Pressure dependence of elastic constants in wurtzite and zinc-blende nitrides and their influence on the optical pressure coefficients in nitride heterostructures

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ABSTRACT

We have studied the nonlinear elasticity effects in III-N compounds. Particularly, we have determined the pressure dependences of elastic constants in wurtzite and zinc-blende InN, GaN, and AlN by performing ab-initio calculations in the framework of plane-wave pseudopotential implementation of the density-functional theory. We have found that C_{11}, C_{12} in zinc-blende phase and C_{11}, C_{12}, C_{13}, C_{33} in wurtzite phase depend significantly and almost linearly on hydrostatic pressure, for all considered nitrides. Much weaker dependences on pressure have been observed for C_{44} in both wurtzite and zinc-blende phases. Further, we have examined the influence of pressure dependence of elastic constant on the pressure coefficient of light emission, dE_E / dP, in wurtzite and cubic, InGaN/GaN and GaN/AlGaN quantum wells. We show that the pressure dependence of elastic constants results in significant reduction of dE_E / dP in nitride quantum wells and essentially improves the agreement between experimental and theoretical values.

INTRODUCTION

The electronic and optical properties of semiconductor heterostructures depend crucially on the strain arising from the lattice mismatch. Commonly, the strain effects in quantum structures, i.e. quantum wells (QWs), wires or dots (QDs), are described using the standard elasticity theory with elastic constants independent on the strain (so-called linear theory). Nevertheless, there are circumstances where this simple approach is insufficient.

Nonlinear elastic properties of GaAs and InAs have recently attracted significant attention. Frogley *et al.* proposed that pressure dependences of elastic constants in GaAs and InAs are required to explain anomalously small pressure coefficient of band-gap in strained InGaAs layers [1]. Ellaway *et al.* calculated pressure dependences of elastic constants for InAs and discussed their influence on the properties of InAs/GaAs QDs [2]. They noticed that hydrostatic strain component in the InAs/GaAs QDs is significantly overestimated by calculations based on linear theory of elasticity.

For the case of III-N compounds, the nonlinear elasticity effects have not been systematically studied yet. A pioneering paper in this field was published by Kato and Hama who calculated the pressure dependence of elastic compliances for wurtzite AlN [3]. Recently, Vaschenko *et al.* have used results of these calculations to estimate the influence of the nonlinear elasticity on pressure coefficients of the light emission (dE_E / dP) in hexagonal GaN/AlGaN QWs [4].

In this work we study the nonlinear elasticity effects in nitride binary compounds. Particularly, we have determined the pressure dependences of elastic constants, in zinc-blende and wurtzite InN, GaN, and AlN by performing ab-initio calculations in the framework of plane-wave pseudopotential implementation of the density-functional theory [5,6]. Further, we examine the influence of pressure dependence of elastic constant on dE_E / dP in wurtzite and cubic, InGaN/GaN and GaN/AlGaN QWs.

PRESSURE DEPENDENCE OF ELASTIC CONSTANTS

The pressure dependence of elastic constants, in zinc-blende and wurtzite GaN, InN and AlN has been determined by carrying out the total energy calculations based on a plane-wave pseudo-potential implementation of the density-functional theory [5]. The numerical computations have been performed with the VASP package [6].

