

# Direct evidence of tensile strain in wurtzite structure $n$ -GaN layers grown on $n$ -Si(111) using AlN buffer layers

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(Received 10 May 1999)*

We present results on precise frequency measurements of first-order Raman-scattering spectra from a thin  $n$ -GaN layer grown by molecular-beam epitaxy on  $n$ -Si(111) substrate using an optimized AlN buffer. It is found that the optical-phonon line at  $565.43\text{ cm}^{-1}$ , which we attributed to the high-frequency  $E_2(\Gamma)$  phonon mode indicates that the grown GaN layer possesses wurtzite structure. No evidence of cubic GaN zinc-blende structure is observed. At the same time, the frequency of the  $E_2(\Gamma)$  phonon mode deviates significantly from that of the bulk GaN and exhibits negative shift, while the triply degenerate Si optical phonon mode exhibits small positive shift in comparison to that of free standing Si substrate. The obtained experimental data demonstrate the complex nature of the strain distribution at the GaN/AlN/Si(111) interface. We show that the epitaxial growth of GaN induces changes on both sides of  $n$ -GaN/AlN/ $n$ -Si(111) interface: the GaN layer itself exhibits biaxial tensile strain while the Si surface at interface is under biaxial compressive strain. This behavior appears to be a common problem for heterostructures independent of the growth technique employed. [S0163-1829(99)07447-0]

## I. INTRODUCTION

Recent breakthroughs in epitaxial growth of direct wide-band-gap group III-V nitride semiconductors, which form a continuous alloy system and whose room-temperature minimum band gap extends from 1.89 eV for InN to 3.44 eV for GaN and to 6.2 eV for AlN, have categorized them as the most promising materials for a variety of devices. They encompass optoelectronic as well as electronic devices which operate in the wide spectral range from the red to ultraviolet regions, and high power amplifiers.<sup>1-4</sup> Owing to high chemical stability at elevated temperatures, excellent mechanical properties, good thermal conductivity, a high breakdown field, and a large electron saturation velocity of GaN, gallium nitride-based structures are an important class of materials. Despite the significant technological accomplishments of the past few years, there is a great deal of need for understanding of the fundamental processes which could pave the way for rapid development of these structures for devices.

Gallium nitride-based layers have been grown epitaxially on different substrates such as sapphire, silicon carbide, zinc oxide, and gallium arsenide. The heteroepitaxial growth of polar gallium nitride-based compound semiconductor layers on nonpolar conductive Si substrates is a current challenge and attracts increased attention. The motivation lies in the properties of these structures for both fundamental studies and device applications. They may be key compounds for possible monolithic integration of gallium nitride-based compounds on Si-based device structures. Furthermore, they may allow production of large area epilayers with high me-

chanical strength and excellent thermal conductivity due to the well-known advantages of Si. However, there exist several serious problems which prevent formation of high-quality layers, and until recently there were only a few attempts to grow high-quality gallium nitride layers on silicon.

One of the principal difficulties in growing gallium nitride-based polar layers on the nonpolar substrates is the formation of antiphase disorder with different sublattice pairing for the cations and anions with the silicon. In addition to the undesirable effect of antiphase disorder, there are problems of mismatch in the lattice constants and in thermal-expansion coefficients of the substrate and epitaxial films. Due to the difference of the temperature-dependent mismatch in the lattice constant and the thermal-expansion coefficients of GaN and Si, the deformation fields and corresponding generation of high-density dislocations at the interface of GaN layers grown on Si(111) is much higher than that of homoepitaxially grown films. In addition, there is the issue of formation of an intermediate oxide and/or nitride layer on the Si surface.

GaN layers grown on Si can assume either the hexagonal—wurtzite or cubic—zinc-blende structures and their simultaneous presence leads to formation of stacking faults. Consequently, recent attempts to grow GaN layers directly on Si substrates resulted in polycrystalline films which are not suitable for devices. The most favorable and practical solution to overcome many of these difficulties is the growth of an optimized AlN buffer layer between the Si substrate and the GaN layer. The growth of AlN on Si(111)

substrate is easier than that of GaN due to strong bonds between Al and Si atoms.

