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Citation: J. Appl. Phys. **72**, 1454 (1992); doi: 10.1063/1.351707

View online: http://dx.doi.org/10.1063/1.351707

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Hydrogen activated radiative states in GaAs/GaAlAs heterostructures and InGaAs/GaAs multiquantum wells

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(Received 3 January 1992; accepted for publication 29 April 1992)

Direct observation of optical emission from H-related complexes in molecular beam epitaxy grown bulk GaAs and GaAlAs, as well as InGaAs/GaAs strained multiquantum wells (MQWs), is obtained from liquid He photoluminescence experiments. Hydrogenation is achieved by low-energy ion irradiation from a Kaufman source. The volume incorporation of hydrogen, for equal treatment, is dependent upon the density of impurities and defects where H can bind. For moderate H treatment, in addition to passivation of shallow acceptors, in GaAs we observe novel emission bands, δ, peaking at 1.360, and γ, peaking at 1.455 eV. After heavy hydrogen treatment in GaAs of low radiative efficiency—even p type originally—there appears a deeper structure α at $\sim$1.20 eV, of the kind known for "internal" transitions in the Ga vacancy-donor complex. Equivalent bands are found in bulk GaAlAs and also in InGaAs/GaAs MQWs. The results allow an approximate estimate of the various optically active Ga-vacancy levels, as affected by the different degrees of hydrogenation of the dangling bonds, and a comparison with theoretical values. Moreover, they provide evidence for the creation of a H-related donor whose binding energy is of order 25 meV. Finally, the γ band is suggestive of a transition between localized conduction and valence states associated with the local distortion that is introduced in the lattice when H binds to impurities, defects, and lattice atoms.

I. INTRODUCTION

The incorporation of hydrogen in silicon and III-V semiconductors leads to passivation of deep nonradiative centers, with enhancement of carrier lifetime and luminescence efficiency. Shallow dopants are also passivated.[1] Recently,[2,3] we have reported for bulk GaAs that for moderate H treatment, a novel shallow-to-shallow level radiative transition is activated whose intensity peaks some 60–65 meV below band gap. In the limit of prolonged H treatment, instead, photoluminescence (PL) at 80 K shows that all near-gap recombination lines are drastically attenuated. The dominant luminescent feature in the spectrum becomes a novel, very broad band, the α band, falling about 0.3 eV below band gap.[3]

The purpose of the present work is fourfold: first, to extend measurements of the α band in heavily H-treated GaAs to liquid helium temperature and to compare with other GaAs material, differing in quality; second, to explain its main features in terms of the different states of charge of the gallium vacancy (V_{Ga}); third, to determine the quenching temperatures of the H-related emission peaks in order to support the picture drawn for the states involved; and finally, to compare the behavior of bulk GaAs with that of two kinds of InGaAs/GaAs MQWs containing different amounts of lattice defects. The last point is meant to prove that the H-related bands are stronger when there is a greater abundance of defects present, which allow a more effective incorporation of hydrogen.

II. EXPERIMENTAL DETAILS

Hydrogenation was produced by ion-beam irradiation at a temperature of 300 °C. Two kinds of structures were studied: bulk GaAs and InGaAs/GaAs MQWs. The GaAs material, a 0.8-μm-thick layer grown by molecular beam epitaxy (MBE), was slightly p type ($\sim 10^{14}$ cm^{-3}) due mainly to unintentional doping. It was grown over a liquid encapsulated Czochralski (LEC) semi-insulating substrate, and it was capped by a 1.1 μm layer of undoped MBE-$Ga_{0.83}Al_{0.17}As$, meant to protect GaAs from possible surface bombardment damage. A beam of hydrogen ions, produced by a Kaufman source, was directed to the GaAlAs surface, and penetrated deep into GaAs by diffusion.

