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Piezoelectric coefficient of aluminum nitride and gallium nitride

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The piezoelectric coefficient d_{33} of aluminum nitride (AlN) and gallium nitride (GaN) thin films grown on silicon substrates by molecular beam epitaxy have been measured using a laser interferometer. X-ray diffraction reveals that the AlN and GaN films consist mainly of crystals with a hexagonal wurtzite structure. In order to grow epitaxial GaN films, an AlN film was first deposited on silicon as the buffer layer, so the d_{33} measurement for GaN was actually performed on GaN/AlN/Si multilayer systems. The relative permittivity and electrical resistivity of each constituent layer of the film and the potential drop across each layer were determined as a function of frequency. The potential drops were then used to calculate the piezoelectric coefficient d_{33} of GaN. After correcting for substrate clamping, d_{33} of AlN and GaN were found to be (5.1 ± 0.1) and (3.1 ± 0.1) pm V^{-1}, respectively. © *2000 American Institute of Physics.* [S0021-8979(00)07722-7]

INTRODUCTION

Recent advances in film growth technology for III–V nitrides have led to a rapid development in devices based on aluminum nitride (AlN) and gallium nitride (GaN). These devices include blue-green lasers,[1] light emitting diodes,[2] ultraviolet photodetectors,[3] AlGaN/GaN heterostructure field effect transistors,[4,5] and AlN bulk acoustic wave devices.[6] AlN and GaN usually grow in the [0001] direction (when they have the hexagonal wurtzite crystal structure) or in the [111] direction (when they have the cubic zinc-blende structure). These are polar axes, hence, AlN and GaN exhibit piezoelectric properties. As these nitride films can withstand high temperatures, they are uniquely suited for applications in high temperature piezoelectric and acoustic devices. The physical properties of GaN films prepared by various methods have been reported.[7] However, there appears to be limited data on the piezoelectric coefficients of GaN,[8] especially for composite films of GaN on AlN buffer layers deposited on silicon substrates. As both AlN and GaN are piezoelectric, the AlN buffer layer will enhance the piezoelectric properties of the GaN film when the composite film is used as a strained piezoelectric layer in a semiconductor–insulator–semiconductor structure.[4] In this study, a laser interferometer is used to measure the piezoelectric coefficient d_{33} of a wurtzite GaN film on an AlN buffer layer. The effect of substrate clamping on the measured coefficient is discussed.

AlN AND GaN FILMS GROWN BY MOLECULAR BEAM EPITAXY

AlN films were deposited on Si(111) substrates in a molecular beam epitaxy (MBE) system (SVTA BLT-N35 MBE system). Before deposition, the silicon substrate was cleaned by ultrasonic degreasing and etched in buffered HF to remove the oxides on the surface. After thermally cleaning the substrate at 940 °C for 1 h, the temperature was decreased to 600 °C and a 450-nm-thick AlN film was deposited at a rate of 0.6 μm h^{-1}.

GaN/AlN/Si(111) and GaN/AlN/Si(100) films grown by MBE were supplied by SVT, USA. The GaN film and AlN buffer layer have thicknesses of 140 and and 30 nm, respectively.

CHARACTERIZATION OF THE NITRIDE FILMS BY X-RAY DIFFRACTION

Since GaN has two polymorphs, the cubic (zinc-blende) and the hexagonal (wurtzite) structures, which have different piezoelectric coefficients, it is important to identify the structure of the nitride films. Our previous x-ray diffraction measurements[9] showed that the GaN layer in both the GaN/AlN/Si(100) and GaN/AlN/Si(110) systems consisted largely of hexagonal crystals with the *c*-axis oriented along the normal of the substrate. Tsuchiya *et al.*[10] suggested that the ratio of zinc-blende to wurtzite structure in a GaN sample could be estimated from the ratio of the integrated x-ray diffraction intensities of the cubic (001) and the hexagonal $(10\bar{1}1)$ planes measured by ω scans. In a θ–2θ scan, the positions of the diffraction peaks associated with the cubic (111) plane