In this work, we present experimental evidence for the local structural and strain properties at interface of  $n$ -GaN/AlN/ $n$ -Si(111) heterostructures grown by molecular-beam epitaxy (MBE). These data were obtained by precise measurements of Raman scattering spectra. Results of numerous investigations associated with Raman studies of strain-related phenomena in GaN have been published.<sup>5–15</sup> To the best of our knowledge, the Raman-scattering spectra of gallium nitride layers grown on silicon substrates have yet not been reported. The experimental observation of the phonon line at  $565.43\text{ cm}^{-1}$ , which we attributed to the high-frequency  $E_2(\Gamma)$  optical-phonon mode, indicates that the GaN epilayer is wurtzitic. No evidence of cubic GaN zincblende structure was observed. Furthermore, the obtained experimental data demonstrate the complex nature of the strain distribution at the  $n$ -GaN/AlN/ $n$ -Si(111) interface. We show that the epitaxial growth of GaN induces structural changes on both sides of the  $n$ -GaN/AlN/ $n$ -Si interface.

## II. EXPERIMENTAL DETAILS

The sample studied was grown by reactive molecular-beam epitaxy (RMBE) using ammonia ( $\text{NH}_3$ ) (Ref. 16) as the nitrogen source. The GaN layer investigated was grown on a conductive  $n$ -type Si(111)-oriented substrate using an optimized thin AlN buffer layer. The AlN layer was deposited at  $800^\circ\text{C}$  followed by the undoped GaN film, which was grown at  $750^\circ\text{C}$  and near stoichiometric conditions. The thickness of the AlN buffer layer was ( $\sim$ ) 5 nm and that of the GaN layer was ( $\sim$ ) 370 nm. During the growth, the crystalline quality of the GaN layer was monitored *in situ* by the reflection high-energy electron diffraction (RHEED). The RHEED patterns were streaky and showed a sharp ( $1 \times 1$ ) structure (with a weaker half order) indicating layer-by-layer growth, while maintaining a reasonably smooth surface.

The micro-Raman-scattering measurements were performed at room temperature in the backscattering configuration from the epilayer surface of the GaN/AlN/ $n$ -Si(111) heterostructure. The spectra were excited by a  $514.532\text{ nm}$  line of an  $\text{Ar}^+$ -ion laser and  $647.087\text{ nm}$  line of a  $\text{Kr}^+$ -ion laser. The typical power of the incident light at the surface of the sample was approximately 1 mW with the diameter of the light spot of  $1\ \mu\text{m}$ . The scattered light was analyzed by a triple monochromator Jobin-Yvon T 64000 spectrometer.

## III. RESULTS AND DISCUSSION

The electrical characterization of gallium nitride layer grown on AlN/ $n$ -Si(111)-oriented substrate indicated  $n$ -type conductivity. In Fig. 1(a), we show the room-temperature Raman spectrum for the  $n$ -GaN/AlN/ $n$ -Si(111) sample in the frequency range from 400 to  $940\text{ cm}^{-1}$ . This spectrum is obtained for the backscattering configuration represented in standard notation as  $z(y,x+y)^-z$ , where  $z$  axis is parallel to the  $[0001]$  crystallographic direction of GaN. The other two axes are chosen to form an orthogonal system with the  $c$  axis. As expected, we detect a very sharp and intense line around  $521\text{ cm}^{-1}$ , corresponding to the triply degenerate zone-center optical-phonon mode of the covalent (111)-

