Influence of pressure on the optical properties of $In_xGa_{1-x}N$ epilayers and quantum structures

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The influence of hydrostatic pressure on the emission and absorption spectra measured for various types of InGaN structures (epilayers, quantum wells, and quantum dots) is studied. While the known pressure coefficients of the GaN and InN band gaps are about 40 and 25 meV/GPa, respectively, the observed pressure-induced shifts in light emission energy in the InGaN alloys differ significantly from concentration-interpolated values. With increasing In concentration, and thus decreasing emission energy, the observed pressure coefficients become very small, reaching zero for emission energies ~2 eV (roughly the value of the InN band gap). On the other hand, the pressure coefficient derived from absorption experiments exhibit a much smaller decrease with decreasing energy when referred to the same scale as the emission data. First-principles calculations of InGaN band structures and their modification with pressure are performed. The results are not able to explain the huge effect observed in the *emission* experiments, but they are in good agreement with the optical *absorption* data. Significant bowings of the band gap and its pressure coefficients are found, and they are especially large for small In concentrations. This behavior is related to the changes in the upper valence band states due to In alloying. Some possible mechanisms are discussed which might be expected to account for the low pressure coefficients of the light emission energy and the difference between the sensitivity of the emission and absorption to pressure.

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I. INTRODUCTION

$In_xGa_{1-x}N$ ternary compounds are materials forming active layers in newly developed optoelectronic light emitters working in the green-blue spectral range. Having band gaps that are composition tunable in a large range of energies (1.9–3.5 eV depending on the indium content) this material is well suited to form quantum wells in many optoelectronic devices based on group III nitrides.[1] In spite of very intensive research, the mechanism of the light emission from such devices is still unclear. For example, the degree of localization of carriers/excitons involved in the radiative recombination has been widely disputed. Different authors have pointed out a leading role of either localized states/localized excitons[2] or free-carrier recombination.[3] A variety of factors have been considered as influencing the optical properties of such devices. It is believed that quantum confinement causing a shift of the emitted light to higher energies (blueshift) appears only when the thickness of the InGaN quantum well is below 3–4 nm.[4] Quite often a red shift of the emitted photon with respect to the $In_xGa_{1-x}N$ alloy band gap as obtained by linear interpolation in x is observed. This is usually associated with two effects. The first one results from the built-in macroscopic polarization which has two contributions, piezoelectric polarization due to strain induced by lattice mismatch,[5] and spontaneous polarization produced by charge accumulation at the interfaces between the epitaxial layers. The latter is present even in the unstrained bulk nitrides and originates from a relative shift of the cation and anion sublattices along the c axis of the polar wurtzite structure.[6] The effective electric field, directed along the c axis (epitaxial growth direction) caused by spontaneous and piezoelectric fields leads to a bending of the potential profile in a structure consisting of InGaN layers. As a result a spatial separation of photoexcited electrons and holes takes place which is accompanied by a decrease in their energetic separation. Thus, when the built-in electric field and the quantum well width increase, the emission energy, related to the carrier recombination, decreases. The second effect leading to a red shift of the emitted light energy, as well as to a Stokes shift, is related to fluctuations in the In concentration in the quantum well or epitaxial layer of InGaN.[4,7,8] Formation of (pseudo) quantum dots or discs corresponding to regions of higher In concentration has been suggested by many researchers. These In concentration fluctuations are believed to result from a phase separation in the $In_xGa_{1-x}N$ alloy,[9,10] particularly for high values of x. In the epitaxial layers, the In concentration can locally differ significantly from the average (nominal) value. Similarly to the optical effects found in InGaN layers and structures subjected to the internal electric fields, in the case of In content fluctuations the light emission also occurs in the regions with the lowest energy gap, i.e., in

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the regions with high In content (pseudodots), where localized electronic states or excitons can be formed.

All the effects mentioned above make an unambiguous determination of the band gap E_G, versus x difficult. In particular, this applies to the determination of the magnitude of E_G from the measured emission energy E_e. Further, it is widely accepted now that the gap bowing parameter for $In_xGa_{1-x}N$ is large. This reflects the strong drop of the E_G value for $In_xGa_{1-x}N$ with low In content ($x \leqslant 0.25$).[11] An increase of the Stokes shift and a commonly reported broadening of the absorption edge in $In_xGa_{1-x}N$ alloys accompany a rise in x value. Another puzzling observation pointing out a particular role of In in InGaN alloys, is the finding of a small x-dependent pressure coefficient of E_e in thick layers as well as quantum structures of $In_xGa_{1-x}N$.[12,13] The previous studies were limited to structures with x below ~ 0.25, and the emission energy above 2.4 eV. They showed that with decreasing emission energy dE_e/dP is reduced drastically. In particular, for $x \sim 0.2$ the pressure coefficient $dE_e/dP = 15$ meV/GPa, is almost three times smaller than that measured for GaN (40 meV/GPa) (Ref. 14) and two times smaller than that calculated for InN (30 meV/GPa),[15,16] respectively. This low value of the pressure coefficient was originally associated with localization of carriers or excitons participating in the radiative recombination since it is well known that localized electronic states in semiconductors exhibit weak sensitivity to the external pressure.[12,13] So far, these experiments strongly favored the suggested carrier localization as the critical factor determining the optical properties. However, recently the investigation[17] of the InGaAsN alloy system brought evidence that for a wide range of compositions, the band structure may react to pressure in a way very different from its binary counterparts and from predictions using a simple virtual-crystal approximation. In particular, the pressure coefficients of the light emission/absorption showed a strong dependence on the applied pressure and even aproached zero for certain values of pressure and nitrogen concentration.[17]

