Free carrier and/or exciton trapping by nitrogen pairs in dilute $GaP_{1-x}N_x$

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The electronic properties of nitrogen pairs have been investigated in dilute $GaP_{1-x}N_x$ samples ($x \leqslant 0.24\%$) by excitation photoluminescence (PLE) spectroscopy and by temperature-dependent photoluminescence (PL). PLE spectra show that three channels are mainly responsible for populating N pairs: (i) exciton tunneling from the isolated nitrogen atom level toward energetically shallow N pairs; (ii) capture of a free exciton by all pairs; and (iii) capture of a free electron and subsequent binding of a hole by energetically deep pairs. On this basis, the quenching with increasing temperature of PL lines associated with different N pairs is described quantitatively.

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I. INTRODUCTION

There is currently a renewed interest for isoelectronic impurities in III-V semiconductor compounds.[1–8] Indeed, the progress in epitaxial growth techniques has recently allowed incorporating a few percents of N atoms in $GaAs_{1-x}N_x$ and $GaP_{1-x}N_x$,[1–4,8] much more than expected on the basis of thermodinamic arguments,[9] with unexpected, large variations in the electronic properties of the host lattice. These changes include a giant reduction in the host band gap that allows making optoelectronic devices such as light emitters in the telecommunications and visible ranges.[1–8]

In the late 1960s, Thomas and Hopfield showed that the narrow emission (or absorption) lines observed in GaP:N for low N concentration ($\sim 10^{18}$ cm^{-3}) could be attributed to the recombination of excitons bound to an isolated nitrogen atom, N_0^a line,[10] or to nitrogen pairs with increasing lattice separations and decreasing exciton binding energy, NN_i lines.[11–13] Later, it was shown that the assumption of a monotonic ordering of the NN_i lines is not fully correct[14–16] and that the NN_2 line, at least, is associated with a three-N atom complex.[15] A typical low-temperature photoluminescence (PL) spectrum is shown in Fig. 1 for a $GaP_{1-x}N_x$ sample with $x=0.05\%$, together with the conventional emission line labeling.

The problem of how a neutral complex can bind an exciton in GaP:N and other materials is a fundamental issue addressed in many theoretical studies.[16–23] Some models[18] rely on the strain fields arising from the huge size difference between P and N to explain the binding of the exciton as a whole, while other models[17,19,23] focus on the very high electronegativity of single and pairs of N atoms, which provides a short-range potential attracting first an electron and then a hole. In the latter framework, N-related complexes show an acceptorlike behavior, as qualitatively predicted by the empirical model described in Refs. 10–13. As a matter of fact, a detailed investigation of the excited states of *e-h* pairs bound to N complexes provided some evidence that energetically deep N pairs do indeed behave as acceptors. However, N complexes progressively lose their acceptorlike character as their energy comes closer to that of the conduction band minimum, apparently approaching an excitonic behavior for the energetically shallower pairs and for the isolated nitrogen atom.[24] These observations can be explained qualitatively as in the following. The energy of the ith PL line is given roughly by the difference between the energy gap of GaP, E_{gap}, and the binding energy for an electron and a hole to the ith N complex, $E_i^{PL}=E_{gap}-(E_b^{h+}+E_{b(i)}^{e-})$. Since the binding energy of the hole (~ 40 meV) is nearly independent of the complex under consideration,[24,25] E_i^{PL} depends solely on the electron binding energy, $E_{b(i)}^{e-}$, which, in turn, is determined by the strength of the short-range attractive potential for the electrons. $E_{b(i)}^{e-}$ quickly decreases on going from deep to shallow complexes, vanishing for those complexes whose energy distance from the conduction band is approximately equal to