The strained $In_{0.09}Ga_{0.91}As$/GaAs MQWs—30 wells of 200 Å spaced by 300 Å barriers—were MBE-grown either on GaAs (100) or on a 4.1 μm GaAs buffer over Si (100); InGaAs was unintentionally doped and protected by a thin GaAs layer.[4] In all cases, the H-ion energy was 100 eV and the current density of order tens of μA/cm^2; the doses impinging on the surface ranged between

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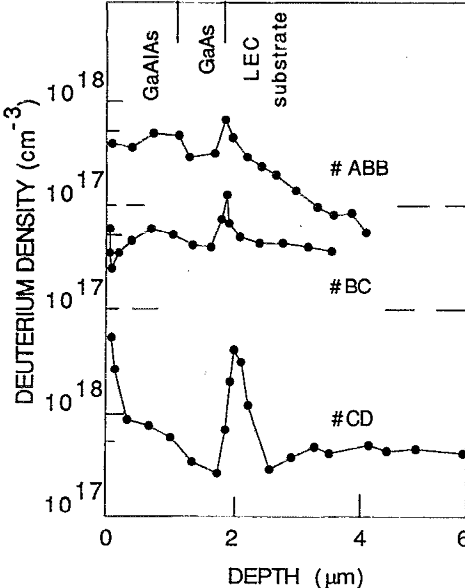

FIG. 1. Secondary ion mass spectroscopy (SIMS) profiles for three deuterated samples, treated respectively with 9×10^{16} (sample ABB), 7×10^{17} (BC), and 7×10^{18} (CD) impinging deuterium ions/cm^2. The profile in the neighborhood of the GaAlAs surface is greatly affected by error (courtesy of C. Grattepain and J. Chevallier).

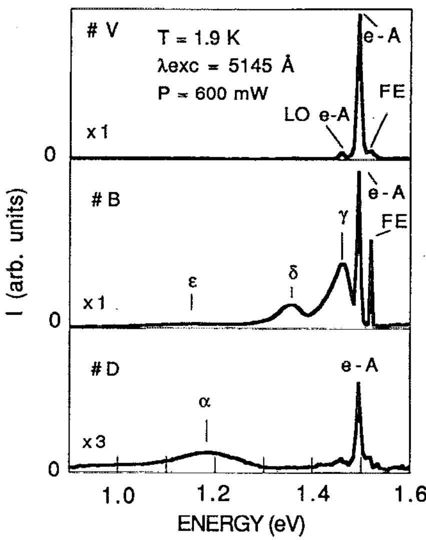

FIG. 2. PL spectra for three MBE-GaAs samples. Sample V: virgin, excitonic lifetime 120 ps. Sample B: irradiated with 1.4×10^{17} H ions/cm^2, lifetime 320 ps. Sample D: irradiated with 1.7×10^{19} H ions/cm^2, lifetime below instrumental limit (40 ps).

$\sim10^{16}$ and $\sim10^{19}$ ions/cm^2, corresponding to exposures from minutes to hours.

Deuterium profiling by secondary ion mass spectroscopy (SIMS) in our GaAlAs/GaAs samples, Fig. 1, indicates that, at a low dose of 9×10^{16} H-ions/cm^2, a density above 10^{17} cm^{-3} has diffused over the two MBE layers and part of the LEC substrate, with a spiky accumulation extending tenths of a micrometer near the MBE/LEC GaAs interface. This is due to H trapping at native interface states. Longer H treatments result in a deeper and deeper penetration with moderate changes in the bulk density value, showing that the H solubility is set by those H-trapping defects that are most abundant. The extra density at the inner interface, instead, increases up to 40 times the background at the highest H dose of 7×10^{18} ions/cm^2. The drop in all near-gap PL transitions—not occurring for the GaAlAs capping layer[2]—is caused by the resulting strong electric field.

Photoluminescence measurements have been made for GaAs/GaAlAs at temperatures ranging between 2 and 250 K, using as a pump either Ar$^+$ or Ti-sapphire lasers. The InGaAs/GaAs MQWs were instead investigated at 10 K, using He-Ne laser excitation.

III. RESULTS

A. GaAs/GaAlAs

Figure 2 shows three typical photoluminescence (PL) spectra at 1.9 K. In the virgin sample *V*, weak free exciton (FE) and acceptor-bound exciton (BE) recombination is visible, with no evidence for donor-related transitions (for better detail of the excitonic region, see Fig. 3). The spectrum is dominated by the free electron-acceptor transition *e-A*, resulting from the overlap of at least three different impurities—Zn, Si, C—and their phonon replica.