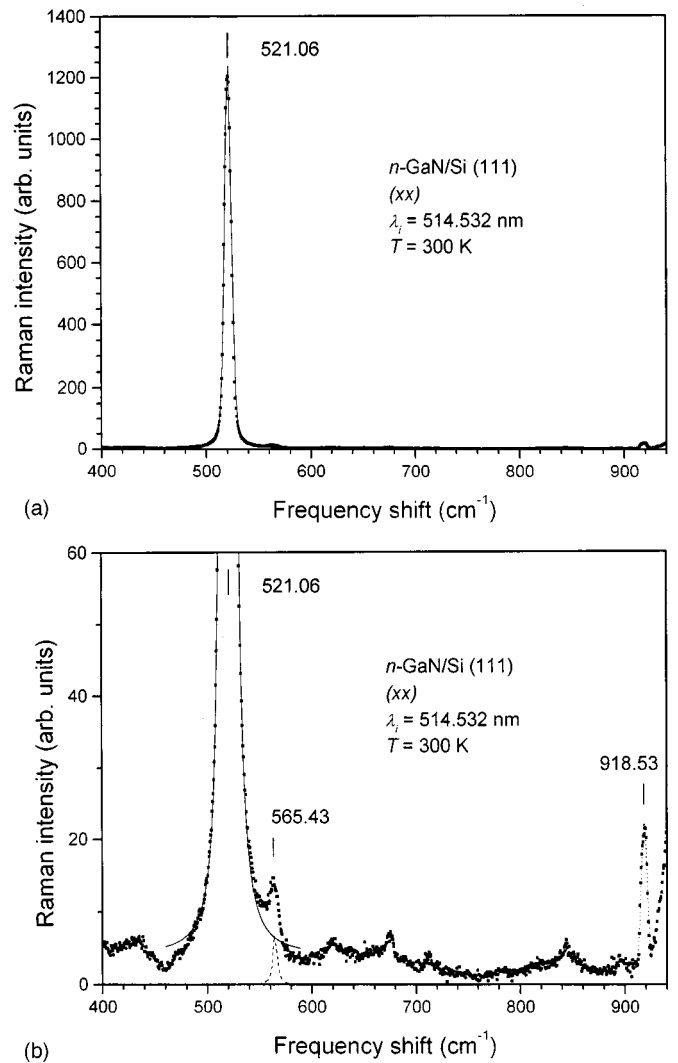


FIG. 1. (a) Room-temperature Raman spectra of  $n$ -GaN/AlN/ $n$ -Si(111) heterostructure sample recorded in the backscattering configuration  $z(y,x+y)^-z$ ; (b) The same in the expanded intensity scale. The solid curve corresponds to the Voigt profile fitted to the experimental data for the Si optical phonon at  $(521.06 \pm 0.05)\text{ cm}^{-1}$ . The dashed curve corresponds to the true Lorentzian profile of  $E_2(\Gamma)$  high-frequency optical phonons in the GaN layer. The dotted curve at  $918.53\text{ cm}^{-1}$  corresponds to the Gaussian instrumental profile of the spectrometer recorded with the Ne spectral line.

oriented  $n$ -Si substrate. At the falling edge of the higher frequency range of this rather intense and well-known completely symmetric line,<sup>17</sup> we observed a new weak structure. This structure is more evident in the spectrum recorded at the extended intensity scale presented in Fig. 1(b). In the higher frequency neighborhood of this Si line, it is clearly seen that an additional line around  $565\text{ cm}^{-1}$  with very small intensity appears. Nevertheless, we see that this line is sufficiently resolved with a well reproducible structure.

In order to ascertain that the new structure indeed relates to the GaN layer and to gain a more detailed understanding of its origin, we performed the same type of measurements for a reference uncovered freestanding surface of a (111)-oriented  $n$ -Si substrate. The experimental conditions were