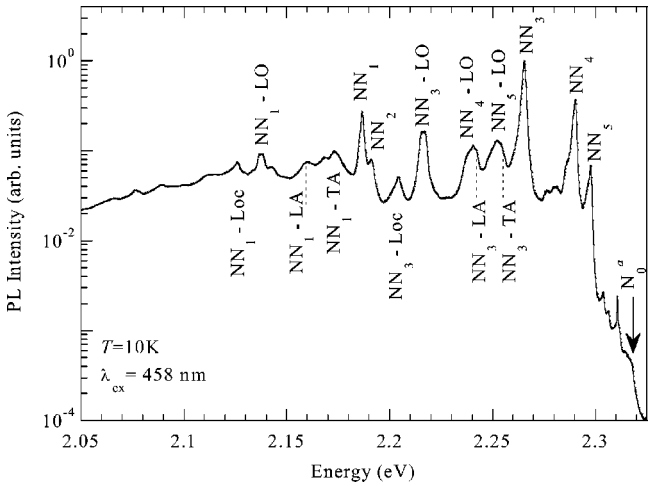

FIG. 1. Peak-normalized photoluminescence (PL) spectrum at 10 K of the $GaP_{1-x}N_x$ sample with $x=0.05\%$ studied in this paper. The NN_i lines and their phonon replicas are labeled according to the classification introduced by Hopfield and Thomas (Refs. 4,11–13). LO stands for Longitudinal Optical, LA and TA for Longitudinal Acoustical and Transverse Acoustical, respectively; Loc denotes Local mode. The position of the N_0^a line (2.317 eV) is highlighted with an arrow.

E_b^{h+}. In this case, the two-step mechanism of the electron and hole pair capture can be ruled out and excitons are captured as a whole by the N single atoms or pairs. The recombination on N pairs lying in an intermediate energy range, instead, may show a "mixed" character, thus making difficult to identify as "strictly excitonic" or "acceptorlike" this recombination.

In this paper, the detailed nature of the recombination on different nitrogen pairs and the trapping (and release) of carriers on (from) N complexes are studied by measuring the excitation photoluminescence (PLE) and photoluminescence quenching with increasing temperature of different N pairs for different N concentrations. It is found that N pairs can be populated through: (i) phonon-assisted exciton tunneling from the isolated N atom; (ii) capture of a free exciton; and (iii) capture of a free electron and subsequent binding of a free hole. Nitrogen pairs with an energy close to that of the conduction band minimum (CBM) are primarily populated through the excitonic channels (i) and (ii), whereas deep N pairs show a stronger coupling with the electrons by channel (iii), thus providing complementary evidence of the trend observed in Ref. 24. Moreover, the shift of the band gap to lower energy with increasing nitrogen concentration leads to a decrease in the capability of a same N pair to bind an electron and a hole separately. These results strongly support and quantify previous models as well as allow to quantitatively reproduce with a limited number of fitting parameters the quenching with increasing temperature observed for the PL intensity of different NN_i lines.

II. EXPERIMENTAL

The $GaP_{1-x}N_x$ epilayers studied in this work were grown by gas-source molecular beam epitaxy on a (001) GaP substrate. Most of the measurements were performed on a sample with $x=0.05\%$, but a sample with nitrogen concentration of 0.24% was also studied to monitor the effects of increasing x on the properties of N complexes. The epilayer thickness is 250 nm, as determined by x-ray diffraction measurements. The excitation source for PLE measurements was provided by a 150 W halogen lamp, whose light was monochromatized by a 25 cm long monochromator. The resulting resolution was 1.6 nm. In PL measurements, the samples were excited by the 458 or 350 nm line of an Ar^+ laser. The PL signal was dispersed by a double 0.75 m monochromator and detected by a cooled photomultiplier with a GaAs cathode used in a single-photon counting mode or by a silicon charge-coupled device (CCD).

III. EXCITATION PHOTOLUMINESCENCE

In PLE measurements with detection energy at E_{det} the signal is proportional to the absorption coefficient at the energy of the excitation photons and to the probability that photogenerated carriers relax and are captured by the complex emitting at E_{det}. The low-temperature PLE spectra, shown in Fig. 2 for a $x=0.05\%$ sample, were obtained by detecting the luminescence signal at the emission energy of lines NN_1, NN_3, NN_4, and NN_5, from bottom to top of the