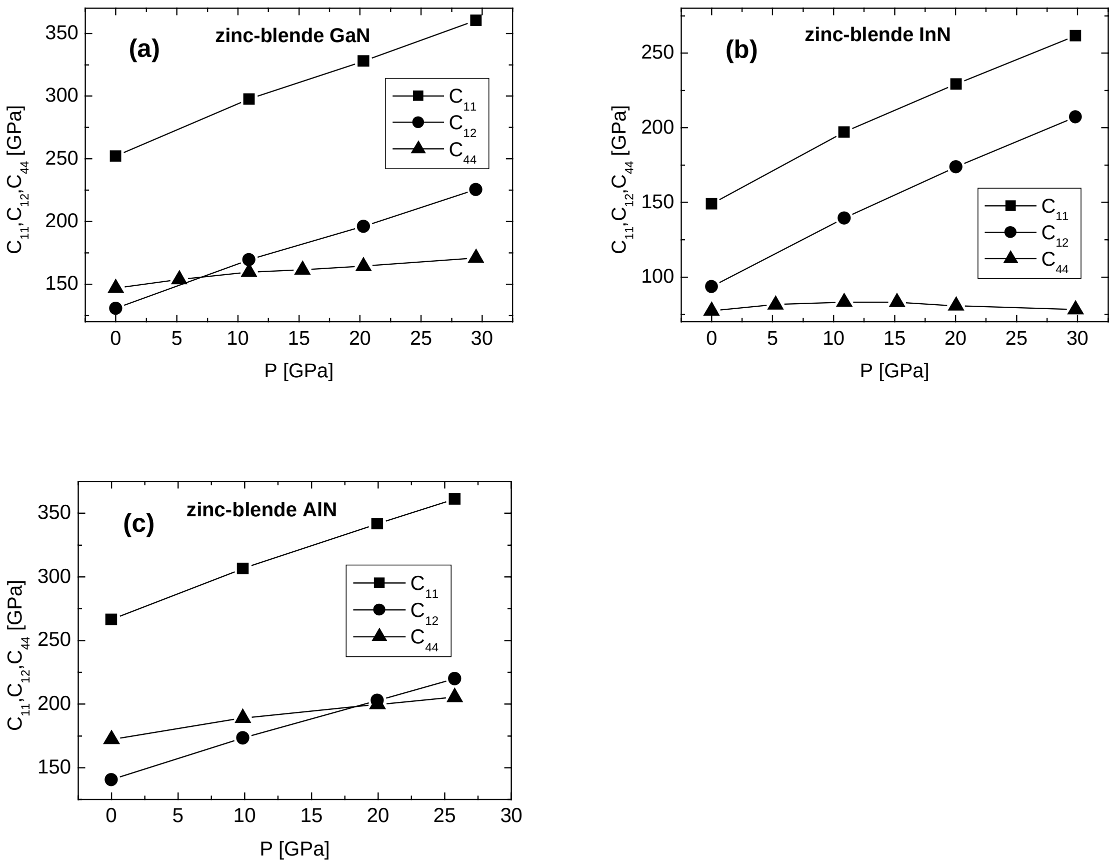

Figure 1. Elastic constants for zinc-blende GaN (a), InN (b) and AlN (c) plotted as a function of hydrostatic pressure. Solid lines are added to guide the eye.

Following the arguments of Ref. [7], the pressure dependent elastic constants are calculated as $C_{\alpha\beta}(P) = \frac{1}{V(P)} \frac{\partial^2 E_{tot}(V(P))}{\partial\varepsilon_\alpha \partial\varepsilon_\beta}$, where $E_{tot}(V(P))$ is the total energy per unit cell, $V(P)$ is the unit cell volume at given pressure P, which is found by solving $P = -\frac{\partial E_{tot}}{\partial V}$, and ε_α,

ε_{β} are the elements of the infinitesimal Lagrangian strain tensor. Details of the approach are described in Ref. [8].

In figures 1a ,1b and 1c we present the elastic constants C_{11}, C_{12} and C_{44} in zinc-blende GaN, InN, and AlN as a function of hydrostatic pressure. One can see that C_{11}, C_{12} vary almost linearly with pressure. The C_{44} elastic constants show much weaker dependence on pressure and slightly sub-linear character. In figures 2a, 2b and 2c we present $C_{11}(P)$, $C_{12}(P)$, $C_{13}(P)$, $C_{33}(P)$ and $C_{44}(P)$ obtained for wurtzite GaN, InN, and AlN. Again, we notice that C_{11}, C_{12}, C_{13}, C_{33} vary almost linearly with pressure, while C_{44} elastic constants possess much weaker and sub-linear dependence on pressure.