Passivation of nonradiative centers in GaAs is optimized when the sample has been irradiated with $\sim10^{17}$ H-ions/cm^2. At this dosage, the exciton lifetime[2] and radiative emission intensities reach their highest values. Sample B corresponds to such a H dose: the FE transition is 25 times stronger than in the virgin sample, and the intensities at the novel H-related bands ϵ (1.150 eV), δ (1.360), and γ (1.455) reach a maximum. (We checked that these bands are not related to the cap layer by pumping below the GaAlAs threshold). The *e-A* emission remains nearly unchanged, as if more than 90% of the acceptors had been passivated. This is in agreement with the remarkable contraction of the (A^0,X) line in Fig. 3 relative to the FE line, reported earlier.[2]

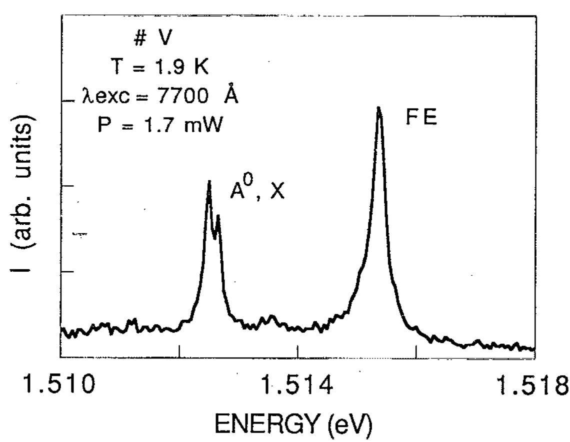

FIG. 3. Detail of the excitonic region of virgin sample V of Fig. 2.

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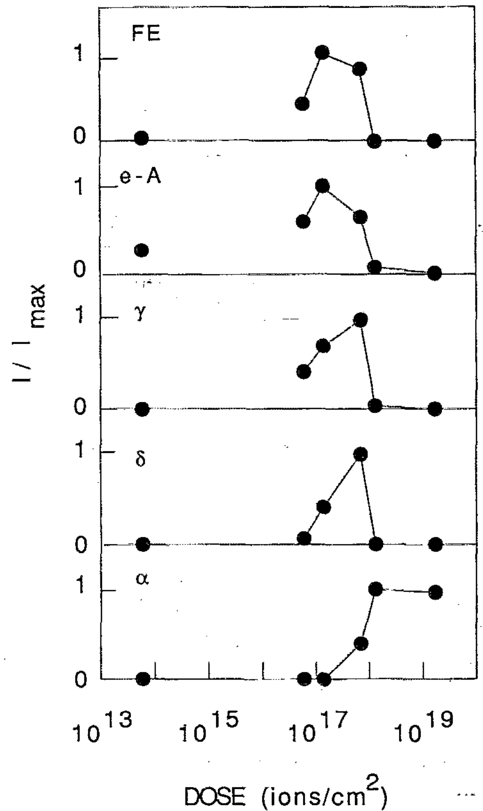

FIG. 4. Integrated emission of the observed emission bands, normalized to their highest value, as a function of the H dose (total number of ions impinging per unit area during the hydrogenation process).

The dependence of the various bands on H dose (including the α band, to be discussed immediately below), is shown in Fig. 4. It is seen that the γ and δ emissions behave differently with the degree of hydrogenation: while the γ to FE ratio, in the range 5×10^{16} to 10^{18} H-ions/cm^2, varies only moderately, the δ to FE ratio correspondingly shows a remarkable increase. It is worthwhile stressing that the dependence on excitation level is also different—linear for γ, but sublinear for α and strongly sublinear for δ. Moreover, γ shifts upwards and shrinks with excitation intensity,[3] while δ remains fixed.

The α band appears only in the very high H-dose range, where the δ and γ bands are washed out and the overall integrated luminescence drops well below the initial value. The α band shifts upwards in the range 1.14–1.20 eV with increasing excitation power (see Fig. 5 for sample D). Note that all the spectra shown have been taken after chemical etching of the GaAlAs layer. Data prior to this would exhibit a band similar to γ at 1.708 eV and to α at 1.38 eV, i.e., at energies shifted by roughly the gap difference of 0.25 eV between the two materials.

