

# Effect of pressure on optical phonon modes and transverse effective charges in GaN and AlN

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(Received 12 January 2001; published 22 June 2001)

The pressure behavior of phonon modes of the hexagonal and cubic modifications of GaN and hexagonal AlN was investigated experimentally. The mode pressure coefficients were determined from Raman measurements at hydrostatic pressures up to 6 GPa. The low-frequency  $E_2$  phonon in GaN exhibits a weak softening which is qualitatively similar to that of zone-boundary transverse acoustic modes of zinc-blende III-V semiconductors. In AlN the  $E_2$ (low) phonon frequency is essentially constant under pressure. For both materials an increase of the LO-TO splitting is observed, which results from the interplay between the pressure dependence of the high-frequency dielectric constant and Born's transverse dynamical effective charge. The latter turns out to be nearly constant under pressure, a behavior deviating from that of other III-V semiconductors. The experimental findings are compared to results of *ab initio* calculations.

DOI: 10.1103/PhysRevB.64.035205

PACS number(s): 78.30.-j, 77.22.-d, 63.20.-e, 62.50.+p

## I. INTRODUCTION

The group-III nitrides GaN and AlN are used in optoelectronic semiconductor devices<sup>1</sup> and therefore are the current subject of intense investigations in basic and applied research. At ambient conditions the thermodynamically stable phase of GaN and AlN is the hexagonal wurtzite ( $2H$ ) modification. Under nonequilibrium conditions the growth of the zinc-blende ( $3C$ ) GaN has been achieved.<sup>2</sup> The nitrides are characterized by high bond ionicity, short bond length, low compressibility, and high thermal conductivity. All these properties are desirable for utilization in a variety of applications involving high-temperature and high-power operation.<sup>3</sup> High-pressure Raman experiments are particularly suitable for studying the relationship between bonding and lattice-dynamical properties and their scaling with the lattice constants.<sup>4</sup> An important motivation for high-pressure investigations stems from the fact that group-III-nitride layers are commonly subjected to large built-in strain since they are often grown on different substrates having considerable lattice mismatch.

Previous Raman measurements and theoretical investigations of GaN and AlN obtained, in part, contradictory results. One concerns the softening under pressure of the low-frequency  $E_2$  modes in the hexagonal materials and whether it is more pronounced in GaN or in AlN.<sup>5,6</sup> The  $E_2$ (low) modes are related to the transverse acoustic (TA) phonon branch of the cubic modification. Due to the different stacking sequence in the hexagonal structure, the cubic Brillouin zone is folded along the  $[111]$  direction. Thus, the cubic zone-edge transverse acoustic  $TA(L)$  phonon folds back onto the hexagonal zone center ( $\Gamma$  point) giving rise to the  $E_2$ (low) mode.<sup>7</sup> For the cubic III-V and II-VI semiconductors it is well known that zone-edge TA phonons exhibit negative mode Grüneisen parameters.<sup>8,9</sup> A correlation between the degree of mode softening and the critical pressure for first-order structural phase transitions has been pointed out.<sup>8,10</sup> A relation between the  $E_2$ -mode shift under pressure and phase stability for the hexagonal modifications of the

nitrides, however, has not been established. Moreover, a structural stability analysis based on calculations of both total energies and phonon dispersion curves of tetrahedrally coordinated compounds has revealed a more complex situation.<sup>11</sup>

The pressure dependence of the LO-TO splitting in GaN is another issue of controversy. In a polar lattice, the splitting of the optical phonon modes is determined by two parameters, Born's transverse dynamical effective charge  $e_T^*$  of the lattice ions and the screening of the Coulomb interaction, which depends on the electronic part  $\epsilon_\infty$  of the dielectric constant in the phonon frequency regime. In a recent paper, it was claimed that the LO-TO splitting of GaN decreases with pressure,<sup>12</sup> as is the case for many zinc-blende III-V compounds. However, our preliminary experimental results for  $2H$ -GaN clearly indicate a small increase in the LO-TO separation at reduced volumes.<sup>13</sup>

In this work we report results of high-pressure Raman experiments on the hexagonal and cubic GaN phases as well as on hexagonal AlN. We also present *ab initio* calculations of the corresponding vibrational spectra, which help to clarify the existing discrepancies about the pressure dependence of the  $E_2$  modes, the LO-TO frequency splitting, and the effective charge  $e_T^*$ . In particular, we show that for the group-III nitrides studied many of these quantities display an unusual pressure behavior as compared with other tetrahedrally coordinated III-V compounds.

