Anomalous composition dependence of the band gap pressure coefficients in In-containing nitride semiconductors

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The pressure-induced changes in the electronic band structures of In-containing nitride alloys, $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ are examined experimentally as well as by *ab initio* calculations. It is found that the band gap pressure coefficients, dE_g/dp, exhibit very large bowing with x, and calculations with simulation of clustered distributions of the In atoms over the cation sites show a strong enhancement of this effect. This relates well to the experimental data obtained from pressure dependent photoluminescence measurements for $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ layers, performed in this work, and combined with existing data for $In_xGa_{1-x}N$ layers. We discuss possible explanations of the anomalously large magnitude of the dE_g/dp bowing in these nitride alloys.

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I. INTRODUCTION

Nitride semiconductor alloys, materials of great importance for use in light emitting devices,[1–3] exhibit several anomalous features. In a previous work,[4] it was shown that anomalously large band gap bowings and a strong modification of the energy band structure can be caused by indium clustering. Spatial variations in the In concentration are commonly used as explanation of the enhanced light emission from In-containing alloys of group-III nitrides.[5–9] In-content fluctuations may cause localization of excitons, thus reducing the rate of nonradiative recombination due to dislocations. Experimental demonstrations of these effects have been reported by several authors and structural studies supplied evidence for the existence of In-rich areas in $In_xGa_{1-x}N$ layers and quantum wells of sizes ranging from tens of nanometers to a few micrometers.[5–7] On the other hand, results of modeling by Bellaiche *et al.*[9] suggest that coexistence of regions with different In-fluctuation scales is highly probable. Concerning optical properties of nitrides, some of the most important fluctuations in In concentration in $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ layers seem to occur on a spatial scale comparable to the range of the exciton wave function, i.e., 2.5–3 nm. It has been suggested that this size of band potential fluctuations causes strong exciton localization[9] and leads to the observed characteristic S shape of the curve giving the luminescence energy vs temperature.

Variations in the band gaps with indium concentration in $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ alloys, with special emphasis on the effects of In clustering, were analyzed in Ref. 4 by *ab initio* calculations for a wide range of x $(0<x<1)$. It was demonstrated that the band gap, E_g, exhibits strong bowing, in particular when In atoms are clustered. The applied approach assumes In clustering on the scale of 1–2 nm. Then, an artificial crystal is constructed by means of periodic arrangements of such building blocks (supercells). Although a real epitaxial layer consists of a complicated combination of differently arranged In cations, the applied model represents the most segregated case: three or four In cations as first neighbors of a selected nitrogen anion.[4] We found that the unusual behavior of E_g as a function of In concentration in the clustered alloy reflects an increase in the valence bandwidth due to hybridization of In p and d states and uppermost N-derived valence band states originating from this particular N anion. Analysis of the lattice relaxation in $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ alloys showed that the strong interaction of In atoms and neighboring N atoms was caused by the bonds between In and N atoms in the clustered alloys being shorter than in InN itself. Our theoretical results were compared with a large number of existing experimental data. The measured E_g values were located between calculated limiting lines corresponding to homogeneous and maximally In-segregated cases.[4] Further it was shown that the effect of large band gap bowings in nitrides leads to a strong limitation of the real range of band gap tuning with composition in ternary and quaternary nitride alloys.[10]

In the present paper, we extend the research on these subjects by including the effects of applying external pressure. We examine the effects of In clustering on the bowing of the band gap pressure coefficients, dE_g/dp, in the In-containing nitride alloys. The existing experimental data on the pressure effects in nitride alloys are rather scarce, especially, we have not found any results concerning $In_xAl_{1-x}N$ alloys under pressure. Therefore, to verify the theoretically obtained variation in dE_g/dp with indium concentration in $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ alloys we decided to perform pressure dependent photoluminescence (PL) measurements for these alloys assuming that E_{PL} in the studied alloys correspond to the band-to-band radiative transitions.

The measured values of the PL pressure coefficients, dE_{PL}/dp, are compared with *ab initio* calculations of dE_g/dp performed with special emphasis on the effects of In clustering. We show that dE_g/dp exhibits anomalous bowing, which is particularly large when In atoms are clustered, and

TABLE I. Structure, In content, and growth parameters (temperature and N_2 pressure) of the measured samples, and the obtained dE_{PL}/dp values.