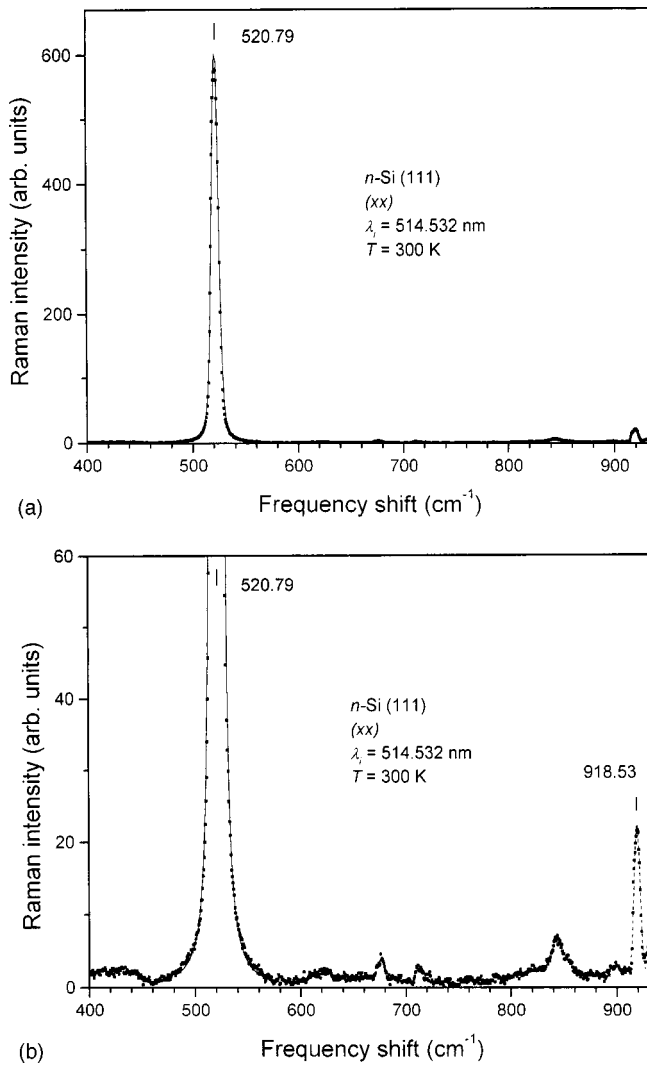


FIG. 2. (a) Room-temperature Raman spectra of uncovered virgin  $n$ -Si(111) substrate, recorded under the same experimental conditions as for the  $n$ -GaN/AlN/ $n$ -Si(111) heterostructure; (b) The same in the expanded intensity scale. The solid curve corresponds to the Voigt profile fitted to the experimental data for the Si optical phonon at  $(520.79 \pm 0.05)$   $\text{cm}^{-1}$ . The dotted curve at  $918.53$   $\text{cm}^{-1}$  corresponds to the Gaussian instrumental profile of the spectrometer recorded with the Ne spectral line.

identical to those for the GaN/AlN/Si case allowing a straightforward comparison. These spectra associated with a clean Si surface are given in Figs. 2(a) and 2(b), respectively. One can see that the line at  $565$   $\text{cm}^{-1}$  appears only in the spectra recorded for the  $n$ -GaN/AlN/ $n$ -Si(111) heterostructure. This line also appears in the spectra excited by a  $647.087$  nm line of a  $\text{Kr}^+$ -ion laser indicating its Raman-scattering origin.

Due to the far off-resonant conditions, the AlN buffer layer itself with a thickness of  $5$  nm is too thin for detection. Furthermore, in the spectra no evidence was found for neither optical transverse  $F_2(\text{TO})$  nor the longitudinal  $F_2(\text{LO})$  phonon modes for the zinc-blende structure of GaN. These modes are also allowed by selection rules for the scattering geometry used and are expected at  $555$  and  $742$   $\text{cm}^{-1}$ , respectively. The absence of these modes indicates the pres-

ence of the hexagonal wurtzite phase in the GaN layer grown on AlN/ $n$ -Si(111) substrate. Therefore, we attribute the additional line at  $565$   $\text{cm}^{-1}$  to the Brillouin zone-center  $E_2(\Gamma)$  high-frequency optical-phonon mode of gallium nitride. This nonpolar phonon mode propagates parallel to the uniaxial  $c$  axis, which is the growth direction of the GaN layer in our experiments. This assignment is also supported by the group-theory selection rules. For GaN crystallized in a hexagonal wurtzite structure, belonging to the space group  $C_{6v}^4-P6_3mc$  with four atoms in the unit cell at  $\mathbf{k}=0$ , the point group theory predicts eight sets of phonon modes. Among them is the twofold degenerate high-frequency  $E_2(\Gamma)$  optical-phonon mode which is Raman active<sup>18</sup> in the backscattering configuration  $z(y, x+y)^{-}z$ .