The purpose of the present work is to check and discriminate between the band structure and localization effects taking also into account the pressure dependence of the piezoelectric effect in $In_xGa_{1-x}N$. In order to achieve the goal we have performed, first, a systematic high-pressure study of the photoluminescence in the InGaN system choosing samples emitting at various wavelenghts (410–630 nm, 2–3 eV) and comparing these results to those obtained earlier. The experimental part was completed by the measurements of photocurrent spectra (absorptionlike data) for three different InGaN light emitting diodes (LED). The aim of these measurements is to discriminate between mechanisms responsible for the light emission and the light absorption. Light emission probes only certain recombination paths (e.g., related to the local extrema of the band structure caused by In fluctuations and related carrier/exciton localization). The light absorption, on the other hand, gives information about the alloy band structure averaged over the sample. Secondly, band structure calculations including pressure effects were performed. To simulate the $In_xGa_{1-x}N$ alloy for different x values, from one to eight gallium atoms were substituted by indium in a 32-atom supercell. As a result of the calculations we obtain (i) the dependence of the band gap and its pressure coefficient on the content of indium, (ii) the total density of states (DOS) and the contributions to the DOS from the individual atoms (Ga,In,N) for each case. This allows us to identify mechanisms responsible for the "peculiar" behavior of the band structure. While comparing the calculated band structure dependence on external pressure with the experimental pressure induced evolution of the light emission and absorption in InGaN we discuss additionally the effect of pressure dependence of the piezoelectric fields, which might significantly influence the optical transition energies in the heterostructures.

In the next section the experiment is described, and in Sec. III some details of the calculations are given. Results and discussion are included in Sec. IV and V.

II. SAMPLES AND EXPERIMENT

The present work comprises measurements of photoluminescence as a function of hydrostatic pressure performed on a set of InGaN quantum dot and quantum well structures covering the broad range of emission energies from 2 to 3 eV. Earlier data obtained for quantum wells[12,13] and epilayers[18] are also included for a complete discussion. The sample data are collected in Table I. The quantum dot structure (sample A) was grown in the Stranski-Krastanov growth mode by the molecular beam epitaxy (MBE) method.[19,20] The quantum well samples, labeled B–F, were grown under a high V/III ratio to prevent the formation of QD's.[19,20] The variable parameter in this set of samples is the quantum dot height/quantum well thickness which varies from 1 nm (emission at 3 eV) up to 4.5 nm (emission at 2 eV). Pressure experiments were performed in a low-temperature diamond anvil cell, cryogenically loaded with argon, serving as pressure transmitting medium. The measurements on MBE grown quantum dots and quantum wells were performed at 80 K in the pressure range 0–8 GPa. The photocurrent (absorptionlike) measurements were performed on an InGaN multiquantum well LED grown at University Santa Barbara (sample SB), and also on two types of commercially available Nichia LEDs (samples NB,NG). The experiments were performed at 300 K, using the UNIPRESS clamp piston-cylinder pressure cell equipped with a sapphire window and electrical connections. Light gasoline was used as a pressure transmitting medium. The resistance variations of a calibrated InSb semiconductor gauge was used to monitor the pressure. Prior to the experiment, the commercial blue and green Nichia diodes were decapsulated. For the electroluminescence (EL) measurements (at current of 2 mA) light emitted by the LED's was dispersed by a SPEX 500M spectrometer and detected by a photon counting system. In the studies of the pressure dependence of the photocurrent (PC) spectra, white light of a xenon lamp was monochromatized by a CVI 242, and then chopped with a frequency 78 Hz. The photocurrent was measured with a lock-in amplifier.

III. METHOD OF CALCULATIONS

The band structures of $In_xGa_{1-x}N$ were obtained by means of the supercell technique. Substitution of one to eight

TABLE I. Structure and parameters of InGaN samples quoted in this paper.

Sample symbol	structure	width/height Å	growth method	In content	measurement temperature	source
A	Quantum dot	10	MBE	15%	80 K	this paper
B	Quantum well	20	MBE	20%	80 K	this paper
D	Quantum well	35	MBE	20%	80 K	this paper
E	Quantum well	40	MBE	20%	80 K	this paper
F	Quantum well	50	MBE	20%	80 K	this paper
NB	Quantum well	15	MOCVD	20% (22%)	295 K	Ref. 11 (Ref. 14)
NG	Quantum well	25	MOCVD	45% (22%)	295 K	Ref. 11 (Ref. 14)
U	Quantum well	30	MOCVD	18%	295 K	Ref. 12
S1	Epilayer		MOCVD	8%	4 K	Ref. 17
S2	Epilayer		MOCVD	14%	4 K	Ref. 17
SB	Quantum well	30	MOCVD	13%	295 K	Ref. 8

gallium atoms by indium in a 32-atom supercell corresponds to indium concentrations x ranging from 0.0625 to 0.50. For each case we calculated the electronic band structures at different values of the hydrostatic pressure, and the equilibrium volumes were determined. In order to include the lattice relaxation effects in the neighborhood of the In impurity the full nonspherical shapes of potentials and charge distributions were taken into account, and for this purpose we used the full-potential version[21] of the linear muffin-tin-orbital (LMTO) method.[22] All (nonoverlapping) muffin-tin spheres were chosen to have the same size. As usual, in open structures, empty spheres (muffin-tin spheres without nuclear charge) were inserted in the interstitial regions to improve the packing fraction. The basis set includes three sets of partial waves of s,p, and d character on each atomic site, with a total of 44 LMTO orbitals per formula unit. The local approximation (LDA)[23] to the density-functional theory was used, and we applied the Perdew-Zunger[24] parametrization of the Ceperley-Alder exchange-correlation.[25] The fundamental gaps derived from the LDA band structures are generally 50–100 % too small. To make a comparison of our results with experiment easier we shifted the conduction bands of $In_xGa_{1-x}N$ rigidly up. First the shifts necessary to reproduce the experimental gaps of GaN and InN were determined. Subsequently, for the $In_xGa_{1-x}N$ alloy a shift linearly interpolated between those of the pure constituents was applied. Both the wurtzite and the cubic phases were studied, and only minor differences were found in the size of the fundamental band gap and its pressure behavior in these two phases. This agrees with our previous calculations of the band structures of the III-V nitrides[15] and the studies of defects in hexagonal and cubic GaN by Neugebauer and Van de Walle.[26]