Sample	Structure	In content x	Growth temperature (°C)	Growth pressure (mbar)	Pressure coefficient (meV/GPa)
N2013b	$In_xGa_{1-x}N$/300 nm GaN:Mg	0.09	820	900	29
N2061b	$In_xGa_{1-x}N$/300 nm GaN:Mg	0.10	780	900	33
N2013a	$In_xGa_{1-x}N$/500 nm GaN:Mg	0.14	820	900	29
Nb2062	$In_xGa_{1-x}N$/500 nm GaN:Mg	0.15	780	900	27
N1871b	37 nm $In_xGa_{1-x}N$/300 nm GaN:Mg	0.18	730	300	33
A383	110 nm $In_xAl_{1-x}N$/700 nm GaN buffer	0.16	810	75	31
A1630	90nm $In_xAl_{1-x}N$/1900 nm GaN buffer	0.18	820	75	15
A1289	90 nm $In_xAl_{1-x}N$/1900 nm GaN buffer	0.17	825	75	14
T1365	$In_xAl_{1-x}N$/GaN buffer	0.18	750	133	15
T1347	$In_xAl_{1-x}N$/GaN buffer	0.25	750	27	31
T1346	$In_xAl_{1-x}N$/GaN buffer	0.28	750	133	17

the effect is most pronounced in the AlN based material. We find that the results of pressure measurements on $In_xGa_{1-x}N$ confirm our theoretical predictions. The measured values of dE_{PL}/dp span over the region determined on one hand by uniformly distributed In cations and on the other hand by the case described in Ref. 4 as the most clustered arrangement of In atoms in the chosen supercell. For $In_xAl_{1-x}N$ the situation is more complicated. In the present work we examine a limited number of samples with In content in the vicinity of $x=0.2$ close to the lattice-matched conditions with GaN. A large scatter of the experimental results can be attributed to the high degree of In segregation, but also other photoluminescence mechanism(s) could influence the observations.

Knowledge of the pressure effects is especially important in the nitride semiconductors due to the mismatch-induced strains, which develop in heterostructure layers being used as components of nitride optoelectronic devices. The relations between dE_g/dp and lattice constants or energy gaps can be useful in the design of optoelectronic devices where not only the values of the band gaps for a given lattice parameter, but also their pressure coefficients are needed.

II. EXPERIMENT

Photoluminescence studies under pressure are performed on a set of $In_xGa_{1-x}N$ samples made in Warsaw and on $In_xAl_{1-x}N$ samples from laboratories in Valbonne[11] and Lausanne.[12] In contents, growth parameters, and thicknesses of the samples are summarized in Table I. All the samples were grown using metal-organic vapor phase epitaxy (MOVPE). In the case of $In_xAl_{1-x}N$ samples a sapphire substrate employing a 700–1900 nm thick GaN buffer layer was used. The $In_xGa_{1-x}N$ samples were deposited on a free-standing HPVE GaN substrate. The samples were grown at different N_2 pressures (20–900 mbar), and different growth temperatures (730–820 °C). Using samples from different laboratories makes the results of our studies more general. However, we are not able to control and tune the In arrangement. The In atoms presumably arrange themselves accidentally, and application of a variety of growth conditions supplies samples with various degrees of In clustering.

The high-pressure PL measurements were performed at 77 K in the case of $In_xGa_{1-x}N$ layers and at 10 K in the case of $In_xAl_{1-x}N$ layers, with the use of a diamond anvil cell (Diacell Products MCDAC-1). Argon was employed as the pressure transmitting medium. The samples with the substrate polished down to a thickness of 30 μm, were loaded into the cell along with a small ruby crystal. The R_1-line ruby luminescence was used for pressure calibration. The sample PL was excited by the 275 nm line of an Ar^+ laser or the 325 nm line of a He-Cd laser, and dispersed by a double monochromator. The signal was detected by means of a cooled charge-coupled device (CCD) camera.