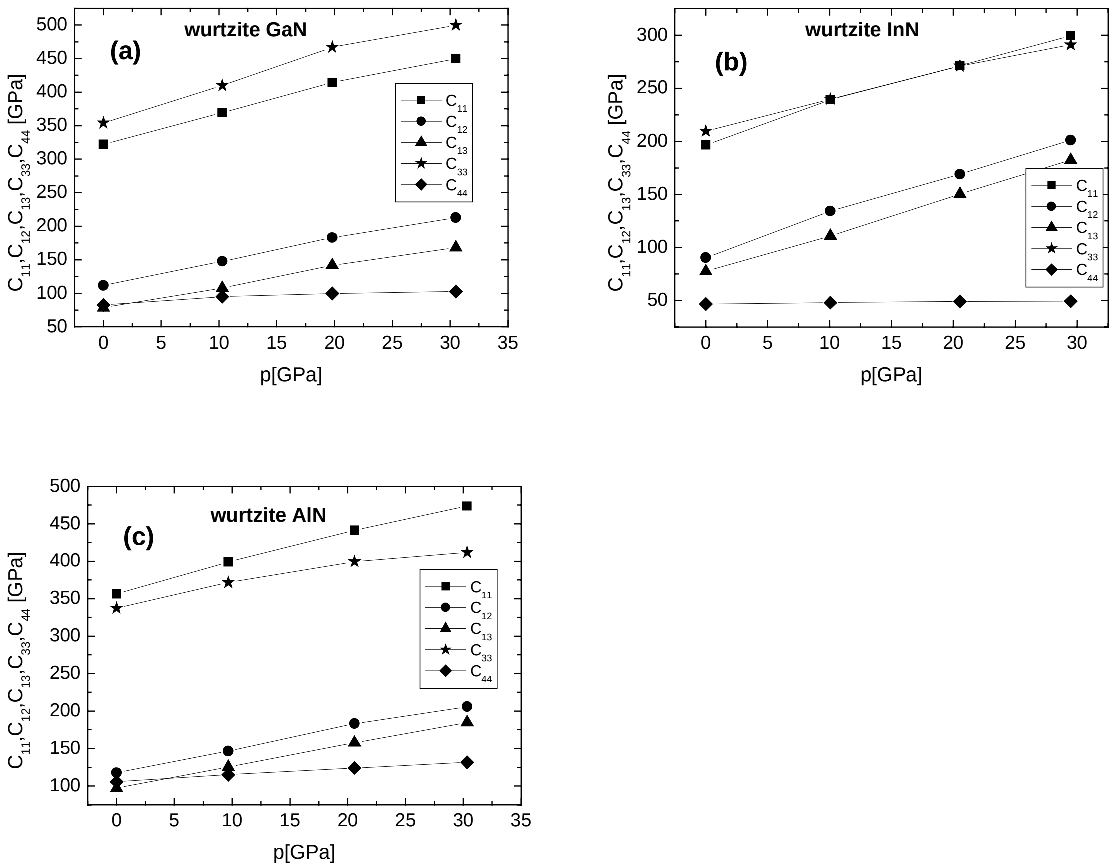

Figure 2. Elastic constants for wurtzite GaN (a), InN (b) and AlN (c) plotted as a function of hydrostatic pressure. Solid lines are added to guide the eye.

In table I we have collected all vales of elastic constants (in GPa) and their pressure derivatives for the ambient pressure. Generally, the elastic constants obtained for ambient pressure are in good agreement with previous calculations [9,10] and experiments [11]. To verify the values of the pressure derivatives of elastic constants, one can easily calculate the derivative of bulk modulus at zero pressure, B_0' for zinc-blende nitrides. For GaN, InN and AlN B_0' equals to 3.33, 3.79 and 3.34 which agrees well with previous calculations and experiments [11, 12].

Table I. Elastic constants and their pressure derivatives at ambient pressure as calculated in this paper.

	$C_{11}(0)$	$C_{12}(0)$	$C_{13}(0)$	$C_{33}(0)$	$C_{44}(0)$	C'_{11}	C'_{12}	C'_{13}	C'_{33}
zb-GaN	252	131			146	3.63	3.18		
zb-InN	149	94			77	3.75	3.81		
zb-AlN	267	141			172	3.77	3.12		
w-GaN	322	112	79	354	83	4.66	3.59	3.18	5.69
w-InN	197	90	78	210	47	3.45	3.17	3.58	3.00
w-AlN	356	118	97	337	106	4.11	3.19	2.95	3.00

PRESSURE COEFFICIENTS OF THE LIGHT EMISSION IN NITRIDE QWS

In this section we show the influence of nonlinear elasticity (i.e. the pressure dependence of elastic constants) on dE_E / dP in wurtzite and zinc-blende GaN/AlGaN and InGaN/GaN QWs. To do so, we calculate energetic positions of the lowest electron and the highest hole states in the QWs for various hydrostatic pressures employing **k·p** envelope function theory. The shift of the band edges caused by the hydrostatic and biaxial strain has been accounted for within the deformation potential theory. For each pressure P, the values of the biaxial strain in the heterostructures have been determined from the Hook's law. The pressure dependent elastic constants for InGaN and AlGaN alloys have been used assuming the Vegard-like law. In wurtzite heterostructures piezoelectric fields in barriers and QWs have been calculated using the model from Ref. [13]. Strain dependent piezoelectric constant have been also taken into account [14]. Details of the calculations for wurtzite QWs are given in Ref. [15], while the model for zinc-blende structures is described in Ref. [8].