IV. EXPERIMENTAL RESULTS AND DISCUSSION

As mentioned earlier, all previous high pressure measurements performed on $In_xGa_{1-x}N$ structures (with emision energies between 2.4 and 3.2 eV) have found very small pressure coefficients of the energies of the emission peaks.[12,27,28] The magnitudes of the measured coefficients were much lower than what could be expected from interpolations of the data known for the pure binaries GaN and InN. It appears that the pressure coefficient is a function of the emission energy, and that it decreases with decreasing emission energy. Having now a larger set of samples emitting in a very broad energy range we can study this tendency in more detail. Figure 1 shows the emission spectra from our MBE grown quantum structures measured at $T=80$ K. Samples A, B, and D have very similar emission intensities, but in E and F the quantum efficiency is significantly reduced. Figure 2 shows the photoluminescence measured at pressures close to 0 and 6 GPa. It is seen that with decreasing emission energy, the shift induced by pressure in the energy of the photoluminescence peaks decreases and even tends to change sign for sample F. As mentioned already in Sec. II we used LED photocurrent measurements to evaluate the influence of pressure on the light absorption. This technique was chosen because standard optical absorption experiments are of little use in the case of the narrow quantum well structures examined here. The photocurrent is extremely sensitive to the absorption in the region of the depletion layer (which coincides

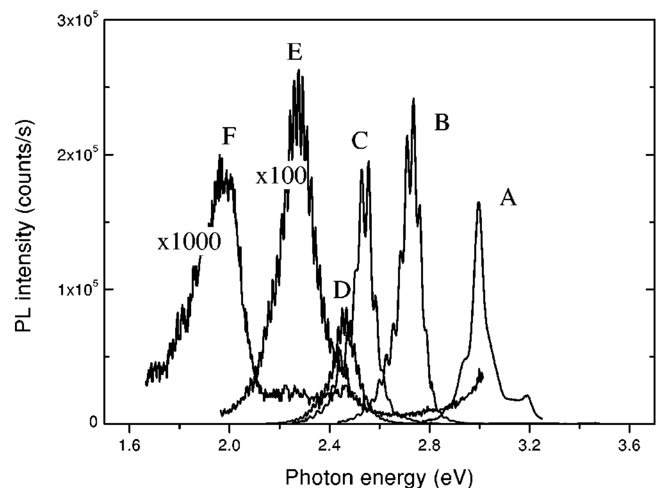


FIG. 1. Photoluminescence of MBE grown GaN/InGaN samples consisting of QD's (A) and QW's (B)–(F) measured at ambient pressure and $T=80$ K.

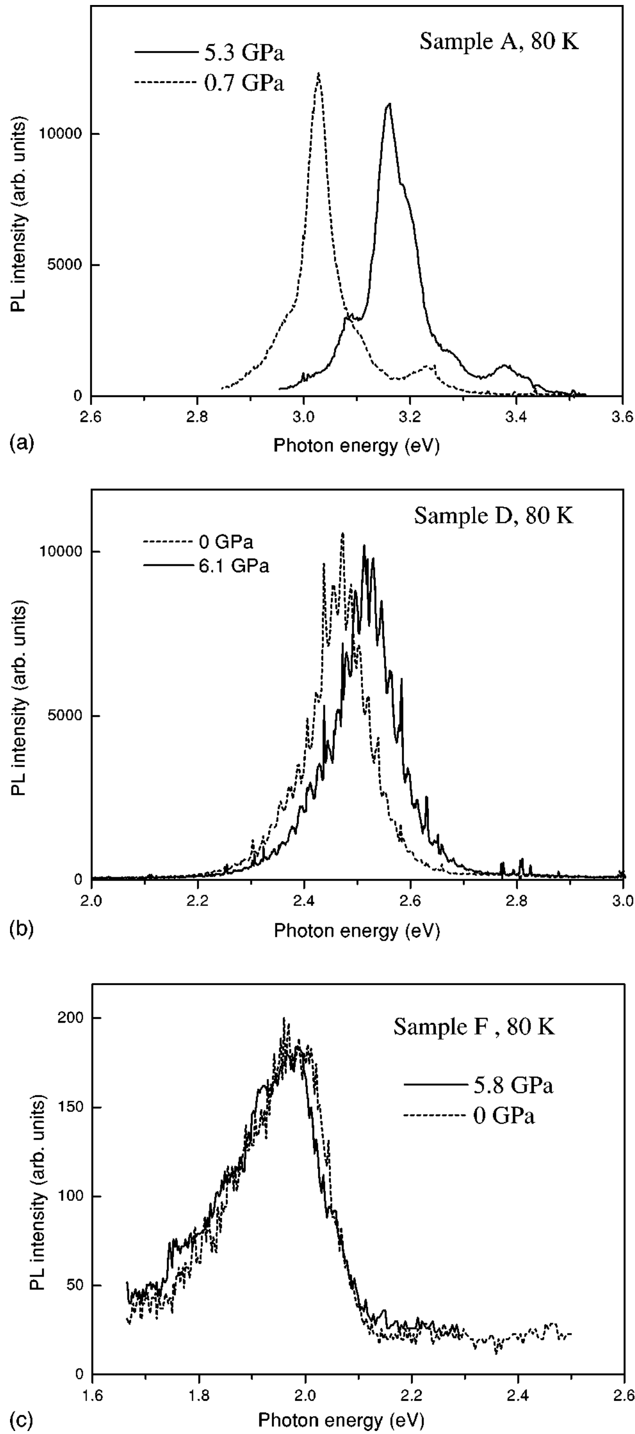


FIG. 2. Pressure induced changes of photoluminescence spectra from MBE grown InGaN quantum structures: (a) sample A, (b) sample D, (c) sample F.