III. THEORY

The electronic structures of the $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ alloys under pressure are calculated by the same method as described in Ref. 4 for ambient pressure, i.e., by *ab initio* approaches with corrected band gaps based on the local density approximation (LDA) to density functional theory. We use pseudopotentials as implemented in the Vienna *ab initio* simulation package (VASP) (Ref. 13) to determine the atomic coordinates in the supercell. Subsequently, the electronic band structure is obtained by the linear-muffin-tin-orbital (LMTO) method[14] in a full-potential version[15] with a semiempirical scheme[16] for correction of the band gaps, which are underestimated by the LDA. Two types of alloys are considered by using a supercell scheme, (i) with uniformly distributed In atoms in the supercell (uniform alloy) and (ii) with In atoms grouped in a small region of the supercell (clustered alloy). The indium concentrations, $x=0.12$, 0.19, 0.25, 0.37, 0.50, 0.56, 0.62, 0.75, and 0.87, have been realized by substituting 2, 3, 4, 6, 8, 9, 10, 12, and 14 Al or Ga atoms by In in a 32-atom supercell.

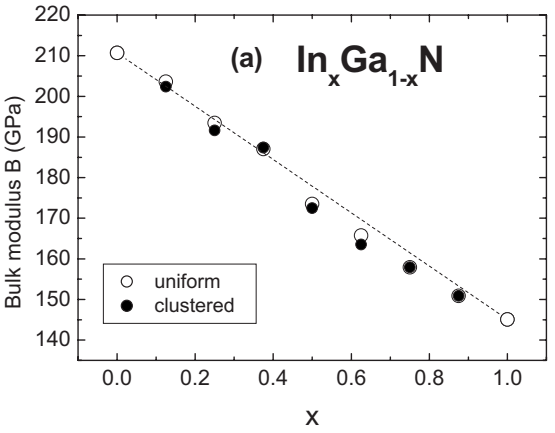

FIG. 1. Calculated bulk modulus as a function of x, for two kinds of $In_xGa_{1-x}N$ alloys; uniform and clustered distribution of indium atoms, respectively.

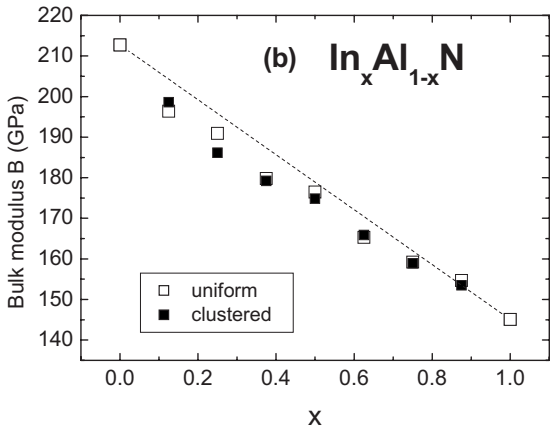

FIG. 2. Calculated bulk modulus as a function of x, for two kinds of $In_xAl_{1-x}N$ alloys; uniform and clustered distribution of indium atoms, respectively.

Structural parameters

For each value of x, the structures of $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ have been optimized by minimization of the total energy with respect to volume and shape of the supercell. Two types of alloys have been considered: uniform and clustered. The obtained values of the lattice parameters a and c, were given in Ref. 4 [Figs. 1(a) and 1(b)] for $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ as a function of x. In the case of uniformly distributed In atoms the dependence of a and c on x was almost linear, whereas in the alloys with clustered In atoms the deviations from linearity were slightly larger.

In modeling the response of a crystalline material to pressure, first the dependence of its properties (in particular electronic band structure) on changes in the volume is calculated. Second, the relation between volume and applied hydrostatic pressure is obtained and expressed as the bulk modulus, B.