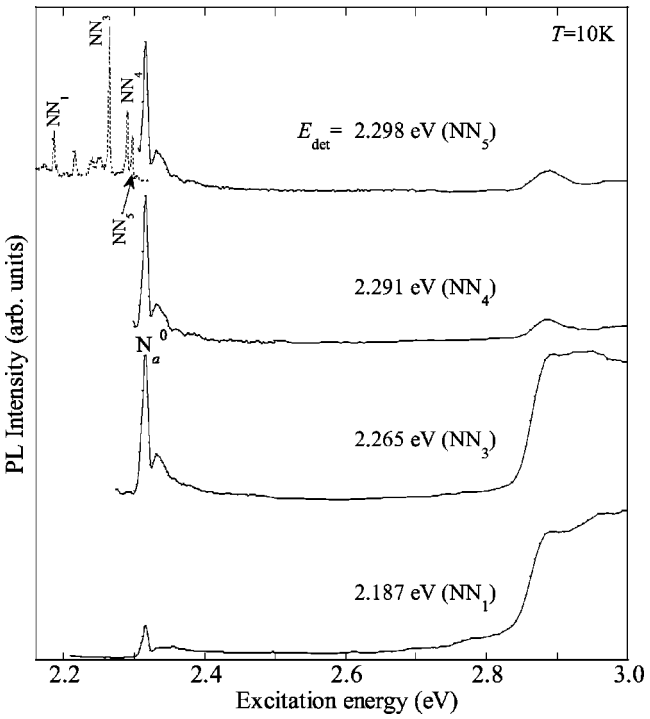

FIG. 2. Peak-normalized photoluminescence excitation spectra of the sample with $x=0.05\%$ at 10 K. Detection energies are in resonance with the four strongest NN_i lines. The PL spectrum of the sample excited with the 350 nm line of an Ar^+ laser is also shown for reference (thick dotted line).

figure, where a PL spectrum is also shown for reference purposes. Three main features are common to all PLE spectra: (i) a sharp resonance at 2.317 eV, the energy of the N_0^a line due to a single-N complex; (ii) a rather distinct peak at 2.33 eV, the energy of the free indirect (X_{1c}) exciton;[13,24–27] (iii) a steep edge in the luminescence signal at ~2.85 eV, due to the direct absorption of free carriers from the top of the valence band to the Γ_{1c} CB minimum. In the spectra relative to lines NN_4 and NN_5, the strong reduction of the height of this edge leads to the uncovering of a fourth feature: a quite pronounced peak at 2.89 eV, which can be attributed to an excitonic level introduced near the Γ_{1c} CB minimum by the isolated nitrogen atom. This level, recently predicted by supercell calculations,[28] has been observed in previous reports,[27,29] but its closeness to many critical points of the GaP band structure made its identification quite problematic. Nevertheless, the attribution of this resonance to a state associated with the single-nitrogen complex is supported by its relative importance with respect to the direct absorption edge—which scales with that of the N_0^a line (see Fig. 2)—and by the fact that its energy remains pinned with increasing N concentration[29]—a typical behavior for N-related complex states in GaP.[4,27,29,30]

The relative weight of the spectral features observed in PLE is determined by the importance of the three channels responsible for populating N complexes and depends noticeably on the complex under investigation. The height of the peaks associated with the isolated nitrogen atom (i.e., the N_0^a line and the peak at 2.89 eV) is proportional to the probability of tunneling from the isolated N atom to the investigated

complex. The sizable intensity of the N_0^a in all PLE spectra is consistent with previous observations highlighting the importance of tunneling between N-related complexes in determining the relative intensity of the NN_i lines in $GaP_{1-x}N_x$ (Ref. 31). The intensity of the excitonic peak at 2.33 eV is proportional, instead, to the probability of binding a free exciton as a whole, whereas the height of the edge at 2.9 eV and energies above is related to the complex probability of capturing a free electron (and hence a hole, according to the model described in Refs. 10–13). For high-energy emitting complexes, namely, nitrogen pairs as NN_4 and NN_5, the most important feature in the PLE spectrum is the N_0^a resonance. The edge at the Γ_{1c} critical point is almost absent, and the only relevant feature in the high-energy part of the spectrum is the N-related peak at 2.89 eV. The NN_1 spectrum, on the contrary, is dominated by the absorption edge at Γ_{1c}, while the NN_3 spectrum shows similar intensities for the N_0^a peak and Γ_{1c} edge. These findings indicate first that the feeding channel associated with the binding of an electron is available only to deeper N complexes. Second, the probability of exciton tunneling from a single N complex is higher toward shallower N pairs with more delocalized wave functions. Third, the exciton capture probability is similar for all N pairs, which all exhibit comparable heights for the 2.33 eV peak.