with the InGaN active layer) thus amplifying the sensivity of the experiment. In Fig. 3 the photocurrent spectra measured for three different InGaN structures are shown. The same figure also shows examples of the pressure induced shift of the photocurrent edge. In order to consistently calculate the position of the relatively broad edges we used a sigmoidal fit proposed recently by Martin *et al.*[29] In Fig. 4 the results are combined with those reported earlier, and the figure shows the measured pressure coefficients as a function of the emission peak energy. A linear relationship is observed. Moreover, the pressure shifts of the electroluminescence spectra, measured at $T=300$ K for the three LED's (SB,NB,NG) have magnitudes very similar to the measured at $T=80$ K. One should notice that the samples which are represented in this figure were grown by different methods and at different temperatures, and therefore they presumably have different In fluctuation scales. Also, as we can learn from the data in Table I, there is no correlation between the nominal indium concentration of the emitting material and the emission energy and its pressure coefficient. It is possible, however, that the dimensions of the quantum structure (dot height or quantum well width) may play certain role in determining the pressure behavior of the emission. Comparing structure data gathered in Table I with the pressure behavior of emission shown in Fig. 4 we can notice the apparent correlation of the increasing well width and decreasing pressure coefficients. Figure 4 also shows data from absorptionlike experiments performed on InGaN light emitting diodes. These data give higher pressure coefficients than those derived from the emission experiments at the same wavelengths. Also for the absorption data there seems to be a linear dependence of the pressure coefficients on the absorption energy, however, with a somewhat larger slope than obtained by a linear interpolation between the band gap pressure coefficients of GaN ($\sim$40 meV/GPa) and InN ($\sim$25 meV/GPa). The solid line represents the pressure coefficient of the calculated band gaps presented in the following section. The calculated values of the pressure coefficients for the pure constituents are 37 meV/GPa and 25 meV/GPa for GaN and InN, respectively. The absorption experiment and the theory are seen to agree well. But, there is still a dramatic difference between absorption and emission data. Here, we would like to discuss the situation when hydrostatic pressure is applied to the heterostructure composed from materials having different compressibilities. It is indeed the case for the structure such as GaN/InGaN. InN is almost two times more compressive than GaN. If this type of structure is subjected to hydrostatic pressure, the harder material reduces the compressibility of the softer one, thus leading to somewhat weaker in-plane deformation of the quantum well material. This problem was already discussed[27,28] and it was shown that the relative reduction of the emission pressure coefficient should not exceed the half of the relative difference of the respective bulk moduli (compressibilities). Accordingly this effect should not lead to the reduction of the pressure coefficients higher than 10% for the sample presented here. Another reason for the very weak pressure sensitivity of the light emission could be that the pressure anomaly of the InGaN band structure (seen in the absorption) is enhanced by additional carrier localization effects which are more decisive in the emission (recombination) mechanisms. Another hypothesis to be discussed in the following section is possible contributions to the observed anomalies from internal electric fields.

V. THEORETICAL RESULTS

A. InGaN band structure under pressure

By substituting from one to eight gallium atoms by indium in the 32-atom supercell we simulated the band struc-