## II. EXPERIMENTAL DETAILS

A 50  $\mu\text{m}$  thick hexagonal crystal of GaN was grown on  $6H$ -SiC by hydride vapor phase epitaxy.<sup>14</sup> For high-pressure experiments the SiC substrate of the  $2H$ -GaN sample was completely removed by mechanical polishing. The AlN samples were synthesized in the form of needle-shaped single crystals (whiskers) by a direct reaction between evaporated aluminum and nitrogen at high temperature and pressure.<sup>15</sup> An AlN whisker was cut into small pieces of about  $50 \times 100 \times 100 \mu\text{m}^3$  in size. For comparison we have

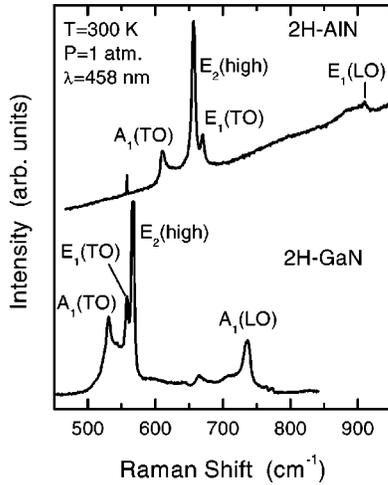


FIG. 1. Representative Raman spectra of  $2H$ -AlN and  $2H$ -GaN measured at room temperature and ambient pressure. Mode assignments are indicated.

also studied a  $1 \mu\text{m}$  thick cubic GaN epilayer grown on GaAs using molecular beam epitaxy.<sup>16,17</sup> The GaAs substrate was thinned down to a final thickness of about  $50 \mu\text{m}$ . Results of low-temperature studies of optical excitations in the cubic GaN samples were reported in Ref. 17.

Raman-scattering experiments under high hydrostatic pressure conditions were performed at room temperature by using a diamond-anvil cell with a 4:1 methanol-ethanol mixture serving as pressure-transmitting medium. Pressure was measured *in situ* by the ruby luminescence method.<sup>18</sup> The 458 and 514 nm lines of an  $\text{Ar}^{2+}$ -ion laser were used for excitation. The scattered light was detected in backscattering geometry and analyzed by a triple-grating spectrometer equipped with a liquid-nitrogen-cooled charge coupled device detector.

### III. THEORETICAL APPROACH

The calculations of the dielectric and dynamic properties are based on density-functional theory with the exchange-correlation energy treated in the local-density approximation. We used a plane-wave pseudopotential method including nonlinear core corrections in the Ga pseudopotential.<sup>19</sup> The dielectric constant, Born's effective charge, and phonon frequencies of GaN and AlN were calculated within the framework of linear-response and density-functional perturbation theory.<sup>20</sup> In order to obtain converged structural parameters at a given pressure, a value of 75 (80) Ry was required for the kinetic-energy cutoff of the plane-wave expansion for the wurtzite (zinc-blende) structure. For the convergence of the dynamical quantities a 60 Ry cutoff was sufficient in all cases. Further computational details including structure optimization procedures are given elsewhere.<sup>21,22</sup>

### IV. RESULTS AND DISCUSSION

Figure 1 shows representative Raman spectra of the hexagonal GaN and AlN samples in the frequency range of the high-frequency  $E_2$  mode measured at ambient temperature