In the off-resonant spectra obtained for this scattering configuration  $E_2(\Gamma)$  optical-phonon line has the highest intensity in comparison with other allowed phonon modes. In Figs. 1(b) and 2(b) the other low-intensity peaks that are present in the spectra obtained in the expanded intensity scale are similar. They correspond to the second-order Raman scattering by different combinations of optical or/and acoustic Brillouin zone-edge phonons of silicon.

The surface flatness of the GaN layer was sufficient to achieve a good signal-to-noise ratio. The gallium nitride layer is transparent to the  $514.532$  nm excitation line, which is also far from resonance with electronic levels. Therefore, the ratio of the absolute intensity of the Si optical-phonon line at  $521.06$   $\text{cm}^{-1}$  to that of the  $E_2(\Gamma)$  optical-phonon line of the thin  $370$  nm GaN layer for our  $n$ -GaN/AlN/ $n$ -Si(111) heterostructure sample is approximately  $10^3$ . In order to detect reliably such a line with rather weak intensity close to the very strong Si phonon line, we performed several measurements for slightly shifted grating positions of the spectrometer with increased acquisition times. We also limited the spectral resolution to  $5.6$   $\text{cm}^{-1}$  without analyzing the polarization of scattered light. It is important to note that, initially it was presupposed that the sharp Si line itself could be used for frequency calibration for this line. However, various experimental conditions and methods of analysis used by different authors led to some discrepancies in the data for the Si optical-phonon mode.<sup>19–21</sup> Very recently, high-accuracy pressure-dependent Raman-scattering measurements for etched and (100)-oriented Si by using a diamond-anvil cell revealed the value of  $523.88$   $\text{cm}^{-1}$  for the frequency of optical-phonon mode at low temperature  $T = 6$  K under ambient pressure.<sup>15</sup> However, the Si(111) surface close to the substrate-gallium nitride layer interface can also be perturbed during the growth of thin AlN and GaN layers with thicknesses of  $5$  and  $370$  nm, respectively. The frequency of optical-phonon modes depends on the strain fields present in the heterostructures. It is clear that the strain fields play a key role in the formation of high-crystalline quality semiconductor heterostructures with potential impact on devices. Therefore, it is important to understand the strain effect at the  $n$ -GaN/AlN/ $n$ -Si(111) heterointerface.

For this reason, in order to establish the macroscopic-strain state at the surface of a Si(111) substrate that is close to the AlN heterointerface layer, we carefully measured the shift in the frequencies of the two phonon lines. We have applied the nearby Ne spectral line at  $918.53$   $\text{cm}^{-1}$  to check the exact values of the spectral resolution, instrumental line

TABLE I. Experimental frequencies  $\omega$  for the Raman-active  $E_2(\Gamma)$  high-frequency optical phonons in GaN obtained in this work and that of orders;  $d$  is the thickness of GaN layer.

Material	$d$	$\omega$ (in $\text{cm}^{-1}$ )	Temperature	Comments
$n$ -GaN/AlN/ $n$ -Si(111)	370 nm	$565.43 \pm 0.05$	RT	Present work
GaN/GaAs or GaN/Al <sub>2</sub> O <sub>3</sub>		566.5	RT	Ref. 12
GaN, bulk		568	20 K	Ref. 15
GaN, bulk		568	RT	Refs. 14, 6
GaN/Al <sub>2</sub> O <sub>3</sub>	2.0 $\mu\text{m}$	568.5	RT	Ref. 11
$n$ -GaN/GaAs (001)	200 nm	569	RT	$n = 1 - 5 \times 10^{18} \text{cm}^{-3}$ , Ref. 7
GaN/GaN or GaN/Al <sub>2</sub> O <sub>3</sub>		569	RT	Ref. 8
$n$ -Ga <sup>14</sup> N/Al <sub>2</sub> O <sub>3</sub> <sup>a</sup>	1.3 $\mu\text{m}$	$569.2 \pm 0.2$	10 K	$n = 1 \times 10^{18} \text{cm}^{-3}$ , Ref. 9
$n$ -Ga <sup>15</sup> N/Al <sub>2</sub> O <sub>3</sub> <sup>a</sup>	1.0 $\mu\text{m}$	$551.8 \pm 0.2$	10 K	$n = 2 \times 10^{19} \text{cm}^{-3}$ , Ref. 9
GaN/Al <sub>2</sub> O <sub>3</sub>	200 $\mu\text{m}$	570	RT	Refs. 5, 10
GaN/Al <sub>2</sub> O <sub>3</sub>	2.0 $\mu\text{m}$	572	RT	$n = 1 - 100 \times 10^{10} \text{cm}^{-3}$ , Ref. 13