We do not correlate the α band with the earlier ϵ band in sample B on the grounds that they exhibit a totally dissimilar T dependence, as shown in Fig. 6. By taking as a reference the curve for the *e-A* transition with an activation energy of $\sim$17 meV going from δ to γ to ϵ, the dropoff temperature increases only moderately, while the α band in

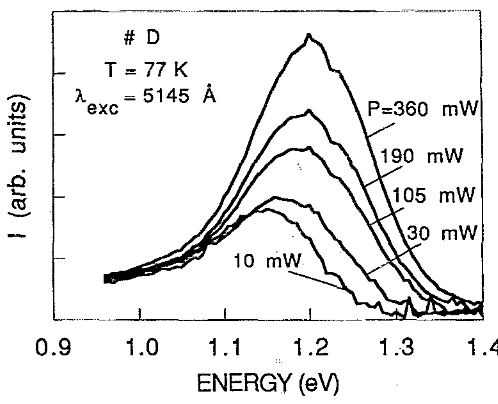

FIG. 5. Excitation power dependence of the α band in sample D as measured at liquid nitrogen. Spectra are normalized at 0.9 eV.

sample D is observed up to 250 K, at 80 K being already the only clearly observable feature.

It is important to stress that we observe a strong α band also in different kinds of hydrogenated LEC material, semi-insulating or moderately n type, but only a weak one in low-doping GaAs samples which, on the basis of their highly efficient excitonic emission, have a comparatively small density of deep recombination centers.[5]

B. InGaAs/GaAs MQWs

The behavior of these samples in the excitonic region have been discussed elsewhere.[6] We fix our attention here on the deeper bands for a comparison with GaAs. Figure 7 gives spectra for virgin samples and for intermediate and heavy hydrogenation, in the two cases of GaAs and Si substrates. All emission originates in the InGaAs wells. The data are normalized to the respective integrated emission in the high energy region. Note the magnification factors used for the deep bands of the GaAs-based MQW, a less defected material, as shown by the narrower, more efficient excitonic (e_1 – hh_1) emission.[6] Although SIMS

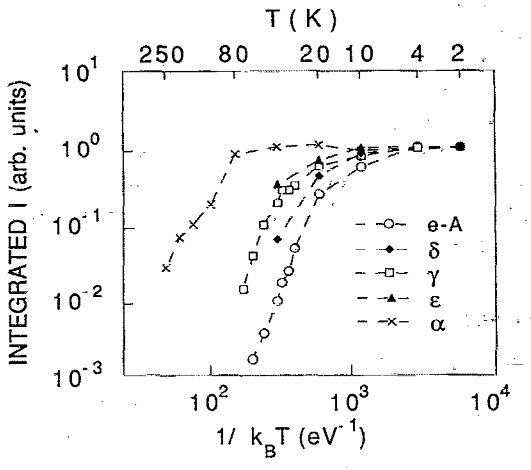

FIG. 6. Temperature dependence of the integrated emission of the bands shown in Fig. 2.

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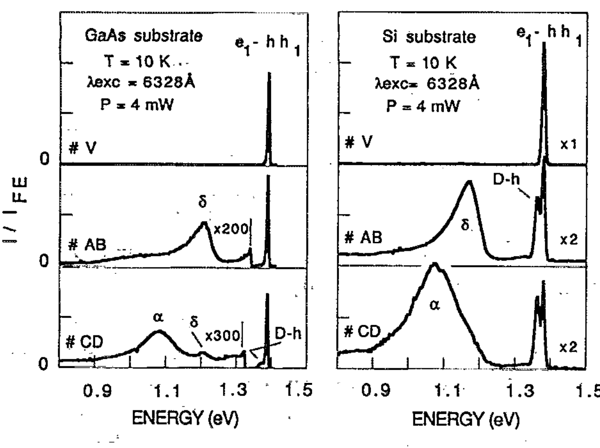

FIG. 7. PL of InGaAs/GaAs MQWs. Left, GaAs-based; right, Si based. The spectra are normalized to the integrated emission of the e_1-hh$_1$ and D-h transitions (about five times stronger in the GaAs-based MQW). Sample V: virgin. Sample AB: irradiated with 9×10^{16} H-ions/cm^2. Sample CD: irradiated with 7×10^{18} H-ions/cm^2.