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(at $\theta = 17.2°$) and hexagonal (0002) plane (at $\theta = 17.3°$) are almost identical, so it is difficult to tell whether the peak is associated with the cubic or hexagonal phase. If the sample is cubic, an additional peak associated with the cubic (001) plane will be found at a tilt angle of 54.7°.[10] For the hexagonal phase, the $(10\bar{1}1)$ peak will appear at a different tilt angle of 61.9°. Hence, by locating diffraction peaks at different tilt angles, we can identify the two phases. If both the cubic and hexagonal phases co-exist in the sample, intensity measurements can be made by ω scans at both tilt angles (54.7° and 61.9°) and the ratio of the two phases can be determined from the ratio of the integrated intensities. Using this method, it was found that the AlN and the GaN/AlN/Si(100) films have a purely hexagonal structure while the GaN/AlN/Si(111) film contains ~2% of the cubic phase.

ELECTRICAL RESISTIVITY AND DIELECTRIC PERMITTIVITY OF AlN AND GaN

In a piezoelectric material with hexagonal symmetry, the piezoelectric coefficient d_{33} can be defined via the converse piezoelectric effect as

$$d_{33} = \frac{\text{strain}}{\text{electric field intensity}} = \frac{\frac{u}{t}}{\frac{V}{t}} = \frac{u}{V}, \tag{1}$$

where u is the displacement induced by an applied voltage V and t is the thickness of the film. In a multilayer sample, irrespective of whether the layer is piezoelectric, there is a potential drop V_n across each layer which is determined by the resistance R and capacitance C of the layer. In addition, if more than one of them are piezoelectric, the measured displacement will be the sum of the displacements induced in all the layers

$$u = \sum_n u_n = \sum_n d_{33}^n V_n, \tag{2}$$

where u_n is the displacement induced in layer n and d_{33}^n is the piezoelectric coefficient of layer n. Hence, it is necessary to determine the R_n and C_n of each layer in order to calculate the piezoelectric coefficients.

Assume that each layer of the sample consists of a resistance R_n and a capacitance C_n in parallel. The impedance, $Z = \mathrm{Re}\,Z + \mathrm{Im}\,Z$, of the multilayer sample is given by

$$\mathrm{Re}\,Z = \sum_n \mathrm{Re}\,Z_n = \sum_n \frac{\frac{1}{R_n}}{(\omega C_n)^2 + \left(\frac{1}{R_n}\right)^2}, \tag{3}$$

$$\mathrm{Im}\,Z = \sum_n \mathrm{Im}\,Z_n = \sum_n \frac{-\omega C_n}{(\omega C_n)^2 + \left(\frac{1}{R_n}\right)^2}, \tag{4}$$

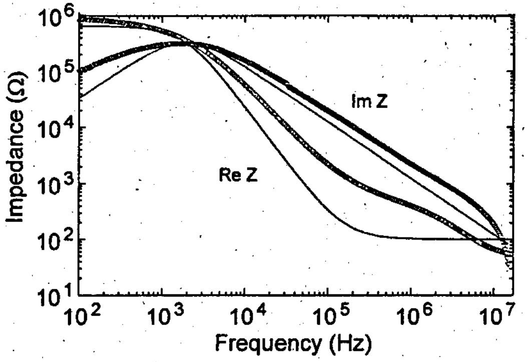

FIG. 1. Measured and calculated impedance curves for the AlN/Si(111) sample. The symbols Δ and ∇ represent Re(Z) and Im(Z), respectively. The lines are theoretical curves calculated according to Eqs. (3) and (4).