In the present work, we calculate the bulk moduli of $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ as a function of x. The values of B have been determined from the dependences of the total energy vs the supercell volume, according to the definition $B = -V_0 \frac{\partial p}{\partial V}\big|_{V=V_0} = V_0 \frac{\partial^2 E}{\partial V^2}\big|_{V=V_0}$, where V_0 is the equilibrium volume and p denotes hydrostatic pressure. The supercell volume has been varied from $0.94V_0$ to $1.06V_0$ in steps of $0.006V_0$. At each volume, full structural relaxation has been carried out to ensure correct extraction of the bulk modulus.[17] The results are presented in Figs. 1 and 2, where B is plotted as a function of x for $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$, respectively. The values of B for InN (145 GPa), GaN (210 GPa), and AlN (213 GPa) are in good agreement with literature data.[18] Importantly, one can see that in the case of $In_xGa_{1-x}N$ alloys, the dependence of B on x is almost linear, whereas for $In_xAl_{1-x}N$ the deviations from linearity are larger. Nevertheless, even for the largest deviation from linearity (i.e., 15 GPa for $In_xAl_{1-x}N$ with $x=0.25$ in the case of clustered distribution of In atoms), the difference in the value of dE_g/dp resulting from this deviation is only about 0.5 meV/GPa, which is still in the range of calculational uncertainty. It is important to note that the influence of In segregation on the magnitude of B is very small.

IV. RESULTS

The measured PL pressure coefficients, dE_{PL}/dp, are shown in Table I together with description of the measured samples, their epitaxial structure, In content, and growth condition parameters.

In the following figures we present results of dE_{PL}/dp studies for selected samples of $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ alloys. There have been some results on the pressure dependence of the PL energy in $In_xAl_{1-x}N$ epitaxial layers. In this work we performed investigation on additional samples to gain a more complete overview of dE_{PL}/dp in $In_xGa_{1-x}N$ layers. In a previous study it was concluded that $dE_{PL}/dp = dE_g/dp$.[19] For $In_xAl_{1-x}N$, no pressure studies have been reported so far.

Figure 3 shows PL spectra for the $In_xGa_{1-x}N$ sample (N2061b) with $x=0.10$, for different choices of applied pressure. The spectra are normalized with respect to their peak intensities. All luminescence lines exhibit linear shifts toward higher energies with increasing pressure.

The hydrostatic pressure dependence of the PL peak energies of this sample and the GaN (template) layer deposited before the studied $In_xGa_{1-x}N$ layers are shown in Fig. 4. The pressure coefficients dE_{PL}/dp correspond to the slopes of the linear fits to the data.

The normalized ambient-pressure PL spectra of the investigated $In_xAl_{1-x}N$ samples, recorded at 10 K, are displayed in Fig. 5. The very intensive narrow lines at the energy 3.48 eV originate from the GaN template, whereas the broader emission bands are presumably associated with band-to-band emission from the $In_xAl_{1-x}N$ layers.

In Fig. 6 normalized PL spectra of the $In_xAl_{1-x}N$ sample (T1365) with $x=0.20$ are displayed as a function of pressure. The spectral positions of the PL peak energies of this sample and band edge PL of the GaN template as a function of pressure are shown in Fig. 7. One can see also the linear fits of the PL pressure coefficient dE_{PL}/dp to the experimental data. The results of pressure studies on $In_xAl_{1-x}N$ alloys should be treated with caution since photoluminescence spectra often consist of several bands (also originating from the GaN template) and their identification during pressure measurements is difficult.

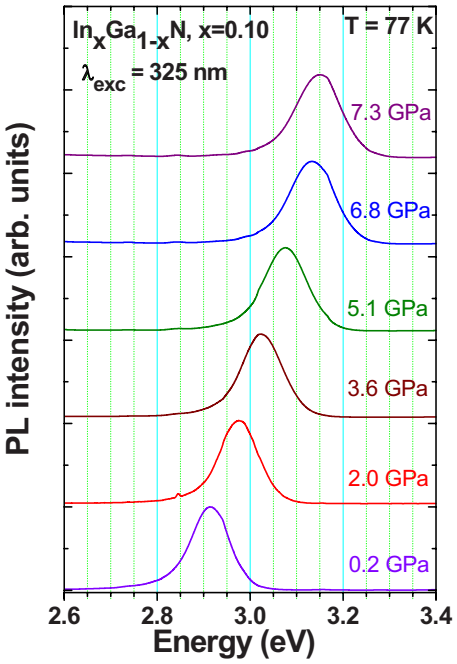

FIG. 3. (Color online) Pressure dependence of the luminescence spectra of InGaN layer measured at $T=77$ K. The spectra are shifted along the vertical axis for clarity.