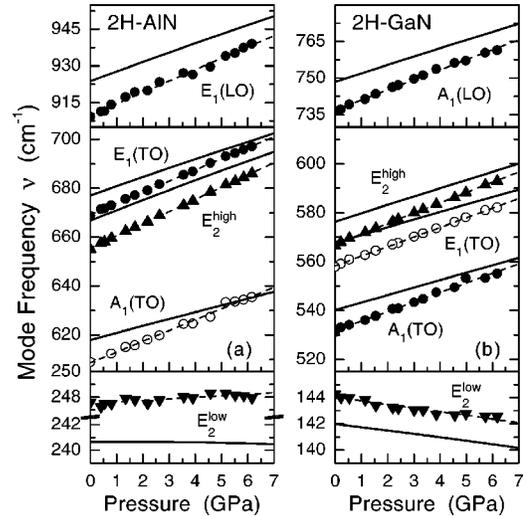


FIG. 2. Measured zone center optical phonon frequencies (symbols) versus hydrostatic pressure for  $2H$ -AlN (left panels) and  $2H$ -GaN (right panels). Solid lines represent the results of *ab initio* calculations. Dashed lines are linear fits to the experimental data.

and pressure conditions. Although forbidden by symmetry, the  $A_1(\text{TO})$  and  $E_1(\text{TO})$  modes appear in the spectra, in addition to the allowed  $E_2$  and  $A_1(\text{LO})$  phonons. This is due to a non-strictly-backscattering configuration in the diamond-anvil cell. The measured frequencies of the GaN and AlN Raman-active phonons are displayed in Fig. 2 as a function of pressure together with the results of the *ab initio* calculations. With increasing pressure the phonon frequencies shift to higher energies, with the remarkable exception of the lower  $E_2$  mode which for GaN exhibits a softening.

Measured and calculated mode frequencies  $\omega_0$  at ambient pressure, their linear pressure coefficients  $\partial\omega/\partial P$ , and mode Grüneisen parameters  $\gamma = -\partial \ln \omega / \partial \ln V = (B_0/\omega_0)\partial\omega/\partial P$  are listed in Table I. To obtain the experimental Grüneisen parameters we used bulk modulus values of  $B_0 = 200$  GPa for GaN,<sup>23</sup> and 208 GPa for AlN.<sup>24</sup> Experimental data for GaN, though, scatter between 188 and 245 GPa.<sup>25</sup> Therefore, the errors of the  $\gamma$  values listed in Table I are mainly determined by the uncertainty in the experimental bulk moduli. The calculated  $\gamma$  values, in contrast, were obtained directly from the theoretical volume dependence of the mode frequencies. The calculated  $B_0$  values at the theoretical equilibrium volumes are 207 GPa for GaN and 210 GPa for AlN.

Data for cubic GaN are also listed in Table I. We point out that, although for the cubic GaN samples the GaAs substrate has not been removed, we have no evidence of built-in strain whatsoever.<sup>13</sup> In fact, within experimental uncertainty no broadening or splitting of the Raman lines is observed under pressure.

The overall agreement between measured and calculated vibrational properties (see Table I) is satisfactory. For the zero-pressure frequencies the calculations deviate by only about 2% from the experimental data. The calculated linear pressure coefficients, however, systematically underestimate the experimental values by about 20%. The observed differences between theory and experiment partly result from the difference in equilibrium lattice constants, the theoretical

TABLE I. Fitting parameters used for the pressure dependence of the phonon frequencies in GaN and AlN and the resulting Grüneisen parameters  $\gamma$ .