where ω is the angular frequency. If there is only one layer [setting $n=1$ in Eqs. (3) and (4)] the resonance frequency $f_r (= \omega_r / 2\pi)$ can be found by setting $d[\mathrm{Im}(Z)]/d\omega$ to 0. This gives

$$f_r = \frac{1}{2\pi RC}. \tag{5}$$

Substitution of Eq. (5) into Eq. (4) gives

$$[\mathrm{Im}\,Z]_{f=f_r} = \frac{R}{2}. \tag{6}$$

Al electrodes of diameter 1 mm were thermally evaporated onto the top surface of the films. A HP 4194A impedance analyzer was used to measure $\mathrm{Re}\,Z$ and $\mathrm{Im}\,Z$ of the samples as functions of frequency f from 100 Hz to 15 MHz. The real and imaginary parts of the impedance of the AlN/Si sample are shown in Fig. 1. The capacitance of the Si substrate is assumed to be negligibly small, so the equivalent circuit of AlN/Si consists of the resistance of Si in series with the AlN equivalent RC circuit. The resistance of the Si(111) substrate is ~100 Ω which is estimated from the value of $\mathrm{Re}\,Z$ at $f \sim 10^7$ Hz. Putting the observed frequency and $\mathrm{Im}\,Z$ at resonance into Eqs. (5) and (6), the R and C values of the AlN film were calculated to be 634 kΩ and 130 pF, respectively. To check the validity of this calculation, the R and C values are inserted into Eqs. (3) and (4) to give the theoretical $\mathrm{Re}\,Z$ and $\mathrm{Im}\,Z$ vs f curve. It is seen from Fig. 1 that reasonable agreement between the experimental and calculated values is obtained. From the R and C values and the geometrical factors, the electrical resistivity ρ and relative permittivity ϵ_r of the AlN film are calculated and shown in Table I.

As an example of the multilayer samples, the real and imaginary parts of the impedance of GaN/AlN/Si(100) are shown in Fig. 2. Again, the resistance of the Si substrate is estimated from the value of $\mathrm{Re}\,Z$ at about 10^7 Hz. The R and C values of the 30-nm-thick AlN layer are calculated from the known resistivity and permittivity and then $\mathrm{Re}\,Z$ and $\mathrm{Im}\,Z$ of this layer are calculated according to Eqs. (3) and (4). The $\mathrm{Re}\,Z$ and $\mathrm{Im}\,Z$ values of the 140-nm-thick GaN layer can then be obtained by subtracting the above estimated values for the AlN and Si layers from the observed $\mathrm{Re}\,Z$ and

TABLE I. The resistance R, capacitance C, resistivity ρ, and relative permittivity ϵ_r for different samples. t is the thickness of the layer.

Sample	Layer	R (Ω)	C (pF)	ρ (Ω m)	ϵ_r	t
AlN on Si(111)	AlN	634×10^3	130	1.1×10^6	8.42	450 nm
	Si	100	0	0.26	3.7	0.3 mm
GaN/AlN on Si(111)	GaN	218×10^3	442	1.2×10^6	8.9	140 nm
	Si	300	0	0.785	3.7	0.3 mm
GaN/AlN on Si(100)	GaN	804×10^3	446	4.5×10^6	8.99	140 nm
	Si	400	0	1.05	3.7	0.3 mm

Im Z for the multilayer sample. From the peak value of Im Z and the frequency at peak for the GaN layer, the R and C values are calculated and given in Table I. The experimentally determined R and C values are then inserted into Eqs. (3) and (4) to give the theoretical Re Z and Im Z vs f curves, and it is seen from Fig. 2 that they compare well with the measured curves.

It should be noted that Im Z of the multilayer sample is dominated by the contribution of the GaN layer. With the R and C values known, the impedance value and hence the potential drop in each layer can be calculated. The magnitude of the potential drop in the GaN layer amounts to about 82% of the voltage applied to the multilayer sample.