In the $In_xAl_{1-x}N$ samples with x less than 0.20 (A383, A1630, A1289, and T1365), with E_{PL} higher than the luminescence energy of GaN, the overlap of the PL peak originating from the $In_xAl_{1-x}N$ alloy and the GaN template increases with increasing pressure due to the larger GaN pressure coefficient. This effect limited the pressure range of measurements and hampered the peak resolution. In turn, in the samples with x above 0.20 (T1346 and T1347) with E_{PL} lower than the luminescence energy of GaN, the PL peak originating from the $In_xAl_{1-x}N$ alloy overlaps with a broad band visible at longer wavelength, which could originate from shallow donor-shallow acceptor pair radiative recombination (DAP), GaN phonon replicas and/or Fabry-Pérot interference among the sapphire substrate, the GaN template, and the sample surface. In such cases the data analysis was performed using a Fourier transform filter.

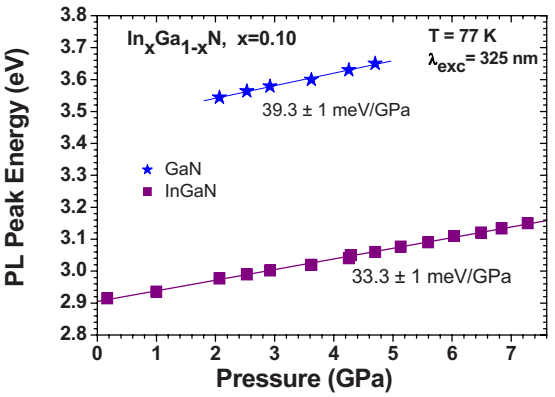

FIG. 4. (Color online) Hydrostatic pressure dependences of the PL peak energies of the $In_{0.10}Ga_{0.90}N$ sample and the GaN epilayer. The slopes of linear fits to the experimental data are equal to PL pressure coefficients.

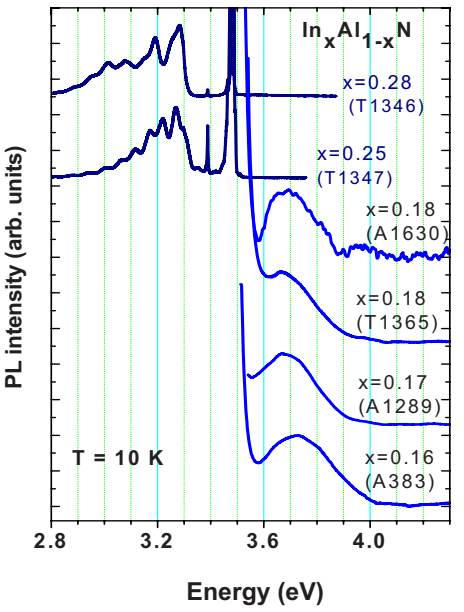

FIG. 5. (Color online) Normalized ambient-pressure PL spectra of $In_xAl_{1-x}N$ layers, recorded at 10 K. The strong, relatively narrow lines visible at the energy 3.48 eV originate from the GaN template. The spectra are shifted along the vertical axis for clarity.

Figures 8 and 9 compare our measured dE_{PL}/dp and calculated dE_g/dp as functions of x for $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$, respectively. The calculated gap variations illustrate the dE_g/dp bowing for two cases: In atoms distributed uniformly in the supercell (solid lines), and In atoms clustered (dotted lines).

The theoretical results for $In_xGa_{1-x}N$ (Fig. 8) start from the value $dE_g/dp=40.6$ meV/GPa for GaN [experimental

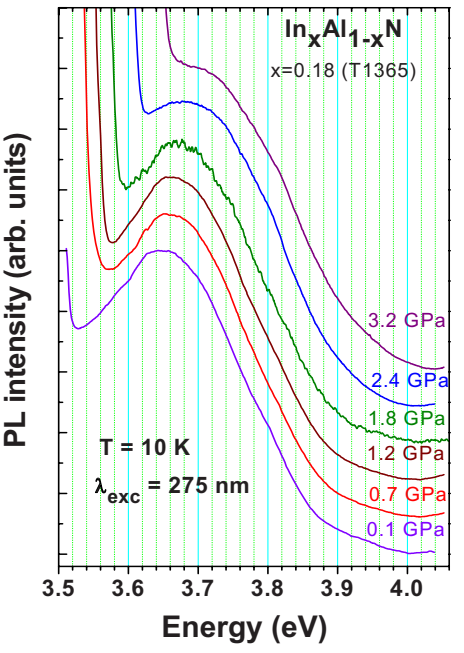

FIG. 6. (Color online) Pressure dependence of the photoluminescence spectra of $In_xAl_{1-x}N$ layer measured at $T=10$ K. The spectra are shifted along the vertical axis for clarity.