Mode	$\omega(\text{cm}^{-1})$		$\partial\omega/\partial P(\text{cm}^{-1}/\text{GPa})$		$\gamma$	
	Expt.	Calc.	Expt.	Calc.	Exper.	Calc.
<i>2H-AlN</i>						
$E_2(\text{low})$	$247.5 \pm 0.5$	241	$0.12 \pm 0.05$	-0.03	$0.10 \pm 0.05$	-0.02
$A_1(\text{TO})$	$608.5 \pm 0.5$	618	$4.4 \pm 0.1$	3.0	$1.51 \pm 0.05$	1.02
$E_2(\text{high})$	$655.5 \pm 0.1$	667	$4.99 \pm 0.03$	4.2	$1.58 \pm 0.01$	1.34
$E_1(\text{TO})$	$669.3 \pm 0.1$	677	$4.55 \pm 0.03$	3.8	$1.41 \pm 0.01$	1.18
$A_1(\text{LO})$	891	898		3.5		0.82
$E_1(\text{LO})$	$910.1 \pm 0.4$	924	$4.6 \pm 0.1$	4.0	$1.06 \pm 0.03$	0.91
<i>2H-GaN</i>						
$E_2(\text{low})$	$144.1 \pm 0.2$	142	$-0.3 \pm 0.1$	-0.24	$-0.4 \pm 0.1$	-0.35
$A_1(\text{TO})$	$531.7 \pm 0.3$	540	$3.9 \pm 0.1$	3.1	$1.47 \pm 0.04$	1.21
$E_1(\text{TO})$	$558.2 \pm 0.1$	568	$3.94 \pm 0.03$	3.3	$1.41 \pm 0.01$	1.19
$E_2(\text{high})$	$567.0 \pm 0.1$	576	$4.24 \pm 0.03$	3.6	$1.50 \pm 0.01$	1.28
$A_1(\text{LO})$	$736.5 \pm 0.2$	748	$4.4 \pm 0.1$	3.5	$1.20 \pm 0.05$	0.98
$E_1(\text{LO})$	$742 \pm 0.2$	757		3.6		0.99
<i>3C-GaN</i>						
TO	$553 \pm 2$	560	$4.0 \pm 0.2$	3.2	$1.4 \pm 0.1$	1.19
LO	$743 \pm 2$	750	$4.5 \pm 0.2$	3.7	$1.20 \pm 0.05$	1.02

values being about 1.5% smaller than the measured ones.

There is a noticeable difference in the behavior of the lower  $E_2$  modes between the two hexagonal nitrides. We find that for GaN the lower  $E_2$  phonon frequency decreases with pressure at a small rate of  $\approx -0.3 \text{ cm}^{-1}/\text{GPa}$ , whereas for AlN the frequency of this mode remains almost constant under compression (see Table I), as was also observed in wurtzite-type BeO.<sup>26</sup> For comparison, Gorczyca *et al.*<sup>6</sup> calculated a softening of  $-0.29 \text{ cm}^{-1}/\text{GPa}$  for the lower  $E_2$  mode of AlN. A mode softening could signal a tendency toward a dynamical instability of the crystal structure. For zinc-blende semiconductors a correlation has been discussed between the often very pronounced softening of the zone-boundary TA modes and the pressure at which structural transitions are observed.<sup>8,10</sup> The mode Grüneisen parameters of the  $E_2(\text{low})$  mode in AlN and GaN are essentially zero or weakly negative, such that a tendency toward a structural instability is not really evident from the mode behavior under pressure. AlN and GaN transform to rocksalt at 23 GPa (Ref. 24) and 30–50 GPa,<sup>27</sup> respectively. For GaN, the energetics of a hypothetical deformation path from wurtzite to rocksalt was recently investigated by Limpijumng and Lambrecht using *ab initio* theoretical methods.<sup>28</sup>

The pressure behavior of the  $E_2$  modes for the two nitrides studied can be understood in terms of the critical balance between central and noncentral elastic forces associated with the stretching and bending of bonds, respectively, which also determines the sign of the Grüneisen parameter for the TA( $L$ ) zone-boundary phonons of tetrahedrally coordinated cubic semiconductors.<sup>29</sup> For the shear-type TA( $L$ ) modes the angular forces tend to make this mode stiffer under pressure, whereas central elastic forces act in the opposite way. For instance, the sign of the mode Grüneisen parameters of zone-edge TA phonons (and consequently of the

thermal expansion coefficient at low temperatures) is positive for diamond ( $\gamma_{TA}=0.4$ ), for which angular forces are dominant,<sup>29</sup> but negative for Si ( $\gamma_{TA}=-1.4$ ) and Ge ( $\gamma_{TA}=-1.53$ ).<sup>8</sup> For GaN the compensation between central and noncentral forces is such that it exhibits a much smaller mode softening than Si. In the case of AlN, the stronger directional (covalent) bonding gives rise to a more balanced situation, intermediate between GaN and diamond. Nevertheless, the pressure coefficients of the  $E_2(\text{low})$  phonons of the nitrides are rather small as compared to other semiconductors, for which the marked ionic character of the former might play a role. The Madelung term due to Coulomb interactions tends to make the  $E_2$  mode stiffer under pressure, thus partially compensating the softening induced by elastic forces.<sup>11</sup>

We now turn to a discussion of the frequency splitting between LO and TO phonon modes. Figure 3 displays the LO-TO splittings of the  $E_1$  and  $A_1$  modes of 2H-AlN and 2H-GaN, respectively, as a function of pressure. In both cases, the LO-TO splitting *increases* slightly with increasing pressure. The calculated pressure slopes (solid lines) are in good agreement with the experimental data except for a small offset due to the slight overestimation of the phonon energies in the calculation.