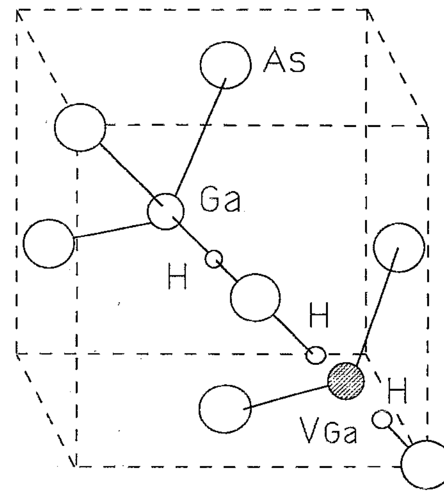

FIG. 8. One of the possible configurations for the H donor/Ga vacancy complex, with the H donor in BC position and two more H atoms passivating broken As bonds.

data for such samples are not available, the orders of magnitude stronger deep bands indicate that hydrogen is much more efficiently incorporated in the defected sample.

The bands observed in the various materials studied are summarized in Table I.

IV. DISCUSSION

A general feature common to all the observations is that the formation of H complexes implies that at least one shallow level (or narrow band) localizes below the bottom of the conduction band (CB). This opens up "internal transitions" that may render optically active centers that would otherwise be nonradiative. Let us first discuss the issue of the donor state. A local density (LDA) calculation predicts, for p-type material and H bound to lattice atoms in bond center (BC) position, a somewhat deep donor level.[7] Experimental evidence for a donor state bound by $\sim$25 meV comes from electroreflectance experiments.[8] A H-related bound state, 14.5 meV below the e_1-hh$_1$ line, is observed in the InGaAs MQWs, particularly evident in the Si-based samples (see Fig. 7). This would very well match a donor having a 25–30 meV binding energy in 3-D.[6] In the spectra of hydrogenated GaAs of Fig. 2, such a donor-free

TABLE I. Energy position of the bands observed at low excitation near liquid He temperature, as measured in eV from the FE line, or e_1-hh$_1$ for MQWs (given in first column). Note that some of the values can be affected by laser excitation intensity and laser wavelength.

Material	FE-line	γ	δ	α	ϵ
GaAs	1.515	0.060	0.155	0.34	0.36
GaAlAs	1.767	0.059	···	0.39	···
InGaAs 200 Å MQW (GaAs substrate)	1.390	0.059	0.180	0.31	···
InGaAs 200 Å MQW (Si substrate)	1.380	0.053	0.210	0.32	···

hole (D-h) emission would overlap the e-A band and be very difficult to detect.

We now examine the α band. The following points are to be stressed: (i) Its peak position shifts downwards with temperature, slightly faster than the band gap. (ii) Its shape is Gaussian, the halfwidth increasing with temperature as $W = A[\coth(E/2kT)]^{1/2}$, where $A=146$ meV and $E=22$ meV. (iii) Its integrated intensity undergoes a quenching process above 200 K, as shown in Fig. 6.

These features strictly characterize the behavior of "internal" transitions between two levels in the Ga vacancy-donor complex in degenerate n-type GaAs,[9] as described by the configurational coordinate model.[10] The peak position in such systems is about 1.20 eV. Donor-acceptor (D-A) type recombination takes place between the excited and the ground state of the complex formed by the two neighboring defects. Since in no case a band of this type was detected in virgin material, unless it was n type doped in the 10^{18} cm^{-3} range, it is apparent that, for p-type material, the donor level needed for "internal" transitions is provided by H. Moreover, H has to bind in BC position near a V_{Ga}, which should be favored by the shift of the As-atom towards the vacancy. Figure 8 illustrates a possible configuration for a V_{Ga} with two H atoms trapped at dangling bonds and one at a BC position, so as to form a kind of H-As-H "molecule." This configuration finds support in recent theoretical considerations.[11] The behavior of the H-induced D-h transition in the data of Fig. 7 support the idea that the stronger the V_{Ga} band, as in the Si-based MQWs, the higher the H-donor density.