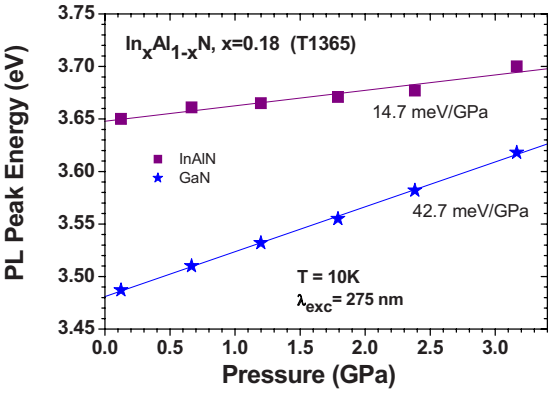

FIG. 7. (Color online) Hydrostatic pressure dependences of the PL peak energies of the $In_{0.18}Al_{0.82}N$ sample and the GaN epilayer. The slopes of linear fits to the experimental data define PL pressure coefficients.

value: 40 meV/GPa (Ref. 19)]. dE_g/dp decreases with x, until it goes through a minimum value of 25 meV/GPa near $x=0.6$ (uniform arrangement), or 16 meV/GPa near $x=0.4$ (clustered arrangement) and finally reaches the value 27.8 meV/GPa in InN [experimental value: 27.3 meV/GPa (Refs. 19 and 20)]. Our measured values (open diamonds) of $dE_{PL}/dp=dE_g/dp$ are combined with existing data for $In_xGa_{1-x}N$ (filled diamonds).[19] Despite the experimental uncertainty discussed in Ref. 19, and scatter of the results, we observe a pronounced bowing of the pressure coefficient, lying somewhere between our theoretical bowings obtained for the uniform and clustered cases. Therefore, for $In_xGa_{1-x}N$ alloys it is natural to interpret the experimental findings as evidence for the existence of short-range In-cation clustering that leads to strong changes in the electronic band structure.

Inspection of Figs. 8 and 9 shows clearly that the theoretical results exhibit a more pronounced bowing of dE_g/dp and clustering related effects in $In_xA1_{1-x}N$ in comparison with $In_xGa_{1-x}N$. In $In_xA1_{1-x}N$ we observe a strong decrease from $x=0$ of dE_g/dp with x for both the uniform and the clustered cases. Starting from the value 48.5 meV/GPa in AlN [experimental value: 49 meV/GPa (Ref. 21)], dE_g/dp of $In_xAl_{1-x}N$ goes through a minimum value of 26 meV/GPa

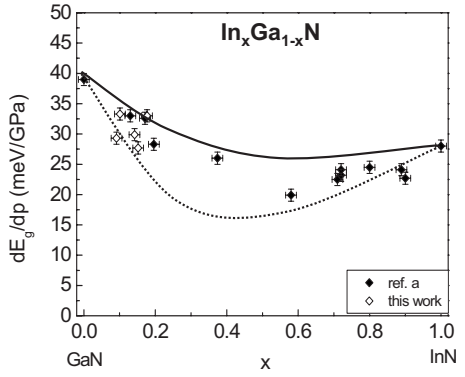

FIG. 8. dE_g/dp as functions of x for $In_xGa_{1-x}N$. Open diamonds are our experimental values. Theoretical results are illustrated for uniform (solid lines) and clustered (dotted lines) arrangement of In atoms. Other experimental values are from ref. a (Ref. 19).