The linear pressure coefficients of the mode splittings are summarized in Table II. We point out that our findings are in contrast to the results of Perlin *et al.*<sup>12</sup> They reported a pressure-induced decrease of the LO-TO separation in hexagonal GaN ( $-0.35 \pm 0.15 \text{ cm}^{-1}/\text{GPa}$ ). They obtained the pressure dependence of the LO and TO modes independently from measurements on two different samples, which may be the reason for the discrepancy. From our data we thus conclude that both GaN and AlN show a behavior different from other III-V compounds, which exhibit negative pressure co-

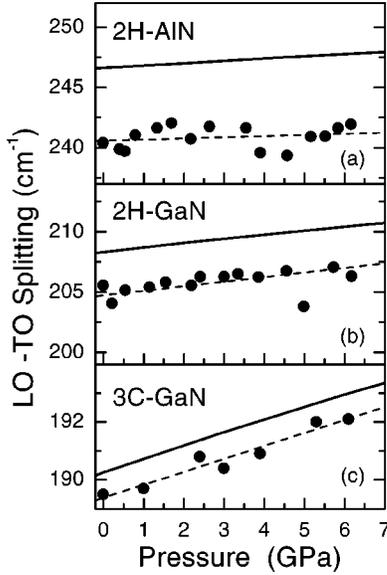


FIG. 3. Experimental LO-TO splittings (symbols) as a function of pressure for (a) the 2H-AlN  $E_1$  modes, (b) the 2H-GaN  $A_1$  modes, and (c) 3C-GaN. Solid lines represent the results of *ab initio* calculations. Dashed lines are linear fits to the experimental data.

efficients for the LO-TO splitting.<sup>30</sup>

The transverse dynamic effective charge can be determined experimentally from the energy splitting of LO and TO phonon modes. This splitting is related to tensor components of the effective charge  $e_T^*$  and the dielectric constant  $\epsilon_\infty$ . While in the cubic case one deals with only one independent tensor component, because of the lower symmetry of the wurtzite structure one has to distinguish between components parallel and perpendicular to the hexagonal  $c$  axis. For modes of the same symmetry with atomic displacements along a direction  $\alpha$  one finds for the corresponding component of  $e_T^*$  (in SI units)

$$(e_T^*)_{\alpha\alpha}^2 = \epsilon_0(\epsilon_\infty)_{\alpha\alpha} V \mu [\omega_{\text{LO}}^2(\alpha) - \omega_{\text{TO}}^2(\alpha)], \quad (1)$$

where  $\epsilon_0$  is the vacuum permittivity,  $\mu$  is the reduced mass of an anion-cation pair,  $V$  is the available volume per pair, and  $\omega$  is the angular mode frequency given in hertz.

The change of the dynamical effective charge under compression can be determined from the measured frequencies of the optical phonons using Eq. (1). The reduction of the unit-cell volume with hydrostatic pressure is described by the Murnaghan equation of state.<sup>31</sup> For the pressure variation of the high-frequency dielectric constant of group-III nitrides