The α band, at low H dosage, is unobservable not only because of the insufficient density of the "donor" states, but also because of a much too low position of the dark Fermi level with respect to the relevant V_{Ga} levels.[9] We explain the excitation intensity dependence of Fig. 5 on the basis of two active levels of the V_{Ga}, presumably corresponding to different numbers of H atoms trapped in the

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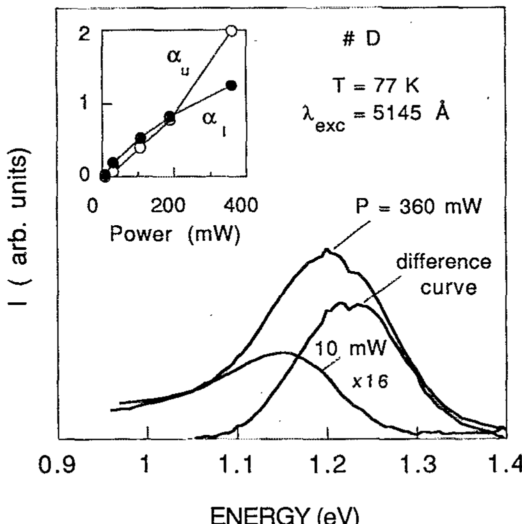

FIG. 9. Deconvolution of the α band of Fig. 5 in two components, whose integrated strength is shown as a function of excitation intensity in the inset. The shape of the lower band α_l is the one actually observed in the limit of very low excitation. The upper band α_u is deduced by difference from the measured spectrum.

vacancy. Figure 9 shows how the α band can be decomposed in a lower component α_l at 1.14 eV (the only one to be seen at very weak excitation–hole quasi-Fermi level falling between the two levels), and an upper one α_u at 1.24 eV, when stronger excitation further lowers the quasi-Fermi level under the deeper state. For the analysis, liquid nitrogen data were used. The advantage was that the α band at this temperature is virtually the only spectroscopic feature observed and that the longer lifetime allows spanning over a larger range of excited carrier densities.

With reference to the schematic representation of Fig. 10,[12] the V_{Ga} acceptor levels binding energy E_A should result from the following relationship:

$$E_A = E_g - E_t + h\nu/2 - E_D + E_r - E_{cc},$$

where E_g is the energy gap, E_t the observed recombination energy, E_D the donor binding energy, E_r the D-A Coulomb interaction, and E_{cc} the configurational coordinate shift between the final state of the optical emission and the energy curve minimum. For the atomic arrangement of Fig. 8, and one electronic charge being neutralized in the transition, we calculate $E_r = 0.388$ eV. This estimate is made by taking the As-V_{Ga} distance equal to the next neighbor separation in the perfect lattice (2.42 Å), and the H(BC)-As distance equal to 1.72 Å.[13] We take 1.508 eV for the gap at 77 K and 0.025 eV for E_D, as discussed above. As for E_{cc}, we adopt, for all the states of charge of the V_{Ga} active in our spectra, the value 0.240 eV, deduced by Williams and White[12] for the unresolved broad band at 1.20 eV of the Si donor/V_{Ga} complex. From our experimental transition energies for bands α_l, α_u, and δ (we make an attempt here, although questionable under many respects, to tie also the last one to transitions within the same complex), the above equation leads to the following values for E_A (in eV):

$$E_{A,\alpha_l} = 0.491 \quad E_{A,\alpha_u} = 0.391 \quad E_{A,\delta} = 0.271.$$

Correlation with the various V_{Ga} states may be established by comparison with those available from tightbinding calculations (in eV):[14]

V_{Ga}^{3-}	V_{Ga}^{2-}	V_{Ga}^{1-}	V_{Ga}^{0}
0.650	0.436	0.283	0.168.