MEASUREMENT OF THE PIEZOELECTRIC COEFFICIENTS BY OPTICAL INTERFEROMETRY

A Mach–Zehnder interferometer[11] (SH120 manufactured by B.M. Industry, France) was used to measure the surface displacement u induced in the piezoelectric sample by an applied ac field. In the experimental setup shown in Fig. 3, the voltage applied to the sample was measured by an oscilloscope with a 50 Ω termination. Initial checking of the setup was carried out using a z-cut lithium niobate crystal with dimensions 14.8 mm×7.2 mm×0.8 mm. The d_{33} coefficient of $LiNbO_3$ was measured as a function of frequency from 5 kHz to 1.4 MHz. The observed value of $d_{33}=9.61\pm0.1\,\mathrm{pm\,V^{-1}}$ agrees very well with the reported value[11] of $9.55\,\mathrm{pm\,V^{-1}}$.

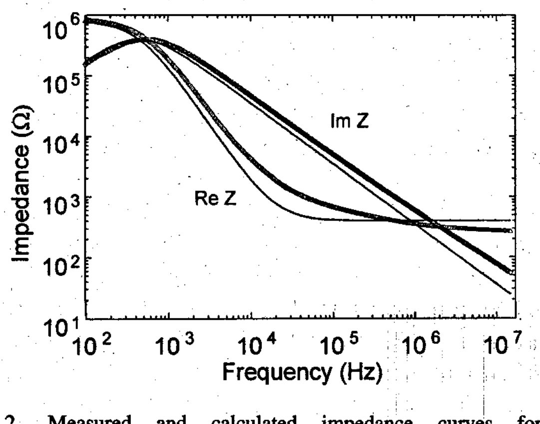

FIG. 2. Measured and calculated impedance curves for the GaN/AlN/Si(100) sample. The symbols Δ and ∇ represent Re(Z) and Im(Z), respectively. The lines are theoretical curves calculated according to Eqs. (3) and (4).

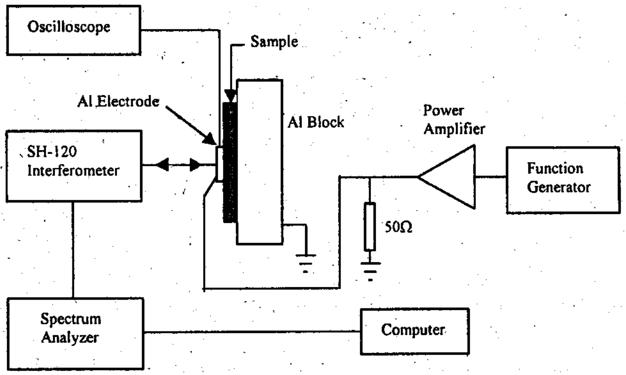

FIG. 3. Experimental setup for the measurement of the displacement induced by an electric field.

To eliminate the effect of substrate bending, a small Al top electrode (diameter 1 mm) was used in the displacement measurement. This small Al electrode also served as a mirror to reflect the probe beam from the interferometer (Fig. 3). It was found that our samples exhibited resonance in the range of 50–100 kHz, so the d_{33} measurements were performed at 10 kHz. The variations of the measured displacement with applied voltage at 10 kHz for AlN/Si(111) and GaN/AlN/Si(111) are shown in Fig. 4. Although not shown, the displacement vs voltage curve for GaN/AlN/Si(100) is very similar to that for GaN/AlN/Si(111). From the slope of these lines, it was found that $d_{33}=(3.9\pm0.1)\,\mathrm{pm\,V^{-1}}$ for AlN on Si(111) and $d_{33}=(2.65\pm0.1)\,\mathrm{pm\,V^{-1}}$ for both GaN/AlN/Si(100) and GaN/AlN/Si(111) composite films.

Since AlN is also piezoelectric, the displacement u induced in the composite film is actually the resultant displacements of the two layers. By putting $d_{33}=3.9\,\mathrm{pm\,V^{-1}}$ for the AlN layer and the known potential drop across each of the two layers in Eq. (2), the d_{33} coefficient of the GaN layer in both of the composite films was found to be $(2.38\pm0.1)\,\mathrm{pm\,V^{-1}}$. Within experimental error, the existence of the 2% zinc-blende structure in the GaN layer of GaN/AlN/Si(111) does not seem to affect the piezoelectric coefficient.