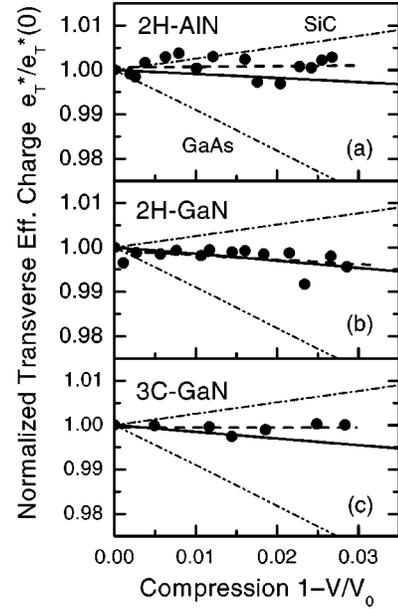


FIG. 4. Born's transverse effective charge (symbols) normalized to its ambient pressure value versus relative volume change for (a) for 2H-AlN (perpendicular tensor component), (b) 2H-GaN (parallel tensor component), and (c) 3C-GaN (cubic), as determined from the mode frequencies using Eq. (1). Solid lines represent the results of *ab initio* calculations. Dashed lines are linear fits to the experimental values. For comparison, the dependence of  $e_T^*$  for 3C-SiC (dot-dashed) and GaAs (double-dot-dashed) is also shown.

there is unfortunately a lack of experimental data. Thus, we used the results of *ab initio* calculations<sup>22</sup> for the logarithmic volume derivative  $r = \partial \ln \epsilon_\infty / \partial \ln V$  with  $r = 0.8$  (0.9) for the hexagonal (cubic) modifications of GaN and 0.4 for 2H-AlN. For comparison, an exponent of  $r = 1.2$  has been determined for hexagonal GaN at around 2 eV by the optical-interference method<sup>32</sup> (using a bulk modulus of  $B_0 = 200$  GPa). The resulting values for  $e_T^*$  are plotted in Fig. 4 as a function of the relative change in volume (data points) together with the theoretical results (solid lines). In order to compare the values obtained for all three materials (Table II), we have normalized  $e_T^*$  in Fig. 4 to its value at ambient pressure. The agreement between experiment and theory is very satisfactory. Our results for GaN agree also well with those from previous calculations.<sup>12</sup>

The effective charge appears to remain *nearly constant* under compression for the two nitrides investigated, in clear contrast to the behavior of 3C-SiC (Ref. 33) and GaAs (Ref. 34) (see Fig. 4). Our findings indicate that the increase of the

TABLE II. Pressure coefficients of the LO-TO splitting  $\Delta\omega$  and transverse dynamical effective charge  $e_T^*$  (in units of the elementary charge  $e$ ).

Material	Mode	$\Delta\omega$ (cm <sup>-1</sup> )		$\partial(\Delta\omega)/\partial P$ (cm <sup>-1</sup> /GPa)		$e_T^*(e)$		$\partial e_T^*/\partial P$ (10 <sup>-3</sup> e/GPa)	
		Expt.	Calc.	Expt.	Calc.	Expt.	Calc.	Expt.	Calc.
2H-AlN	$E_1$	240.8±0.5	247	0.10±0.12	0.21	2.63±0.05	2.54	0.15±0.70	-1.0
2H-GaN	$A_1$	205.3±0.2	208	0.4±0.1	0.39	2.73±0.03	2.74	-1.3±0.7	-2.0
3C-GaN	(cub.)	189±1	190	0.45±0.05	0.50	2.65±0.03	2.65	0.0±0.5	-1.9

LO-TO splittings in the group-III nitrides at high pressures is mainly due to the reduction of the dielectric constant, which is a signature of strong covalent bonding and the related overall increase of direct optical gaps with pressure. The only known example of a tetrahedrally coordinated semiconductor exhibiting a larger Born effective charge at reduced volume is SiC. In this case the lack of  $p$  electrons in the carbon core allows for a larger penetration of the Si wave functions into the carbon core regions, leading to an increase in ionicity and hence of  $e_T^*$  under pressure.<sup>35</sup> This situation holds also for the nitrides since the nitrogen and carbon atomic cores look alike. Thus, the dynamical effective charges of GaN and AlN exhibit under compression a similar but less marked behavior to that of SiC. For other III-V compounds like GaAs both the LO-TO splitting and the dielectric constant decrease with pressure giving rise to a reduction of  $e_T^*$ .

In summary, we observed both experimentally and theoretically that certain lattice-dynamical properties of GaN and AlN show an anomalous pressure behavior if compared to the zinc-blende III-V compounds. The mode Grüneisen parameter of the lower  $E_2$  Raman-active phonon is nearly zero

in AlN and only weakly negative in GaN. This indicates an approximate cancellation of the effects of central and non-central forces on the pressure dependence of the phonon frequency. In contrast to other III-V or II-VI semiconductors, the LO-TO splitting is nearly constant for AlN and increases slightly in GaN with pressure. The transverse effective charges are almost constant under pressure. All these effects are a consequence of the strong directional covalent bonding of the nitrides, which behave upon compression in a manner similar to carbon-based solids like diamond and SiC.