Considering that the V_{Ga}^0 state, i.e., fully H-passivated dangling bonds in the vacancy, is unlikely to fall within the band gap, the agreement with the V_{Ga}^{3-} to V_{Ga}^{1-} sequence is reasonable. One must take into account, on one side, the possibly large theoretical error, and, on the other side, the very broad character of the emission bands, the remarkable uncertainty in the Coulomb energy, and the drastic assumptions made about the E_{cc} term. This should affect in particular the value derived for $E_{A,\delta}$, since the δ band, with its smaller width and quenching temperature compared to the two E_α states, is suggestive of a basically different configurational coordinate model.

Alternative origins for the δ band are, however, possible. A band very similar to ours has often been reported in the literature and attributed either to As vacancies[15] or to copper impurities.[16] In the former experiment, the δ band appeared only after prolonged annealing at 600 °C, in parallel with a conspicuous enhancement of Si donor to free hole transitions. There might be a close analogy with our case, where H-related donors are being developed.

The V_{Ga} involved in the α band is a native defect, rather than a consequence of the prolonged As-H reactions at the surface, resulting in the formation of Ga_{As} plus V_{Ga} and subsequent outward migration of gallium. As a matter of fact, we find only a small difference in the strength of the α band for H doses ranging from 10^{18} to above 10^{19} ions/cm^2. We also rule out deep levels originating from bombardment,[17] because they would correspond to transitions outside the range explored here.

We come now to the γ band. Its totally different behavior from the δ band, as to dependence on laser power and duration of H treatment, is suggestive of a different origin. When H passivates acceptors by sitting in BC po-

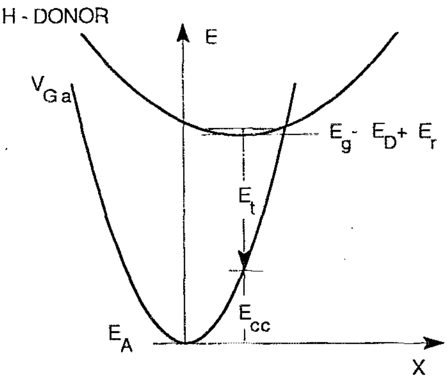

FIG. 10. Schematic configurational coordinate representation for one of the possible states of charge of the V_{Ga}.

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sition, it gives rise to a remarkable bond distortion by pushing its neighbors apart. By a supercell local density approximation (LDA) calculation, we have estimated, for the case of carbon, that Ga moves outwards by 0.55 and C by 0.29 Å in the opposite direction. For a periodically reproduced intrinsic cell made of 32 lattice atoms, and an energy cutoff of 16 Ry, LDA calculations yield a band gap of 1.40 eV. The introduction of one H atom produces a gap shrinkage, respectively, negligible, equal to 40 and to 110 meV for H in tetrahedral, antibonding, and bond center positions, (though the absolute energies are affected by some error, the relative changes are quite reliable). We have not made a similar computation for H in BC between Ga and C. However, because of the comparable distortion with the BC case in the perfect lattice, the band shrinkage should not be too dissimilar.

These estimates, which are consistent, incidentally, with the well-known widths of the localized band tails in amorphous semiconductors, should be taken only as an order of magnitude of the effect since the cell approach implies a much higher H density than the real one. We suggest that localized states of this kind are responsible for the γ band.

It should be noted that analogous distortion-induced states should originate at other H-related complexes, e.g., H bound to lattice atoms in BC position, either in a perfect crystal region, or near defects, as illustrated in Fig. 8 for the Ga vacancy case. We expect the combination of these effects to result in a somewhat broadened band of states, differing in spatial location. Their density, if all bound H atoms are contributing, should be of the order of 10^{17} cm^{-3}, and only weakly dependent on the H dose, since most of the H trapping occurs in the early stage of hydrogenation (see Fig. 2). Now, for a lifetime of 300 ps in optimal sample B,[2] the photocarrier density in the GaAs layer never exceeds 10^{15} cm^{-3}. As a result, as opposed to the V_{Ga}-related bands, the γ band must linearly follow the excitation power. We also expect its intensity to be mainly controlled by the effects of deep trap passivation, i.e., to follow, for increasing H treatment, the evolution of the excitonic strength. Both features are experimentally verified.