<sup>a</sup>Ref. 9: completely relaxed GaN layers MBE grown from natural Ga and natural N (99.63% <sup>14</sup>N) and isotopically pure <sup>14</sup>N.

shape, and frequency shifts. Linearity in the spectral calibration of the spectrometer in this frequency range was proven by detection of the several nearby neon lines. Furthermore, the observed phonon line shapes were well simulated to the experimental points by the Voigt function (solid curves in all the spectra). The Voigt function is the convolution of the Lorentzian function corresponding to the true phonon line shape and the Gaussian function corresponding to the spectrometer profile (dotted curves at  $918.53 \text{cm}^{-1}$ ). In this case, the result of the convolution<sup>22,23</sup> was obtained by fitting a Voigt profile to the experimental line shape by accepting a fixed width for the Gaussian component. Consequently, we significantly improved the measurement accuracy of these frequency shifts. Therefore, the phonon frequency was determined quite accurately and with an estimated accuracy better than  $\pm 0.05 \text{cm}^{-1}$ .

This approach really allowed us to detect the not negligible shift for the Si optical-phonon lines in these spectra. First, we found that the precise value of the room-temperature frequency shift for the Si optical-phonon line is  $(520.79 \pm 0.05) \text{cm}^{-1}$  for the free-standing surface of the (111)-oriented  $n$ -Si substrate. This is the same value as that observed in the spectra recorded with a  $647.087 \text{nm}$  line of a  $\text{Kr}^+$ -ion laser with radically reduced excitation power down to approximately  $10 \mu\text{W}$ . Therefore, we believe that laser heating of the Si surface through the gallium nitride layer was negligible. Second, we found also that the position of this Si phonon mode detected from the gallium nitride side, in the case of the  $n$ -GaN/AlN/ $n$ -Si(111) heterostructure, slightly shifts toward higher energies. The exact position of the line in this case is  $(521.06 \pm 0.05) \text{cm}^{-1}$ . Third, the penetration depth of the  $514.532 \text{nm}$  excitation laser light for the underlying Si is very small (approximately  $< 300 \text{nm}$ ), ensuring a high sensitivity to strain at the Si surface close to the  $n$ -GaN/AlN/ $n$ -Si(111) interface. Fourth, we established that this shift is not induced by a thermal effect, because heating of the Si surface would shift the phonon frequency in the opposite direction. Therefore, the experimental observation of this shift, as small as  $(0.27 \pm 0.05) \text{cm}^{-1}$ , immediately indicates that the silicon surface itself at the  $n$ -GaN/AlN/ $n$ -Si(111) interface really changed by the nitride growth pro-

cess. What is more interesting is that this change is caused by only very thin AlN and GaN layers with thicknesses of 5 and 370 nm, respectively. We attribute this blueshift of the Si optical-phonon line to a biaxial compressive strain of the silicon surface at the  $n$ -GaN/AlN/ $n$ -Si(111) heterointerface due to the large mismatch in lattice constants and thermal-expansion coefficients of GaN, AlN, and Si. Furthermore, we were able to determine the precise value of the  $E_2$  optical-phonon mode at  $565.43 \pm 0.05 \text{cm}^{-1}$  for the GaN layer. This experimental value is given in Table I. Also shown in Table I are the results of recently performed Raman-scattering investigations of strain-related phenomena in GaN thin layers grown by different techniques and on various substrates.<sup>5-15</sup>