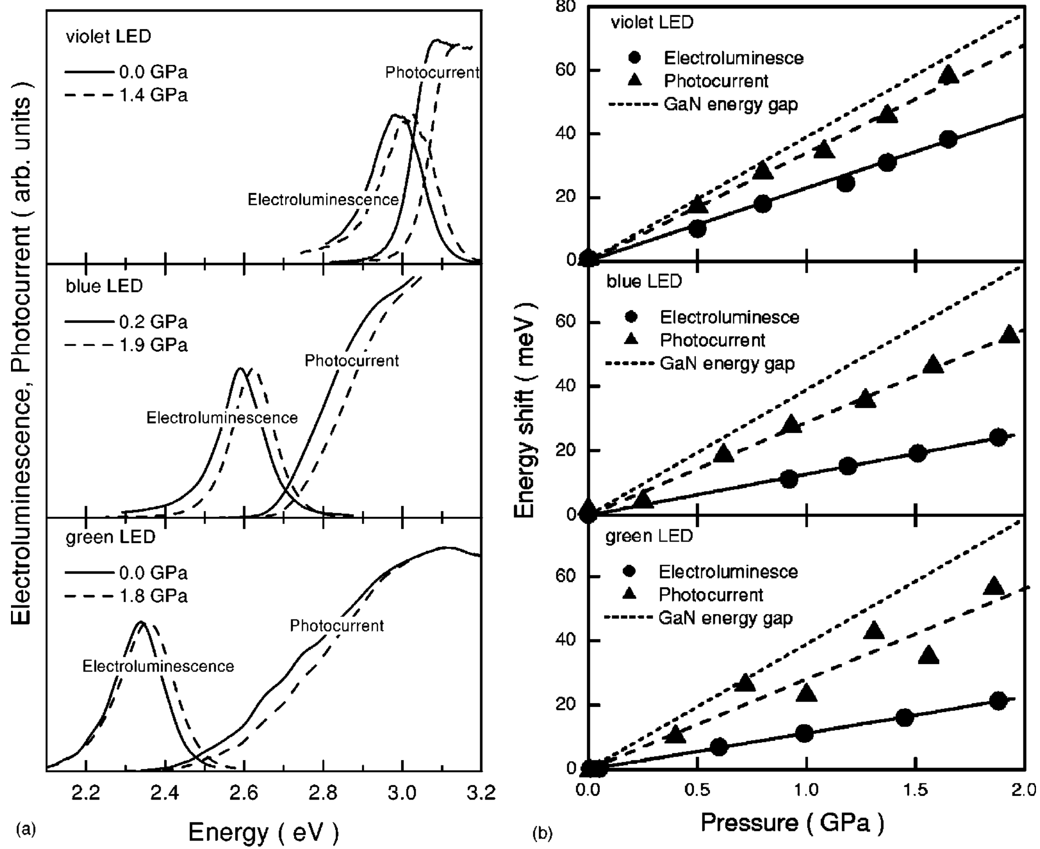


FIG. 3. Photocurrent and electroluminescence spectra for sample SB (violet), NG (green), NB (blue). (a) Emission and photocurrent spectra for two different values of pressure, (b) position of emission peaks and photocurrent edge as a function of pressure.

ture of $In_xGa_{1-x}N$ with indium concentrations x equal to 0.0625, 0.125, 0.1875, 0.25, and 0.50. For each value of x the band structure was calculated for different volumes to find the equilibrium volume and the hydrostatic pressure dependence. The values of equilibrium volumes and bulk moduli are almost linearly dependent on x. Calculations of the lattice relaxations around the In atoms showed that In is always in an almost ideal substitutional position, even in the case where eight In atoms are placed in the supercell. The nearest neighbor N atoms relax symmetrically outwards. The value of this relaxation is 6% of the bond length, for the wurtzite as well as the zincblende structure.

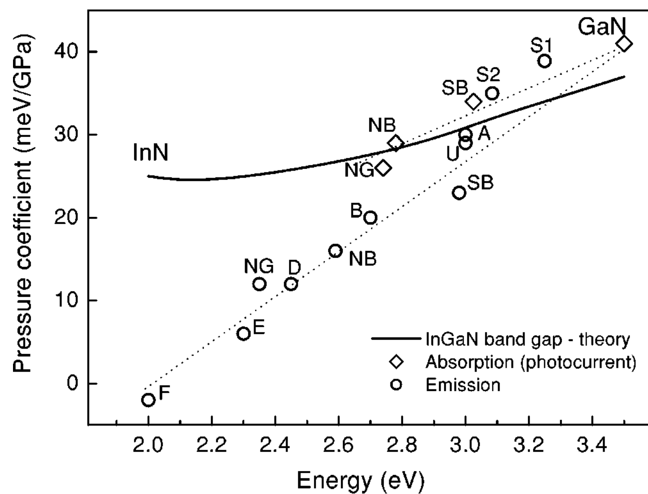


FIG. 4. Available data for absorption and emission pressure coefficients. The solid line shows the results of the theoretical calculations performed in the present work. Dotted lines are to guide the eye. Upper dotted line: photocurrent spectra; bottom dotted line electroluminescence and photoluminescence data. For sample symbols see Table I.

Figure 5 shows the band gap as a function of x for both structures. The results for the wurtzite and the zincblende phases are very similar. Up to 25% In content the energy gap is decreasing rapidly with the number of indium atoms: from 3.5 eV for pure GaN to about 2.6 eV for $x=0.25$, in the wurtzite structure. For larger values of x the gap decreases more slowly, reaching the value of about 2.2 eV (2.1 eV in the zinc-blende structure) for 50% indium. The corresponding bowing parameter (1/2 times the second derivative of the gap with respect to x) is found to be ≈ 3 eV up to $x\approx 0.25$, and then it decreases. Our findings agree qualitatively with the previously reported results (see, e.g., Ref. 29). Looking for an explanation of such a peculiar behavior of InGaN, we consider the total density of states (DOS) as a function of indium concentration. Figure 6(a) shows the DOS as calculated for the uppermost valence bands of $In_xGa_{1-x}N$ in the wurtzite structure for four In concentrations $x=0$, 0.125, 0.50, and 1.0. Similar results for the zinc blende structure are shown in Fig. 6(b). In all cases the bottom of the $N-2s$ band

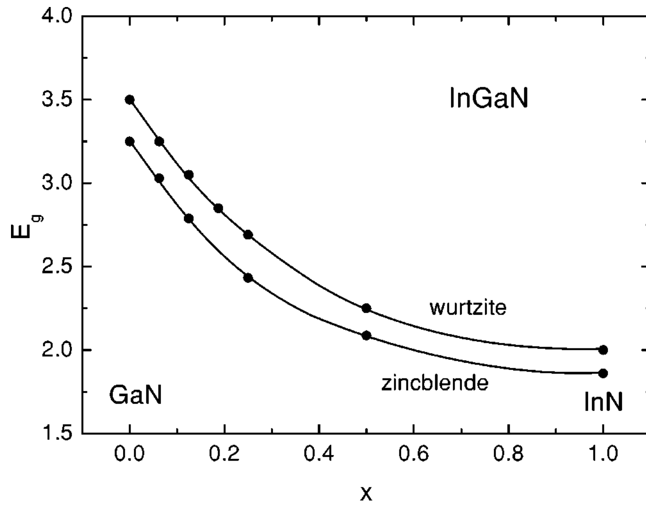


FIG. 5. The calculated InGaN band gap as a function of indium composition for the wurtzite and zinc blende structures.