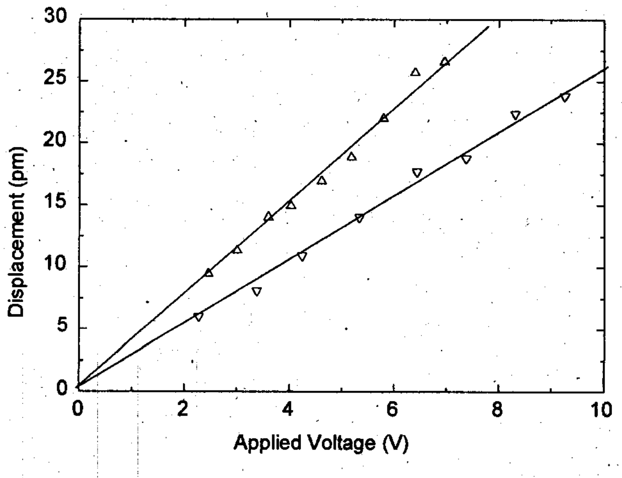

FIG. 4. Displacement as a function of applied voltage at 10 kHz. The symbols Δ and ∇ represent displacements of AlN/Si(111) and GaN/AlN/Si(111), respectively. The lines are least-square fits to the data.

TABLE II. Values of piezoelectric coefficient d_{33} (in pm V^{-1}) for AlN film after correcting for substrate clamping. The compliance values (in $10^{-12}\,\mathrm{m}^2\,\mathrm{N}^{-1}$) used in the calculations are also included.

References	s_{11}^E	s_{12}^E	s_{13}^E	d_{33}
Tsubouchi *et al.*(a)	3.5	−1.0	−0.8	5.1
McNeil *et al.*(b)	2.9	−0.9	−0.5	4.9
Ruiz *et al.*(c)	2.5	−0.7	−0.5	5.0
Wright(d)	3.0	−0.9	−0.6	5.1

(a)See Ref. 12. Compliances calculated from surface acoustic wave phase velocity.

(b)See Ref. 13. Compliances measured by Brillouin scattering.

(c)See Ref. 14. Compliances calculated using the Hartree-Fock theory.

(d)See Ref. 15. Compliances calculated using the plane-wave pseudopotential method.

SUBSTRATE CLAMPING EFFECT

As the AlN and GaN films are deposited on silicon substrates, they are clamped by the substrates. The substrates constrain their expansions and contractions and thus affect the measured strains. As a result, the measured value of d_{33} is less than the true value of an unclamped sample. If one assumes that the thin film is clamped by a substrate such that its lateral strain is 0, then the following relation holds[11]

$$d_{33}=d_{33}'-2\left(\frac{d_{31}'s_{13}^E}{s_{11}^E+s_{12}^E}\right), \tag{7}$$

where d_{33} is the coefficient measured using the laser interferometer, d_{33}' and d_{31}' are the coefficients for an unclamped sample and s_{pq}^E are the elastic compliances of the sample. As seen from Eq. (7), the true coefficient d_{33}' differs from the apparent coefficient by a corrective factor (the second term).

In order to use the earlier equation, the elastic compliances of AlN and GaN are required. The theoretical and experimental compliance data for AlN and GaN are compiled from the literature and are given in Tables II and III. Using these data, and assuming that $d_{31}' \cong -d_{33}'/2$, d_{33} is calculated and shown in Table II and III. It is seen that although there are different sets of reported compliances, the corrected piezoelectric coefficients based on these data are quite similar. By choosing the sets of data reported by Tsubouchi *et al.*[12] and Wright,[15] the corrected d_{33} value for AlN is $(5.1\pm0.1)\,\mathrm{pm\,V^{-1}}$. For GaN, if the more recent data of Takagi *et al.*[18] and Wright[15] are used, the corrected d_{33} value is $3.1\pm0.1\,\mathrm{pm\,V^{-1}}$.