Our value for the  $E_2$  optical-phonon mode at  $565.43 \pm 0.05 \text{cm}^{-1}$  is lower than the room-temperature values of the bulk and homoepitaxial GaN layers. The observed frequency of the  $E_2$  optical-phonon mode is also lower than that of others. This is true excluding the special case<sup>9</sup> of  $551.8 \pm 0.2 \text{cm}^{-1}$  for the  $E_2$  optical-phonon mode of the Ga <sup>15</sup>N layer grown on  $c$ -axis-oriented sapphire by MBE with isotopically pure nitrogen (0.5% <sup>14</sup>N, 95.5% <sup>15</sup>N) and natural Ga: GaN layers grown with natural gallium and natural nitrogen<sup>9</sup> (99.6345% <sup>14</sup>N, 0.3666% <sup>15</sup>N) exhibit the same line at  $569.2 \pm 0.2 \text{cm}^{-1}$ . The significant negative frequency shift of  $(17.4 \pm 0.2) \text{cm}^{-1}$  has an other origin and mainly is induced by the almost full isotope shift due to reduced-mass behavior.<sup>9</sup> The negative frequency shift for the  $E_2$  optical-phonon mode which we observed for our  $n$ -GaN/AlN/ $n$ -Si(111) heterostructure in comparison to bulk GaN<sup>2</sup> is  $2.57 \pm 0.05 \text{cm}^{-1}$ . The difference is remarkable. It is important to note that the frequency for this nonpolar  $E_2$  optical-phonon mode does not depend on the direction of phonon propagation relative to the optical  $c$  axis due to the lack of the anisotropy of the long-range Coulomb contribution. Consequently, the observed shift could not possibly be explained by a small misalignment of the sample during our measurements. Neither could it be attributed to laser heating, since the  $n$ -GaN layer is transparent, nor to the underlying and absorbing Si surface for which we have shown above that the thermal heating by the incident laser beam is also excluded.



At the same time, the corresponding shift for GaN layers grown on sapphire in contrast to our case is positive and ranges from 0.5 to 4.0  $\text{cm}^{-1}$  indicating a compressive strain for these gallium nitride layers. We attribute the negative sign of the shift to the tensile deformation of GaN layer.

These results underscore the importance of the observed phonon line-shape analysis and highly accurate measurements of the frequency shifts. To check the homogeneity of the GaN layer as well as possible in-plane inhomogeneity of the strain field, we have performed several measurements at different points of the sample with a step of  $\sim 0.5$  mm. All these data revealed the same value of the shifts for both Si and GaN phonon lines indicating a high homogeneity of strain distributions. Furthermore, the observation of the low level background scattering is also an indirect indication of the relatively flat and featureless surface morphology of the grown GaN layer.

Due to the large lattice mismatch and mismatch of thermal-expansion coefficients of GaN and AlN with respect to Si, GaN starts to grow commensurate until a critical thickness is reached. The room temperature (RT) lattice constants for GaN (Ref. 24) are  $a = 3.1890$ ,  $c = 5.1864$  and AlN 3.104, 4.966 Å, respectively, and for Si it is 5.4301 Å. The RT thermal-expansion coefficients for GaN are  $\alpha = 5.59$ ,  $c = 3.17$ , AlN 4.2 for  $a$ , 5.3 for  $c$ , ( $\times 10^{-6}/\text{K}$ ), respectively, and for Si it is  $3.59 \times 10^{-6}/\text{K}$ . In the elastic model for GaN grown on AlN, the critical thickness was estimated<sup>25</sup> as  $\sim 3$  nm. For pseudomorphically grown GaN layers with a thickness close to the critical thickness, strain fields due to the mismatch in lattice constants and thermal-expansion coefficients of GaN, AlN, and Si can be accommodated through a large local deformation of the crystalline lattice at the interfaces. When the thickness is beyond the critical thickness, the generation of misfit dislocations becomes energetically favorable, releasing the strain generated at the interfaces and inducing a lattice relaxation with possible breaking up of the epilayers. However, in our Raman measurements we still detect a residual built-in strain. The value of the residual strain may be changed by the growth of GaN layers with different thicknesses. The presence of such a strain in heterostructures can induce changes in the optical and electrical properties, providing a new degree of freedom in the device design. Knowledge about strain fields between gallium nitride layers and substrates is important. For example, some theoretical predictions show that the optical gain or threshold current density in a nitride-based laser can be slightly reduced by introducing anisotropic strain in the  $c$  plane of GaN.<sup>26</sup>