#### ACKNOWLEDGMENTS

We thank D. J. As, D. Schikora, and B. Schöttker for providing the cubic GaN samples. We also thank F. Bechstedt and A. Hoffmann for stimulating discussions. This work was supported in part by the Deutsche Forschungsgemeinschaft (DFG) in the framework of the Schwerpunkte ‘‘Gruppe-III-Nitride,’’ Projects No. Be 1346/8-4 and No. 1032. Most of the calculations were performed on the Cray J90 and T90 of the Supercomputer Center NIC in Jülich.

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- <sup>1</sup>S. Nakamura and G. Fasol, *The Blue Laser Diode* (Springer, Berlin, 1997).
- <sup>2</sup>S. Strite, J. Ruan, Z. Li, A. Salvador, H. Chen, D.J. Smith, W.J. Choyke, and H. Morkoç, *J. Vac. Sci. Technol. B* **9**, 1924 (1991); D.J. As, F. Schmilgus, C. Wang, B. Schöttker, D. Schikora, and K. Lischka, *Appl. Phys. Lett.* **70**, 1311 (1997); J. Wu, H. Yaguchi, K. Onabe, R. Ito, and Y. Shiraki, *ibid.* **71**, 2067 (1997).
- <sup>3</sup>H. Morkoç, S. Strite, G.B. Gao, M.E. Lin, B. Sverdlov, and M. Burns, *J. Appl. Phys.* **76**, 1363 (1994).
- <sup>4</sup>M. Cardona and E. Anastassakis, *Semicond. Semimetals* **55**, 117 (1998).
- <sup>5</sup>P. Perlin, A. Polian, and T. Suski, *Phys. Rev. B* **47**, 2874 (1993).
- <sup>6</sup>I. Gorczyca, N.E. Christensen, E.L. Peltzer y Blanca, and C.O. Rodriguez, *Phys. Rev. B* **51**, 11 936 (1995).
- <sup>7</sup>S.S. Mitra, O. Brafman, W.B. Daniels, and R.K. Crawford, *Phys. Rev.* **186**, 942 (1969).
- <sup>8</sup>B.A. Weinstein and R. Zallen, in *Light Scattering in Solids IV*, edited by M. Cardona and G. Güntherodt (Springer, Berlin, 1984), p. 463.
- <sup>9</sup>S. Klotz, J.M. Besson, M. Braden, K. Karch, P. Pavone, D. Strauch, and W.G. Marshall, *Phys. Rev. Lett.* **79**, 1313 (1997).
- <sup>10</sup>B.A. Weinstein, *Solid State Commun.* **24**, 595 (1977).
- <sup>11</sup>V. Ozoliņš and A. Zunger, *Phys. Rev. Lett.* **82**, 767 (1999); K. Kim, V. Ozoliņš, and A. Zunger, *Phys. Rev. B* **60**, R8449 (1999).
- <sup>12</sup>P. Perlin, T. Suski, J.W. Ager III, G. Conti, A. Polian, N.E. Christensen, I. Gorczyca, I. Grzegory, E.R. Weber, and E.E. Haller, *Phys. Rev. B* **60**, 1480 (1999).
- <sup>13</sup>H. Siegle, A.R. Goñi, C. Thomsen, C. Ulrich, K. Syassen, B. Schöttker, D.J. As, and D. Schikora, in *Gallium Nitride and Related Materials II*, edited by C.R. Abernathy, H. Amano, and J.C. Zopler, *Mater. Res. Soc. Symp. Proc.* 468 (Material Research Society, Pittsburgh, 1997), p. 225.
- <sup>14</sup>Y.A. Vodakov, E.N. Mokhov, and A.D. Roenkov, *Phys. Status Solidi A* **51**, 209 (1979).
- <sup>15</sup>J. Pasternak and L. Roskocova, *Phys. Status Solidi* **26**, 591 (1968).
- <sup>16</sup>D. Schikora, M. Hankeln, D.J. As, K. Lischka, T. Litz, A. Waag, T. Buhrow, and F. Henneberger, *Phys. Rev. B* **54**, R8381 (1996).
- <sup>17</sup>Z.X. Liu, A.R. Goñi, K. Syassen, H. Siegle, C. Thomsen, B. Schöttker, D.J. As, and D. Schikora, *J. Appl. Phys.* **86**, 929 (1999).
- <sup>18</sup>G.J. Piermarini, S. Block, J.D. Barnett, and R.A. Forman, *J. Appl. Phys.* **46**, 2774 (1975); H.K. Mao, J. Xu, and P.M. Bell, *J. Geophys. Res. [Space Phys.]* **91**, 4673 (1986).
- <sup>19</sup>K. Karch, F. Bechstedt, and T. Pletl, *Phys. Rev. B* **56**, 3560 (1997).
- <sup>20</sup>P. Giannozzi, S. de Gironcoli, P. Pavone, and S. Baroni, *Phys. Rev. B* **43**, 7231 (1991); A. Dal Corso, S. Baroni, and R. Resta, *ibid.* **49**, 5323 (1994).
- <sup>21</sup>K. Karch, J.-M. Wagner, and F. Bechstedt, *Phys. Rev. B* **57**, 7043 (1998).
- <sup>22</sup>J.-M. Wagner and F. Bechstedt, *Phys. Rev. B* **62**, 4526 (2000).
- <sup>23</sup>C. Kisielowski, J. Krüger, S. Ruvimov, T. Suski, J.W. Ager III, E. Jones, Z. Liliental-Weber, M. Rubin, E.R. Weber, M.D. Bremser, and R.F. Davis, *Phys. Rev. B* **54**, 17 745 (1996).
- <sup>24</sup>M. Ueno, A. Onodera, O. Shimomura, and K. Takemura, *Phys. Rev. B* **45**, 10 123 (1992).
- <sup>25</sup>See related citations in Z.X. Liu *et al.*, *Solid State Commun.* **108**, 433 (1998).
- <sup>26</sup>A.P. Jephcoat, R.J. Hemley, H.K. Mao, R.E. Cohen, and M.J. Mehl, *Phys. Rev. B* **37**, 4727 (1988).
- <sup>27</sup>P. Perlin, C. Jaubertie-Carillon, J.P. Itie, A. San Miguel, I. Grzegory, and A. Polian, *High Press. Res.* **7**, 96 (1991); *Phys. Rev. B* **45**, 83 (1992).