TABLE III. Values of piezoelectric coefficient d_{33} (in pm V^{-1}) for GaN film after correcting for substrate clamping. The compliance values (in $10^{-12}\,\mathrm{m}^2\,\mathrm{N}^{-1}$) used in the calculations are also included.

References	s_{11}^E	s_{12}^E	s_{13}^E	d_{33}
Sheleg *et al.*(a)	5.1	−0.9	−2.5	4.0
Polian *et al.*(b)	2.6	−1.0	−0.6	3.6
Takagi *et al.*(b)	3.5	−0.9	−0.5	3.0
Wright(c)	3.3	−1.0	−0.6	3.2

(a)See Ref. 16. Compliance obtained from x-ray diffraction measurements.

(b)See Refs. 17 and 18. Compliances measured by Brillouin scattering.

(c)See Ref. 15. Compliances calculated using the plane-wave pseudopotential method.

CONCLUSIONS AND DISCUSSION

A single beam heterodyne Mach–Zehnder interferometer has been used to measure the displacements induced in AlN and GaN deposited on Si substrates. The voltage drop across each layer in a GaN/AlN/Si composite film is evaluated as a function of frequency and used to calculate the piezoelectric coefficients. The values of the unclamped d_{33} coefficients for AlN and GaN are found to be 5.1 and 3.1 pm V^{-1}, respectively. The d_{33} value for GaN is slightly higher than that of epitaxial GaN prepared by chemical vapor deposition.[8]

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[1] S. Nakamura, M. Senoh, S. Nagahama, N. Iwasa, T. Yamada, T. Matsushita, H. Kiyoku, and Y. Sugimoto, Jpn. J. Appl. Phys., Part 2 **35**, L74 (1996).
[2] S. Nakamura, T. Mukai, and M. Senoh, J. Appl. Phys. **76**, 8189 (1994).
[3] M. Razeghi and A. Rogalski, J. Appl. Phys. **79**, 7433 (1996).
[4] A. Bykhovski, B. Gelmont, and M. Shur, J. Appl. Phys. **77**, 1616 (1995).
[5] R. Gaska, J. Yang, A. Osinsky, A. D. Byhovski, and M. S. Shur, Appl. Phys. Lett. **71**, 3673 (1997).
[6] M. Dubois, P. Muralt, and L. Sagalowicz, Ferroelectrics **224**, 243 (1999).
[7] S. Strite and H. Morkoc, J. Vac. Sci. Technol. B **10**, 1237 (1992).
[8] S. Muensit and I. L. Guy, Appl. Phys. Lett. **59**, 1896 (1998).
[9] C. M. Lueng, H. L. W. Chan, C. Surya, W. K. Fong, C. L. Choy, P. Chow, and R. Rosamond, J. Non-Cryst. Solids **254**, 123 (1999).
[10] H. Tsuchiya, K. Sunaba, S. Yonemura, T. Suemasu, and F. Hasegawa, Jpn. J. Appl. Phys., Part 2 **36**, L1 (1997).
[11] D. Royer and V. Kmetik, Electron. Lett. **28**, 1828 (1992).
[12] K. Tsubouchi, K. Sugai, and N. Mikoshiba, *Proc. IEEE Ultrason. Symp.* (IEEE, New York, 1981), p. 375.
[13] L. E. McNeil, M. Grimsditch, and R. H. Trench, J. Am. Ceram. Soc. **76**, 1132 (1993).
[14] E. Ruiz, S. Alvarez, and P. Alemany, Phys. Rev. B **49**, 5188 (1994).
[15] A. F. Wright, J. Appl. Phys. **82**, 2833 (1997).
[16] A. U. Sheleg and V. A. Savastenko, Izv. Akad. Nauk SSSR, Neorg. Mater. **15**, 1598 (1979).
[17] A. Polian, M. Grimsditch, and I. Grzegory, J. Appl. Phys. **79**, 3343 (1996).
[18] Y. Takagi, M. Ahart, T. Azuhata, T. Sota, K. Suzuki, and S. Nakamura, Physica B **219&220**, 547 (1996).