V. CONCLUSION

In conclusion, we have shown that, under appropriate hydrogenation, new radiative states are activated in the band gap of both GaAs, GaAlAs, and InGaAs MQWs. The data provide evidence for a H-related shallow donor, and suggest the existence of localized conduction and valence states due to distortion of the bonds, when H passivates acceptors and other defects, or binds to lattice atoms. We also observe novel deeper bands at 1.14 and 1.24 eV, which we assign to the optical activation of states of the gallium vacancy, made possible by the nearby creation of the H donor in BC or other suitable position. Another H-induced deep transition, observed at 1.36 eV, is also tentatively attributed to a state of the gallium vacancy, though this interpretation is not as straightforward.

ACKNOWLEDGMENTS

The authors are indebted to M. Colocci for helpful discussion and to L. Pavesi for disclosure of new theoretical results prior to publication. A basic contribution to the work came from SIMS profiling results kindly performed by C. Grattepain and J. Chevallier. The work has been supported by the Ministry of University and Research, and Progetto MADESS-CNR.

[1] See, for instance, articles in *Proceedings of the 1990 IUPAP-ICTP Trieste Symposium: Hydrogen in Semiconductors: Bulk and Surface,* edited by M. Stutzmann and J. Chevallier (Physica B 170, North-Holland, 1991); see also articles in *Hydrogen in Semiconductors,* edited by J. I. Pankove and N. M. Johnson, *Semiconductors and Semimetals* (Academic, New York, 1991), Vol. 34.
[2] M. Capizzi, C. Coluzza, P. Frankl, A. Frova, M. Colocci, M. Gurioli, A. Vinattieri, and R. N. Sacks, Physica B **170**, 561 (1991).
[3] M. Capizzi, C. Coluzza, V. Emiliani, P. Frankl, A. Frova, and F. Sarto, Mater. Sci. Forum **83–87**, 599 (1992).
[4] D. A. Woolf, D. I. Westwood, and R. H. Williams, J. Cryst. Growth **100**, 635 (1990); *ibid.* **108**, 25 (1991).
[5] We find a weak band at ~1.22 eV in liquid phase epitaxy GaAs grown by R. A. Logan, and at 1.24 eV in MBE material grown by G. Weimann.
[6] Z. Sobiesierski, D. A. Woolf, D. I. Westwood, A. Frova, and C. Coluzza, Solid State Commun. **81**, 125 (1992); also, M. Capizzi, V. Emiliani, A. Frova, and F. Sarto (unpublished).
[7] L. Pavesi (private communication). See also: Doctoral Thesis #898, EPF Lausanne, 1990; L. Pavesi and P. Giannozzi, Phys. Rev. B **43**, 2446 (1991).
[8] L. Kassel, J. W. Garland, P. M. Raccah, C. Coluzza, A. Neglia, and A. Di Carlo, Appl. Surf. Sci. **56–58**, 356 (1992).
[9] E. W. Williams, Phys. Rev. **168**, 922 (1967).
[10] See, for example, C. C. Klick and H. Schulman, in *Solid State Physics,* edited by F. Seitz and D. Turnbull (Academic, New York, 1957), Vol. 5, p. 100.
[11] A. Amore Bonapasta, LDA calculation (unpublished).
[12] E. W. Williams and A. M. White, Solid State Commun. **9**, 279 (1971).
[13] L. Pavesi, P. Giannozzi, and F. K. Reinhart, Phys. Rev. B **42**, 1864 (1990).
[14] H. Xu and U. Lindefelt, Phys. Rev. B **41**, 5979 (1989).
[15] H. Birey and J. Sites, J. Appl. Phys. **51**, 619 (1980).
[16] E. W. Williams, Solid State Commun. **4**, 585 (1966).
[17] H. Y. Cho, E. K. Kim, S. K. Min, J. B. Kim, and J. Jang, Appl. Phys. Lett. **53**, 856 (1988); A. Jalil, H. Heurtel, Y. Marfaing, and J. Chevallier, J. Appl. Phys. **66**, 5854 (1989).

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