With increasing nitrogen concentration, a drastic change in the relative importance of the N complex feeding processes takes place, as shown by the PLE spectra of the NN_1 pair plotted as continuous lines in Fig. 3 for samples with $x=0.05\%$ and $x=0.24\%$. PL spectra of the samples are also shown in the figure for reference purposes (thick dotted lines). The strength of the free-electron capture process sizably decreases in the case of the NN_1 pair on going from $x=0.05$ to $x=0.24\%$, as shown by the strong reduction of the height of the Γ_{1c} absorption edge in the PLE spectra. This is intuitively accounted for by the fact that the band-gap redshifts while the energy of the N pair levels does not change with increasing N concentration.[1–8,16,27,29] In the simple picture described in the introduction section, this implies a gradual reduction in the binding energy of the electron to N complexes as x increases. In the case of the NN_1 pair under consideration, the PL spectrum shows a clear redshift of the band gap with an ensuing decrease of $E_{b(1)}^{e^-}$ for the $x=0.24\%$ sample. It should be pointed out also that the exciton tunneling rate from the isolated N atom (as well as from shallower pairs) toward the NN_1 pair increases for increasing N concentration, as shown in the figure. This increase can be explained by an increased number of nitrogen complexes in proximity to the investigated pair and, possibly, to a smaller degree of localization of the exciton bound to the pair when the short-range attractive potential for the electron vanishes.

PLE spectra taken at a detection energy of 2.06 eV and shown with long dashed lines are also included in Fig. 3 to support this picture. Since no N complexes have been identified to emit at 2.06 eV, there is no favored mechanism of carrier relaxation towards this particular energy, and the PLE spectrum can be regarded as a good approximation of the absorption coefficient of the material. The complete changeover in the relative weight of the processes responsible for

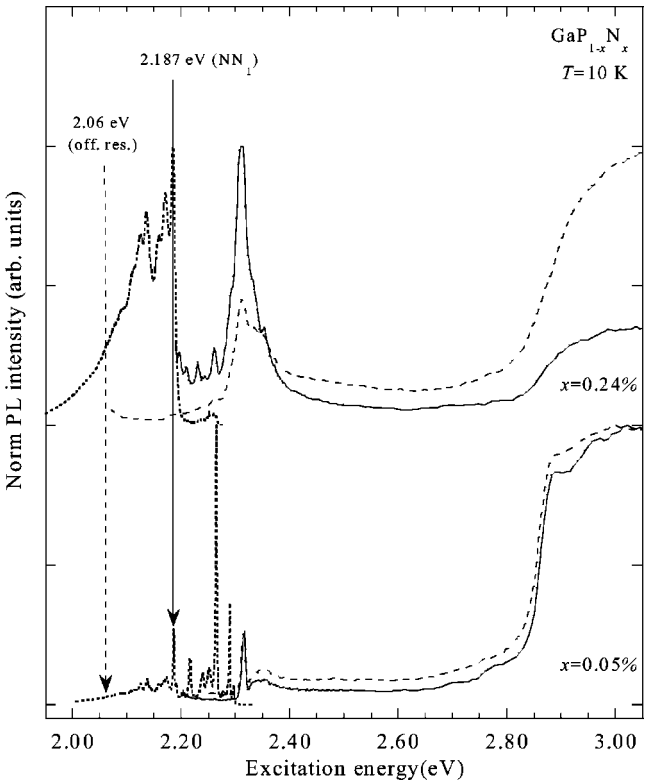

FIG. 3. Peak-normalized photoluminescence excitation spectra at 10 K of samples with $x=0.05\%$ and $x=0.24\%$. Detection energies are 2.187 eV (continuous line), resonant with the NN_1 line, and 2.06 eV (dashed line), not resonant with any of the identified N complexes. The PL spectra of the samples excited with the 458 nm line of an Ar^+ laser are also shown for reference purposes (thick dotted lines).

populating the NN_1 pair is even more surprising when compared to the relatively small variation of the absorption coefficient as x goes from 0.05% to 0.24%.