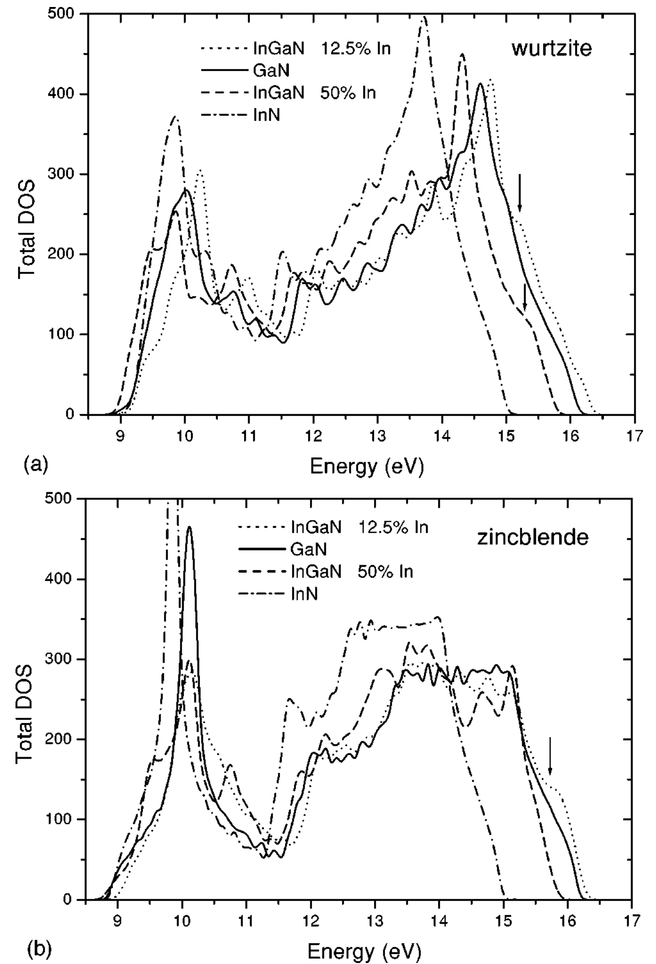
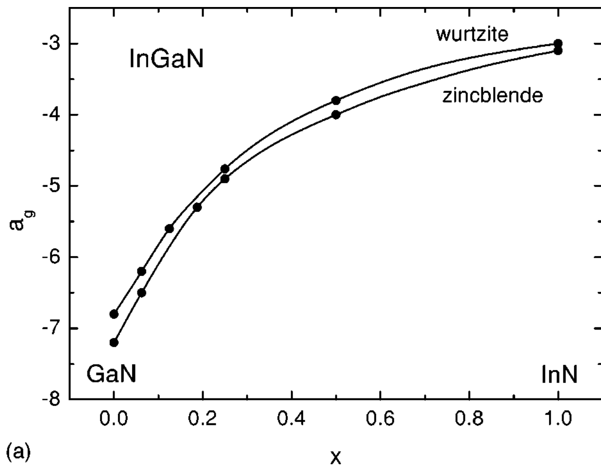


FIG. 6. The valence band density of states for GaN (solid line), InGaN with 12.5% In (dotted line), 50% In (dashed line) concentrations, and for InN (dotted-dashed line). (a) Wurtzite structure, (b) zinc blende structure. In all cases the bottom of the $N-2s$ band is used as energy reference level. The arrows indicate characteristic shoulders appearing in the InGaN DOS due to the indium incorporation.

is used as energy reference level. For both structures we find (i) a change of the shape of the valence band top for 12.5 and 50% indium as compared with pure GaN and InN—the shoulders which appear at the band top are indicated by arrows in Fig. 6, (ii) the valence band width does not vary linearly with x; for 12.5% In it is larger than in pure GaN instead of decreasing linearly as might be expected from the virtual-crystal approximation. We found also that for $x=0.25$ the width of the valence band is practically the same as in GaN (not shown in Fig. 6).

Next, we consider the hydrostatic pressure dependence of the $In_xGa_{1-x}N$ energy gap. In Fig. 7(a) the band gap deformation potentials are shown for the wurtzite and zinc blende structures as functions of x. As found for the band gap we also observe a strong increase of the gap deformation potential with increasing In content. This corresponds to a decrease of the pressure coefficient, which is shown in Fig. 7(b). The bowing is significant in both cases. Again, the wurtzite and zinc blende results are very similar. The pressure coefficients obtained here by the full-potential LMTO for the binary compounds (37 meV/GPa for GaN and 25 meV/GPa for InN in the wurtzite structure) differ slightly from the values obtained earlier[15] by the LMTO-ASA (atomic spheres approximation, i.e., using spherically symmetric potentials),[22] 39 and 30 meV/GPa, respectively. Our calculated pressure coefficients of the energy gap for different In content are in good agreement with the experimental data obtained from absorption experiments (see Fig. 4).