Since many of the performance parameters of devices are determined by the lattice defect structure, it is useful to know how they are affected by deformation fields. In this vein, we see that the effect of these strain fields on the optical phonons in different types of layers is very different. The biaxial strain character at the  $n$ -GaN/AlN/ $n$ -Si(111) hetero-interface alternates from compressive for the Si surface to the tensile for the GaN layer. Therefore, the effective strain value at the interface is relatively small providing structural stability.

Generally, the strain dependence of the frequency shift of the optical-phonon modes in semiconductors is given in terms of the phonon deformation potentials.<sup>27</sup> The phonon frequency shifts depend also on modification of bond length

and bond angles.<sup>28</sup> Because of the lattice distortion of the GaN layer and Si surface due to the strain field, the average bond lengths are no longer equal to the natural bond lengths of unstrained GaN and Si. The bond-length difference depends on the fractional strain contributions. Our data show that the strain-induced frequency shift of the GaN vibrational mode is greater than that for the Si. This fact partially indicates that the variation of the Ga-N bond length caused by the residual strain is larger than that for Si-Si.

The lack of inversion symmetry in a wurtzite-structure semiconductor, such as GaN, leads to spontaneous polarization and results in internal built-in strong electric fields along the growth direction because of the strong piezoelectric properties of these materials. The effect of these electric fields has recently been considered.<sup>29-31</sup> These electric fields are reduced to a different extent by various types of defect formation and should be taken into account in the analysis of experimental data and appropriate applications of external electric fields. This point should be highly emphasized in designing GaN/Si-based device structures

#### IV. CONCLUSIONS

In summary, we have shown that strain fields play an important role in the formation of high-crystalline quality  $n$ -GaN/AlN/ $n$ -Si(111) heterostructures. We have performed precise frequency measurements of the first-order Raman-scattering spectra from thin 370-nm gallium nitride layer grown by MBE on  $n$ -Si(111)-oriented conductive substrate by using an optimized AlN buffer. It was found that the observation of the optical-phonon line at  $565.43 \text{ cm}^{-1}$ , which we attributed to the high-frequency nonpolar optical-phonon  $E_2(\Gamma)$  mode, indicates that the grown GaN layer possesses wurtzite structure. No evidence of the cubic GaN zinc-blende structure was observed. Furthermore, the obtained experimental data demonstrate the complex nature of the strain distribution at the  $n$ -GaN/AlN/ $n$ -Si(111) interface. The negative frequency shift for the  $E_2$  optical-phonon mode that we observed for our  $n$ -GaN/AlN/ $n$ -Si(111) heterostructure in comparison to the bulk GaN is  $(2.57 \pm 0.05) \text{ cm}^{-1}$ . In contrast, the triply degenerated phonon mode of Si exhibits a positive shift as small as  $(0.27 \pm 0.05) \text{ cm}^{-1}$  in comparison to that for the free standing Si substrate. We show that the epitaxial growth of the thin GaN layer induces changes on both sides of the  $n$ -GaN/AlN/ $n$ -Si interface: the GaN layer itself exhibits biaxial tensile strain, while the Si surface at the interface is under biaxial compressive strain. Such an unexpected behavior of the substrate surface to the substrate-thin-layer interface seems to be a common problem for heterostructures for various growth techniques used including MBE growth.

#### ACKNOWLEDGMENTS

This work was supported in part by the Deutsche Forschungsgemeinschaft (DFG) at the TU Bergakademie Freiberg, and by the Air Force Office of Scientific Research and Office of Naval Research at the VCU. B.H.B. gratefully acknowledges financial support from the DFG and the hospitality of the TU Bergakademie Freiberg, and VCU.

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