IV. TEMPERATURE-DEPENDENT PHOTOLUMINESCENCE

The temperature dependence of the PL spectrum of the sample with $x=0.05\%$ is shown in Fig. 4. In the investigated temperature range ($10\ \mathrm{K} \leqslant T \leqslant 160\ \mathrm{K}$), the PL intensity of the NN_i lines gradually decreases by almost four orders of magnitude at a rate that differs from complex to complex. Indeed, the PL signal coming from shallow pairs, as NN_5, is quenched at a lower T than that related to deeper complexes, as NN_1, which can be detected up to $T=130$ K. The PL intensity of deep N complexes, such as NN_1, does not exhibit the maximum at finite temperature (10–40 K) reported in some earlier work.[32,33] In those works, this maximum has been attributed to an important thermal transfer from shallow to deep N complexes via the continuum states. The different behavior with temperature we report here could be accounted for by a higher concentration of nonradiative centers in our samples, which weakens the effect of this carrier transfer.

In order to account for the temperature dependence shown in Fig. 4, we have developed a simple model based on PLE

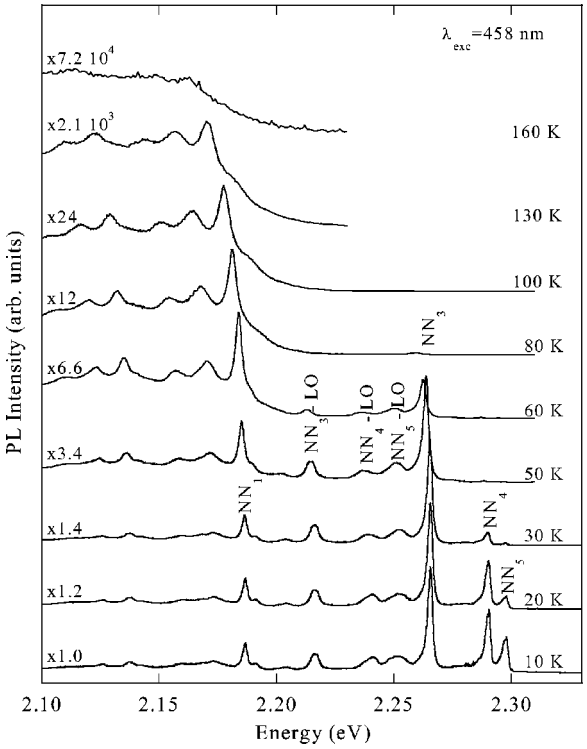

FIG. 4. Peak-normalized photoluminescence (PL) spectra of the studied sample ($x=0.05\%$) at different temperatures. PL normalization factors are given.

results where the rate equation for the emission intensity of excitons bound to the ith complex is approximated by

$$\frac{dn_i}{dt} = \frac{n_{N_a^0}(T)}{\tau_{0i}} + g_i^{ex}(T) + g_i^{e^-} - \frac{n_i}{\tau_i} - \frac{n_i}{\tau_{ion}^j} e^{-(E_i^{ion}/k_BT)} - \frac{n_i}{\tau_{hole}} e^{-(E_b^{h+}/k_BT)}. \quad (1)$$

The first term on the right-hand side of Eq. (1) gives the number of excitons that tunnel from the single N level N_0^a to the ith complex per unit time, τ_{0i} being the tunneling time. The second and third terms are, respectively, the number of photogenerated excitons and electrons captured per unit time. Three decay modes are considered as well. The first, n_i/τ_i, accounts for the excitonic radiative recombinations per unit time, namely, the PL signal we measure, τ_i being the radiative decay time of the ith pair. The second term, $(n_i/\tau_{ion}^j)e^{-(E_i^{ion}/k_BT)}$, where E_i^{ion} is the binding energy of the exciton to the ith complex and τ_{ion}^j is the time over which thermal excitation occurs, gives the number of excitons thermally excited per unit time towards the free exciton level at 2.328 eV (see Refs. 13 and 24–27). The last term, $(n_i/\tau_{hole})e^{-(E_b^{h+}/k_BT)}$, accounts for thermal excitation of a single hole toward the valence band in the case of those N pairs ($i=1$ and 3) that can directly bind a single electron as discussed in Sec. III. τ_{hole} is the time over which thermal excitation of the hole takes place, and E_b^{h+} is roughly equal to 40 meV for all pairs.[24,25] Additional nonradiative decay processes, like the Auger effect,[24,25] do not play an important role at the temperature and power densities of our measurements.