The unusual decrease in both the band gap and its pressure coefficient with In content seems to come from the In-induced changes of the states at the valence band top. To find an explanation for the unusual behavior of the valence band we analyzed the contribution of different states to the valence band top as In is added to GaN. Analyzing the band structure and the density of states up to 50% indium we found no states in the gap. Also, the In contribution to the lower part of the conduction bands is negligible. On the other hand, In(p,d) states contribute significantly to the uppermost valence bands. Partial densities-of-states corresponding to anions and cations for the higher valence bands of pure GaN and of $In_xGa_{1-x}N$ with $x=0.25$, are shown in Figs. 8(a) and 8(b), respectively. Figure 8(b) shows that In states contribute to the whole uppermost valence band hybridizing strongly with GaN states. As a result, the N(p) states, which contribute to the valence band top by about 90%, are pushed up, changing the valence band edge shape. Further evidence for strong interactions between indium and nitrogen states is presented in Fig. 8(c), showing partial DOS contributions from two types of N atoms: type 1, nearest neighbors of In-atoms; type 2, nearest neighbors of Ga atoms only (far away from In atoms). There are dramatic differences at the valence band top in the DOS for the two types of N atoms. The *resonant* character of an In impurity state in the continuum of GaN valence bands was earlier found by empirical pseudopotential calculations.[30] The uncertainty resulting from different arrangements of In atoms in the supercell was estimated for the calculations for 18.75 and 25 % In for the wurtzite structure. This was done by placing the In atoms in



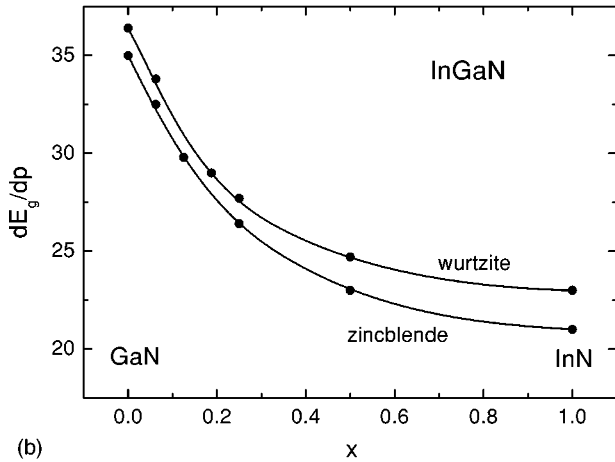


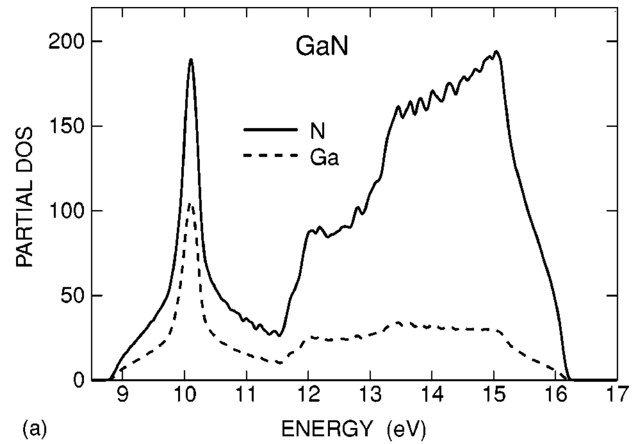
FIG. 7. (a) The $In_xGa_{1-x}N$ band gap deformation potential as a function of indium composition for the wurtzite and for the zinc blende structure. (b) The $In_xGa_{1-x}N$ band gap pressure coefficient as a function of indium composition for the wurtzite and zinc blende structures.

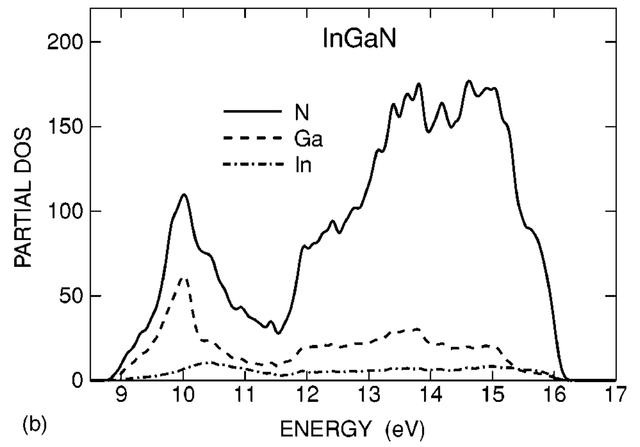
two different ways, one where they were clustering in one corner of the supercell, another with the In atoms distributed as uniformly as possible. The calculated values of the band gap vary by $\sim$0.15 eV, becoming lower in the "clustered" case. The corresponding pressure coefficients are $\sim$2 meV/GPa smaller. The results reported in Figs. 5 and 7 are average values. Obviously, for larger supercells there might be configurations with significantly larger clustering, which would lead to still lower values of the band gap and its pressure coefficient.

B. Internal electric field at high pressures

The optical properties of quantum structures are strongly influenced by internal electric fields.[6] In nitride based quantum wells thicker than 3 nm an electric field of the order of 10^6 Vcm^{-1} via the quantum confined stark effect (QCSE) can lead to an emission energy which is 1 eV lower than the band gap of the bulk material. Therefore, the influence of pressure on the internal electric field should be examined.

Results obtained for many different strained heterostructures (other than nitrides) have shown that the application of hydrostatic pressure tends to reduce the internal strain.[31,32] This comes from the fact that compounds of larger lattice constants (InGaN in our case) are softer than compounds of smaller lattice constant (as would be GaN in our case). Therefore, the creation of a tensile strain by pressure gradually reduces a previously existing strain in the (InGaN) quantum well, and this then leads to a reduction of the electric