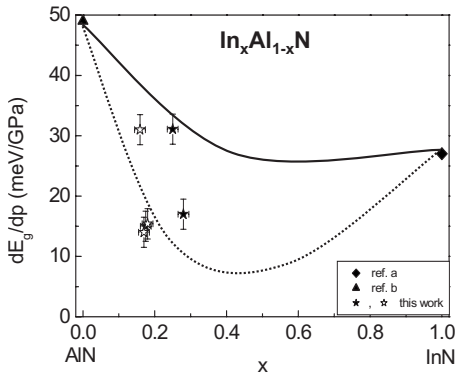

FIG. 9. dE_g/dp as functions of x for $In_xAl_{1-x}N$. Open and filled stars are our experimental values. Theoretical results are illustrated for uniform (solid lines) and clustered (dotted lines) arrangement of In atoms. The experimental data for InN and AlN are from ref. a (Ref. 19) and ref. b (Ref. 21), respectively.

near $x=0.5$ (uniform arrangement), or 8 meV/GPa (clustered arrangement). Also the experimental values of dE_g/dp for $In_xAl_{1-x}N$ are significantly more dispersed than those for $In_xGa_{1-x}N$, however, covering a much narrower range of x. In Fig. 9, we present the results of the two sets of PL measurements under pressure performed on the samples from Valbonne (filled stars) and on the samples from Lausanne (open stars). A large scatter of the measured values may likely indicate considerable differences in In clustering characteristic for different samples, reflecting the role of different growth conditions, in particular different growth pressure and temperature. For example, two $In_xAl_{1-x}N$ samples with very similar In concentrations, but grown at different pressure values ($In_{0.25}Al_{0.75}N$ at 27 mbar, $In_{0.28}Al_{0.72}N$ at 133 mbar), exhibit quite different behavior under applied hydrostatic pressure, being close to the calculated values for the uniform and clustered case, respectively (see Fig. 9).

For both alloys the theoretically predicted influence of In clustering on the pressure variation in the band gap is surprisingly large. The dE_g/dp bowings are so pronounced that the dE_g/dp values are lower (in the clustered case significantly lower) in the alloys around $x=0.5$ than in InN, which has the lowest dE_g/dp among the parent binary compounds. Comparing Figs. 8 and 9 with analogous figures in Ref. 4 illustrating E_g bowings in $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$, one can see that applying pressure in a sense enhances all the effects observed at ambient pressure. Large bowing of E_g in the clustered alloys was explained[4] in terms of an expansion of the VB caused by strong In-N interactions at the VB top. Under pressure all the effects leading to VB widening are enhanced. As follows from the present calculations the VB width increases unusually fast under pressure leading to a large decrease in dE_g/dp for small values of x, which again causes the strong dE_g/dp bowing.

V. SUMMARY

In conclusion, the *ab initio* calculations find unusually large bowings of the band gap pressure coefficients in nitride semiconductors containing indium, especially in the cases

where In clustering occurs. The experimental data, from our measurements and from literature, agree well with our theoretical predictions. The fact that the measured values of dE_{PL}/dp show a large scatter, but generally are situated between theoretical predictions for two extreme arrangements of In atoms in $In_xA1_{1-x}N$ and in $In_xGa_{1-x}N$, may reflect the role of different growth conditions in modifying the degree of In clustering. These results can be useful for understanding and controlling the influence of growth conditions on basic properties of these materials. Further, measurement of the pressure dependence of the band gaps could become an experimental tool for identifying short-range In clustering.

Since the bulk modulus varies linearly with x, the observed strong bowing of dE_g/dp versus In content is attributed to the bowing of the volume deformation potential of the band gap. Similarly as in the case of E_g bowings[4] we associate the observed large bowings of dE_g/dp in the case of In clustering with the strong modification of the VB width caused by strong interaction (hybridization) of In and N states at the top of the VB.[4] This effect is so strongly enhanced under pressure that the resulting bowings of the band gap pressure coefficients are more pronounced than the bowings of the band gaps themselves.[4]

The present work shows that further analysis of the cation-clustering problem in nitrides, including pressure effects, is highly desirable in order to get a clearer picture of the observed phenomena with reliable explanations of such anomalous effects. In particular, there is a need for further PL measurements, and especially for $In_xAl_{1-x}N$ with higher values of In content, x.

ACKNOWLEDGMENTS

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