Under steady-state conditions ($dn_i/dt=0$), Eq. (1) gives

$$n_i(T) = \frac{g_i^{e^-}\tau_i + g_i^{ex}(T)\tau_i + \frac{\tau_i}{\tau_{0i}} n_{N_a^0}(T)}{1 + \frac{\tau_i}{\tau_{ion}^j} e^{-(E_i^{ion}/k_BT)} + \frac{\tau_i}{\tau_{hole}} e^{-(E_b^{h+}/k_BT)}}. \quad (2)$$

We should now estimate $g_i^{ex}(T)$ and $n_{N_a^0}(T)$. The number of free excitons that are captured per unit time by the ith pair $g_i^{ex}(T)$ is proportional to the number of photogenerated excitons in the sample at a given temperature $n^{ex}(T)$ whose rate equation is

$$\frac{dn^{ex}(T)}{dt} = g_0^{ex} - n^{ex}(T)\sum_i \frac{1}{\tau_i^{ex}} - \frac{n^{ex}(T)}{\tau_{ex}} e^{-(E_b^{ex}/k_BT)}. \quad (3)$$

g_0^{ex} is the rate at which photogenerated e-h pairs bind to form excitons, $n^{ex}(T)\Sigma_i(1/\tau_i^{ex})$ represents the number of excitons that are captured per unit time by N complexes, $[n^{ex}(T)/\tau_{ex}]e^{-(E_b^{ex}/k_BT)}$ accounts for the possibility of thermal dissociation of the exciton, τ_{ex} is the dissociation time, and E_b^{ex} is the binding energy of the exciton [$\sim$22 meV (Refs. 13, 24–27)]. Radiative recombination processes have been neglected because of the indirect character of the band gap for $x=0.05\%$. Under stationary excitation conditions, Eq. (3) yields

$$n^{ex}(T) = \frac{g_0^{ex}\left(\sum_i \frac{1}{\tau_i^{ex}}\right)^{-1}}{1 + \frac{\left(\sum_i \frac{1}{\tau_i^{ex}}\right)^{-1}}{\tau_{ex}} e^{-(E_b^{ex}/k_BT)}}. \quad (4)$$

The rate equation for the number of excitons bound to the single-N complex at a given temperature $n_{N_a^0}(T)$ is quite similar to Eqs. (1) and (3)

$$\frac{dn_{N_a^0}(T)}{dt} = g_i^{ex}(T) - n_{N_a^0}(T)\sum_i \frac{1}{\tau_{0i}} - \frac{n_{N_a^0}(T)}{\tau_{ion}^0} e^{-(E_0^{ion}/k_BT)}, \quad (5)$$

where only one feeding mechanism and two decay paths have been considered. In fact, since the isolated nitrogen atom cannot bind the electron by itself, the refilling process associated with the capture of one electron is ruled out, as well as the thermal dissociation of a hole. The probability per unit time that an exciton bound to a single-N complex is thermally excited toward the free exciton level is accounted for by $(n_{N_a^0}/\tau_{ion}^0)e^{-(E_0^{ion}/k_BT)}$, where $E_0^{ion}=11$ meV is the binding energy of the exciton to the isolated nitrogen atom [given by the difference between the energy of the indirect band gap exciton, 2.328 eV (Refs. 13, 24–27), and the energy of the N_0^a line in the PL spectrum, 2.317 eV] and τ_{ion}^0 is the mean time for an exciton to be ionized from the N_0^a level. $n_{N_a^0}\Sigma_i(1/\tau_{0i})$ represents the number of excitons that per unit time tunnel toward N pairs. Since PL and PLE data show that excitons transfer preferentially to N pairs instead of recom-