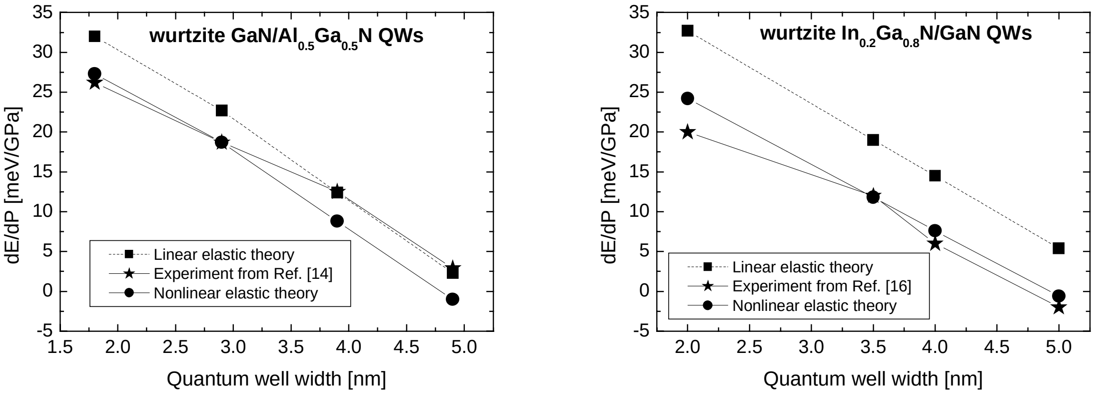

Figure 3. Pressure coefficients of emission energies (dE_E / dP) from wurtzite $GaN/Al_{0.5}Ga_{0.5}N$ (a) and $In_{0.2}Ga_{0.8}N/GaN$ (b) QWs as a function of QW width. Solid and dashed lines are added to guide the eye.

In Fig. 3, we show theoretical values of dE_E / dP for wurtzite GaN/ $Al_{0.5}Ga_{0.5}N$ and $In_{0.2}Ga_{0.8}N$/GaN QWs as a function of QW width, obtained using linear and nonlinear elastic theory. For comparison experimental values of dE_E / dP are also given [14,16]. Generally, one can see strong decrease of dE_E / dP with the quantum well width in wurtzite QWs which was attributed in literature to piezoelectric effects, namely to pressure-induced increase of piezoelectric field. However, it is clear from Fig.3 that application of the nonlinear elastic theory results in further reduction of dE_E / dP in wurtzite QWs by about 4-7meV/GPa comparing to linear elastic theory. The latter effect is independent on QW width and is important especially for narrow QWs in which piezoelectric field plays less important role. This effect is more pronounced for wurtzite InGaN/GaN QWs than for GaN/AlGaN QWs.

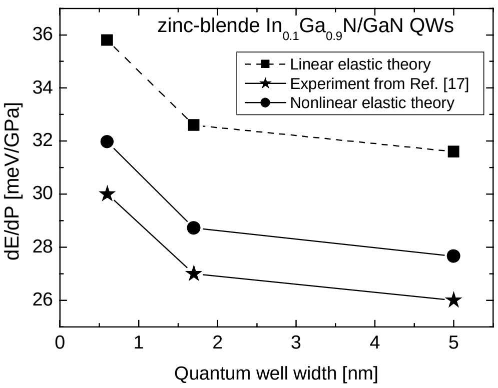

Figure 4. Pressure coefficients of emission energies (dE_E / dP) from cubic $In_{0.1}Ga_{0.9}N$/GaN QWs as a function of QW width. Solid and dashed lines are added to guide the eye.

Zinc-blende nitride QWs, grown in [001] direction, offer much better opportunity to study nonlinear elastic effects than hexagonal heterostructures since the piezoelectric field is not present in these structures. In Fig.4 we show theoretical and experimental [17] values of dE_E / dP obtained for zinc-blende $In_{0.1}Ga_{0.9}N$/GaN QWs as a function of QW width. One can see that linear elastic theory gives values of dE_E / dP which are significantly higher than obtained from experiment. Application of nonlinear elastic theory improves essentially the agreement between theoretical and experimental results for zinc-blende InGaN/GaN QWs.

CONCLUSIONS

In summary, we have calculated the pressure dependence of elastic constants in wurtzite and zinc-blende GaN, InN and AlN. We have found significant and almost linearly increasing dependences on pressure for C_{11}, C_{12} in zinc-blende phase and for C_{11}, C_{12}, C_{13}, C_{33} in wurtzite phase for all considered nitrides. Much weaker dependence on pressure has been observed for C_{44} in both wurtzite and zinc-blende phases. Then, we have studied the influence of nonlinear elastic effects on the pressure coefficients of light emission (dE_E / dP) in wurtzite and zinc-blende nitride QWs. We have demonstrated that pressure dependence of elastic constants results in significant decreasing of the dE_E / dP in both hexagonal and cubic structures as compared to results obtained within linear elastic theory. For hexagonal structures, this effect co-exists with well-known reduction of dE_E / dP by piezoelectric field. For zinc-blende InGaN/GaN QWs, the application of nonlinear elastic theory is essential for quantitative analysis of dE_E / dP since piezoelectric field is absent.

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