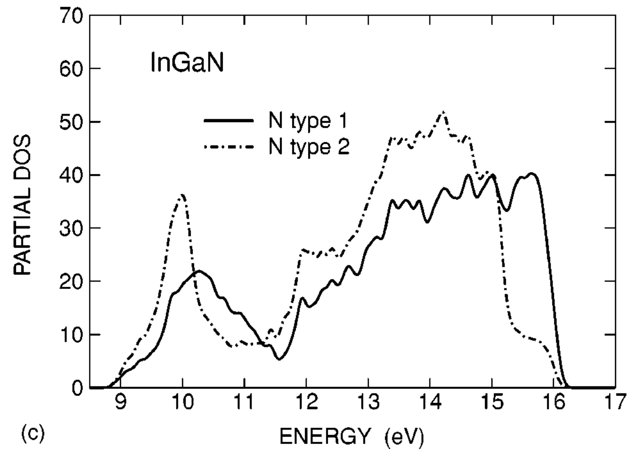


FIG. 8. Partial DOS for (a) pure GaN, solid line: N contribution, dotted line: Ga contribution, dashed line. (b) InGaN (25% In concentration); solid line: N contribution, dotted line: Ga contribution, dashed line: In contribution, (c) InGaN (25% In concentration): solid line: N (type 1 -contribution; dotted line: N (type 2) contribution.

field, which again gives a *positive* contribution to the pressure coefficient of the emission energy. On the other hand, recent experimental results on the influence of hydrostatic pressure on the light emission from strained AlGaN/GaN quantum wells[35] demonstrated that the electric field (or more strictly speaking a potential drop across a quantum well) *reduces* the pressure coefficient of the photoluminescence peak energy. In the case of AlGaN/GaN structures the effect of the internal electric field can be explained[35] within simple linear elasticity theory using piezoelectric tensor data available for GaN and AlGaN (for AlGaN interpolated from binaries). The origin of this effect is the increase of the piezoelectric field caused in part by a nonhydrostatic response of the wurtzite lattice to fully hydrostatic external stress[35] and specific interplay of elastic constants and piezoelectric tensor elements.

A similar approach is more difficult to apply to the case of InGaN/GaN heterostructures because in addition to the electric field, effects related to In content fluctuations can contribute to the observed behavior. Let us, for the sake of simplicity, consider a homogeneous distribution of In and concentrate on the internal electric field which originates from the strain existing in the InGaN/GaN layer grown in the polar (0001) direction. Apart from a ''classical'' piezoelectric component of the internal electric field, we encounter here the presence of the spontaneous polarization which is allowed by the relatively low symmetry of wurtzite. However, since the spontaneous polarizations of GaN and InN are rather similar[6] the most important component of the field is the piezoelectric polarization. We have used linear elastic theory to estimate the strain in InGaN/GaN heterostructures in parallel to the analysis performed for the AlGaN/GaN (Ref. 33) and GaN/sapphire (Ref. 28) systems. First of all, the strain tensor is calculated assuming coexistence of hydrostatic pressure and biaxial stress in the quantum well layer. Then the z component of the piezoelectric polarization vector is determined for quantum wells and barriers. Finally, for simplicity, we consider the case of a single quantum well layer placed in between two thick barriers which enables us to apply a simple formula for the value of the electric field in the quantum well region with semi-infinite cladding layers.[34] The results show that contrary to the AlGaN/GaN case, but in agreement with the intuitive strain-release argument, the piezoelectric field decreases with pressure, the calculated pressure coefficient being $\alpha_E = -0.242$ mV/(Å GPa). A negative α_E causes an increase of the emission energy with pressure due to the QCSE and thus gives a positive contribution to the pressure coefficient of the emission energy. Considering a typical quantum well structure of 50 Å width we may expect the increase of the pressure coefficient of the emission energy to be of the order of 12 meV/GPa. It should be borne in mind, however, that this estimate may be strongly influenced by two factors. First, the use of linear interpolation for the InGaN piezoelectric tensor may be inappropriate as was pointed out by Bernardini and Fiorentini.[36] Secondly, mechanical properties of thin, strongly biaxially strained layers, as is the case of InGaN on GaN, can be different from those of the unstrained material (nonlinear elasticity of biaxially strained material). These mechanical changes can be amplified by the presence of a piezoelectric field. Unfortunately, the material parameters needed to improve on the present type of calculation are not yet avalaible.[36]

VI. CONCLUSIONS

We have studied the influence of hydrostatic pressure on the emission and absorption spectra measured from various types of InGaN structures. The samples examined consisted of epilayers, quantum wells and quantum dots. While the emission energy changes from approximately 3 down to 2 eV, its relevant pressure coefficient varies from 30 meV/GPa down to zero or even a slightly negative value. Thus we can observe the evolution of the pressure coefficient value from characteristic for standard band to band transitions to the magnitude which resembles a highly localized, e.g., an intracenter type of recombination. All data for the pressure coefficients can be arranged as a linear function of the emission energy. This dependence seems to be unrelated to the method of growth and to the details of a particular quantum well structure of the samples. The observed pressure coefficient reduction then reflects a universal property of all the InGaN structures. In the search for a microscopic explanation of the observations we performed *ab initio* calculations of the alloy band structures and their changes with pressure. Significant bowings of the $In_xGa_{1-x}N$ band gap and its pressure coefficient are found, and the bowing effects are especially large for small concentrations of In ($x<0.25$). This behavior is related to the changes in the upper valence band states due to In alloying. Apart from a similarity in trends the band structure calculations are not able to explain the large pressure coefficient reduction observed in the *emission* experiments. In contrast, the pressure coefficients obtained from the *absorption* measurements are not that small, and in this case there is good agreement between the calculated pressure changes of the band structures and the experimental results.

As a possible mechanism which can account for the very low pressure coefficient of the emission energy and the difference between the sensitivity of the emission and absorption to applied pressure we discussed the influence from internal electric fields. Analysis of the effects of these fields performed within the linear elasticity theory (piezoelectric and spontaneous polarizations) in InGaN/GaN heterostructures failed to explain the observed anomalies. The pressure dependence of the internal field should be examined using a more refined model, including better piezoelectric constants and nonlinear elasticity of the InGaN alloys. Further, the effects on the emission properties by In concentration fluctuations and localization of carriers and excitons need to be clarified.

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