- <sup>28</sup>S. Limpijumngong and W.R.L. Lambrecht, Phys. Rev. Lett. **86**, 91 (2001).
- <sup>29</sup>C.H. Xu, C.Z. Wang, C.T. Chan, and K.M. Ho, Phys. Rev. B **43**, 5024 (1991).
- <sup>30</sup>R. Trommer, H. Müller, M. Cardona, and P. Vogl, Phys. Rev. B **21**, 4869 (1980).
- <sup>31</sup>F.D. Murnaghan, Proc. Natl. Acad. Sci. U.S.A. **30**, 244 (1944).
- <sup>32</sup>P. Perlin, I. Gorczyca, N.E. Christensen, I. Grzegory, H. Teisseyre, and T. Suski, Phys. Rev. B **45**, 13 307 (1992).
- <sup>33</sup>J.A. Sanjurjo, E. López-Cruz, P. Vogl, and M. Cardona, Phys. Rev. B **28**, 4579 (1983); J. Liu and Y.K. Vohra, Phys. Rev. Lett. **72**, 4105 (1994); N.M. Balzaretta and J.A.H. Jornada, Solid State Commun. **99**, 943 (1996).
- <sup>34</sup>B.A. Weinstein and G.J. Piermarini, Phys. Rev. B **12**, 1172 (1975); R. Trommer, H. Müller, M. Cardona, and P. Vogl, *ibid.* **21**, 4869 (1980); D. Diego, M. Cardona, and P. Vogl, *ibid.* **25**, 3878 (1982).
- <sup>35</sup>K. Karch and F. Bechstedt, Phys. Rev. Lett. **77**, 1660 (1996).