Lett. **70**, 2984 (1997).

[27] T. Makimoto and N. Kobayashi, Appl. Phys. Lett. **67**, 688 (1995).

[28] S. H. Wei and A. Zunger, Phys. Rev. Lett. **76**, 664 (1996).

[29] L. Bellaiche, S. H. Wei, and A. Zunger, Phys. Rev. B **54**, 17568 (1996).

[30] J. W. Burd, Trans. Metall. Soc. AIME **245**, 571 (1969).

[31] M. G. Craford and W. O. Groves, Proc. IEEE **61**, 862 (1973).

[32] D. J. Wolford, J. A. Bradley, K. Fry, J. Thompson, and H. E. King, in *Gallium Arsenide and Related Compounds*, edited by G. E. Stillman, IOP Conf. Proc. No. 65 (IOP, London, 1982), p. 477.

[33] D. J. Wolford, J. A. Bradley, K. Fry, and J. Thompson, in *Proceedings of the 17th International Conference on the Physics of Semiconductors*, edited by J. D. Chadi and W. A. Harrison (Springer, New York, 1984), p. 627.

[34] D. J. Wolford, W. Y. Hsu, J. D. Dow, and B. G. Streetman, J. Lumin. **18/19**, 863 (1979).

[35] D. J. Wolford, R. E. Anderson, and B. G. Streetman, J. Appl. Phys. **48**, 2442 (1977).

[36] D. J. Wolford, B. G. Streetman, R. J. Nelson, and N. Holonyak, Jr., Solid State Commun. **19**, 741 (1976).

[37] D. J. Wolford, B. G. Streetman, W. Y. Hsu, J. D. Dow, R. J. Nelson, and N. Holonyak, Jr., Phys. Rev. Lett. **36**, 1400 (1976).

[38] A. Jayaraman, Rev. Mod. Phys. **55**, 65 (1983).

[39] G. J. Piermarini, S. Block, J. D. Barnett, and R. A. Forman, J. Appl. Phys. **46**, 2774 (1975).

[40] L. Merrill and W. A. Bassett, Rev. Sci. Instrum. **45**, 290 (1974).

[41] R. A. Noack and W. B. Holzapfel, in *Proceedings of the Sixth AIRAPT International High Pressure Conference*, 1977 (unpublished).

[42] D. J. Wolford and J. A. Bradley, Solid State Commun. **53**, 1069 (1985).

[43] P. Vogl, in *Festkorperprobleme*, edited by J. Treusch (Vieweg,

Braunschweig, 1981), Vol. 21, p. 191.
[44] S. Y. Ren, J. D. Dow, and D. J. Wolford, Phys. Rev. B **25**, 7661 (1982).
[45] D. J. Wolford and J. A. Bradley (unpublished).
[46] D. J. Wolford, B. G. Streetman, and J. Thompson, J. Phys. Soc. Jpn. **49**, 223 (1980).
[47] G. F. Bassani, *Electronic States and Optical Transitions in Solids* (Pergamon Press, Oxford, 1975), p. 240.
[48] J. C. Phillips, *Bonds and Bands in Semiconductors* (Academic Press, New York, 1973), p. 235.
[49] E. Cohen, M. D. Sturge, N. O. Lipari, M. Altarelli, and A. Baldereschi, Phys. Rev. Lett. **35**, 1591 (1975).
[50] A. Baldereschi and N. O. Lipari, Phys. Rev. B **8**, 2697 (1973).
[51] A. Baldereschi and N. O. Lipari, Phys. Rev. B **9**, 1525 (1974).
[52] I. Vurgaftman, J. R. Meyer, and L. R. Ram-Mohan, J. Appl. Phys. **89**, 5815 (2001).
[53] D. L. Rode, in *Semiconductors and Semimetals*, edited by R. K. Willardson and A. C. Beer (Academic Press, New York, 1975), p. 10.
[54] G. F. Glinski and T. N. Loginova, Sov. Phys. Solid State **26**, 1923 (1984).