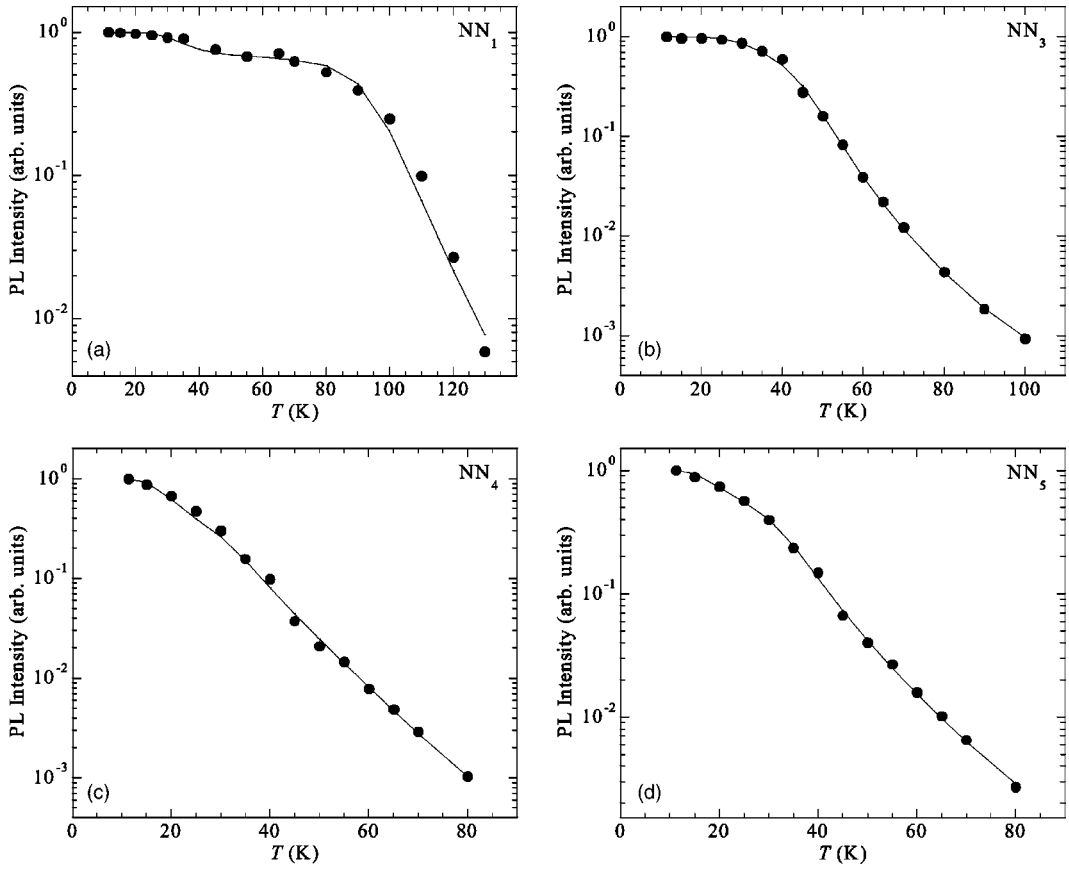

FIG. 5. Temperature dependence of the normalized PL intensity of lines NN_1 (a), NN_3 (b), NN_4 (c), and NN_5 (d). Dots are the experiment data, and the continuous line is a fit performed using Eq. (7).

bining radiatively from the isolated nitrogen atom, thus leading to a low emission intensity of the N_0^a line, radiative recombination has been neglected in Eq. (5). Finally, by solving Eq. (5) under stationary conditions, we get

$$n_{N_a^0}(T) = \frac{g_i^{ex}(T)\left(\sum_i \frac{1}{\tau_{0i}}\right)^{-1}}{1 + \frac{\left(\sum_i \frac{1}{\tau_{0i}}\right)^{-1}}{\tau_{ion}^0} e^{-(E_0^{ion}/k_B T)}}. \quad (6)$$

Since the intensity of the ith line I_{PL}^i is proportional to n_i, by Eqs. (2), (4), and (6), we get the final formula used to fit the normalized PL intensity shown by full circles in Figs. 5(a)–5(d) for several N pairs

$$I_i^{PL}(T) = \frac{a_i + \left[b_i + \frac{c_i}{1 + d e^{-(E_0^{ion}/k_B T)}}\right] \frac{1}{1 + f e^{-(E_b^{ex}/k_B T)}}}{1 + g_i e^{-(E_0^{ion}/k_B T)} + h_i e^{-(E_b^{h+}/k_B T)}}. \quad (7)$$

In order to reduce the number of parameters, E_b^{ex} has been kept equal to the binding energy of the free indirect exciton (22 meV) (Refs. 13, 24–27), and $E_b^{h+} = 40$ meV (Refs. 24 and 25). E_i^{ion} is estimated as the difference between the energy of the free indirect exciton (2.328 eV from Refs. 13, 24–27) and the energy of the NN_i line in the PL spectrum. Parameters a_i, b_i, and c_i weigh the relative importance (at $T=0$ K) of the three feeding processes responsible for populating N pairs, namely, capture of a free electron (a_i), capture of a free exciton (b_i), and exciton tunneling from the isolated nitrogen atom (c_i). The intensity of each line reaches its maximum at $T=0$ K, therefore, the condition

$$I_{PL}^i(T = 0\ \text{K}) = a_i + b_i + c_i = 1, \quad (8)$$

allows us to eliminate one fitting parameter. Since the analysis of the PLE measurements has shown that the complexes responsible for lines NN_4 and NN_5 are populated exclusively through the excitonic channels (b_i and c_i), a_i and h_i have been set equal to zero in fitting these two lines. On the same grounds, since lines NN_1 and NN_3 associated with deep nitrogen pairs are predominantly populated through the capture of free electrons and excitons, the contribution of tunneling from the isolated N atom has been not included ($c_i=0$) in their fits. Finally, the values of d and f, which do not depend on the line considered, have been found by fitting the PLE intensity of line NN_5 and then kept constant when fitting the other lines.

The results of the fitting procedures of the data shown in Figs. 5(a)–5(d) are shown by continuous lines in the same figures, while the values of the fitting parameters are given in Table I, where the values kept constant are indicated by bold characters. The temperature dependencies for all the four different N pairs are reproduced in detail with great accuracy. It should be pointed out that b_i has similar values for all the

TABLE I. Values of the parameters included in Eq. (5), as obtained with a fit of the PL intensity of the four most intense NN_i lines. The values written in bold were kept fixed during the fitting procedure.

	NN_1	NN_3	NN_4	NN_5
a_i	0.66	0.47	**0**	**0**
b_i	0.34	0.53	0.27	0.48
c_i	**0**	**0**	0.73	0.52
d	**0**	**0**	$\mathbf{6.5\times10^2}$	6.5×10^2
f	$\mathbf{1.6\times10^3}$	$\mathbf{1.6\times10^3}$	$\mathbf{1.6\times10^3}$	1.6×10^3
g_i	2.7×10^7	4.5×10^5	7.6×10^2	1.4×10^2
h_i	40	2.0×10^4	**0**	**0**

studied pairs, thus confirming that the likelihood of capturing a free exciton is the same for all N-related complexes.

V. CONCLUSIONS

Different pairs of nitrogen atoms in $GaP_{1-x}N_x$ exhibit different and nontrivial dependencies of the PL intensity on temperature, which can be quantitatively and successfully accounted for in terms of a picture of exciton and carrier relaxation and trapping derived by photoluminescence excitation measurements. These measurements show that nitrogen complexes in $GaP_{1-x}N_x$ are populated mainly by (i) exciton tunneling from the single-N complex; (ii) capture of the exciton as a whole; and (iii) capture of a free electron with subsequent binding of a hole. The relative weight of these processes changes with N complex. Tunneling from single-N complexes occurs preferentially toward N pairs characterized by shallow energy levels and more delocalized excitonic wave functions. For pairs emitting at lower energies, the probability of capturing a free electron and then a hole progressively increases. Conversely, it decreases when an increasing nitrogen concentration leads to a sizable redshift of the band gap, as shown for the NN_1 pair. Finally, the capture of a free exciton does not depend on the N pair investigated.

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