The temperature dependence of the refractive indices of GaN and AlN from room temperature up to 515 °C

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The temperature dependence of the refractive indices of GaN and AlN was investigated in the wavelength range from the near band edge (367 nm for GaN and 217 nm for AlN) to 1000 nm and the temperature range from room temperature to 515 °C. Optical interference measurements with vertical incident configuration were employed to precisely evaluate the ordinary refractive indices.
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Wide band-gap group-III nitrides, gallium nitride (GaN) and aluminum nitride (AlN), have attracted much attention for optoelectronic devices in the green to ultraviolet region.[1–3] To optimize the design of optoelectronic devices, knowledge of the refractive indices of the constituent materials is required. In general, the refractive index of a material varies with temperature, a phenomenon known as the thermo-optic effect. Since the junction temperature of a GaN-based laser diode (LD) exceeds 100 °C,[4] failure to consider the thermo-optic effect would result in a suboptimal LD waveguide design. On the other hand, the thermo-optic effect can be used to actively modulate device characteristics by varying the temperature. For example, when an optical filter such as a distributed Bragg reflector (DBR) made of $Al_xGa_{1-x}N$ is combined with a GaN-based photodiode, the spectral response of the photodetector can be varied by controlling the DBR temperature. Thanks to its large band gap, GaN-based photodiodes are capable of operation at temperatures much higher than 400 °C.[5] Varying the temperature from room temperature to high temperature makes possible a widely variable range of detectable wavelength. It should be noted that a high power is not required to reach temperatures above 400 °C if the device has good thermal insulation, a small volume, and a monolithically integrated heater.

Tisch *et al.*[6] reported the refractive indices of GaN and aluminum gallium nitride ($Al_xGa_{1-x}N$) measured by spectroscopic ellipsometry from room temperature to 300 °C. While refractive index data up to 300 °C are adequate for LD design, extension of the data set to higher temperatures will be needed for other applications as mentioned above. In addition, one must also consider the optical anisotropy of GaN and AlN inherent to its crystal structure (wurtzite). Tisch *et al.*[6] did not separate the anisotropy. In this study, we measure the thermo-optic coefficients ($\partial n/\partial T$) of GaN and AlN by optical interference measurements. A vertical incident configuration was employed to evaluate the ordinary refractive index n_o (light propagating along the c axis). The temperature range of the measurements is from room temperature to 515 °C.

The samples used in this study were commercially available GaN layers grown on (0001)-oriented sapphire substrates by metal-organic vapor phase epitaxy and AlN layers grown on (0001)-oriented 6*H*-SiC substrates by hydride vapor phase epitaxy. 5.18 and 10.6 μm thick GaN layers and 9.23 μm thick AlN layers were used for the measurements. The layer thicknesses were determined by cross-sectional scanning electron microscopy using a magnification calibration standard. The error of the thickness measurement is less than 2%.

The interference spectrum was measured in air. A bundle of one optical fiber for light collection and surrounding six optical fibers for illumination was used as a specular reflection probe. The diameter of each fiber was 450 μm. The distance between the sample and the reflection probe is about 20 mm. The error of the wavelength was less than 0.2 nm for the UV region and 0.5 nm for visible region. The refractive index dispersion curve was calculated from the peak and valley wavelengths of the interference together with the layer thickness. For elevated temperatures the layer thickness change due to thermal expansion of both epilayers and substrates was taken into account. The employed parameters[7–9] are summarized in Table I. Since the strain state of epilayers depends on many factors, there should be an error in the estimation of the thickness change with temperature. However, even if we ignore the thermal expansion, the difference in the calculated thermo-optic coefficients is only 7%. There-

TABLE I. Parameters used in this study.

	Thermal expansion ($\times10^{-6}$ K^{-1})		
	a axis	c axis	Poisson's ratio
GaN	5.59[a]	3.17[a]	0.23[b]
AlN	4.2[a]	5.3[a]	0.287[a]
Sapphire	7.5[c]		
6*H*-SiC	4.3[a]		

[a]Reference 7.
[b]Reference 9.
[c]Reference 8.

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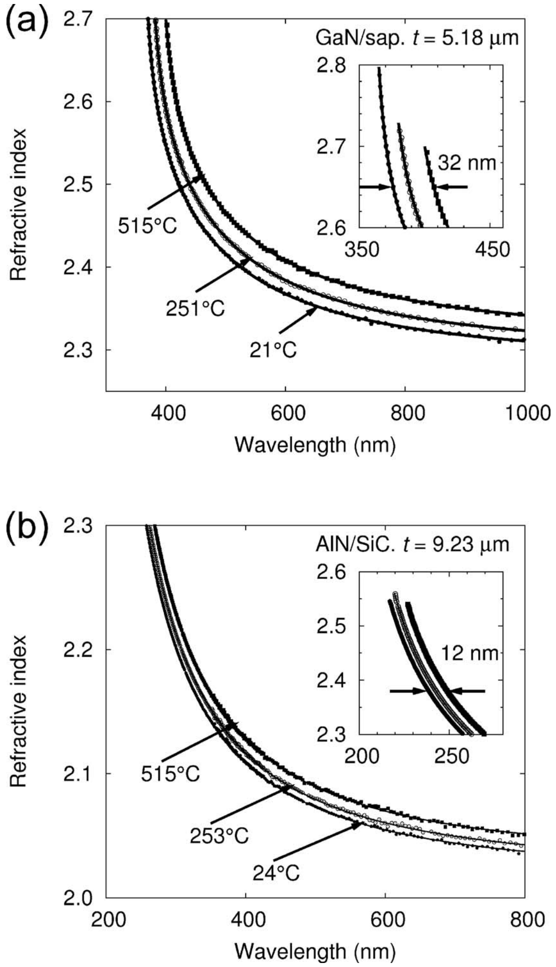

FIG. 1. Dispersion of the refractive indices of (a) GaN and (b) AlN at elevated temperatures. Solid lines are curve fits to the Sellmeier equation. Insets show the dispersion curves near the band gap.

fore the error of the thickness change may have a minor effect (much smaller than 7%). To perform high-temperature measurements with high uniformity and accuracy, the sample was set into a small copper chamber with a sapphire window. The temperature difference between the copper chamber block and the inside (atmosphere) of the chamber was confirmed to be less than 3 °C even at 500 °C.

Figure 1(a) shows the measured dispersion curves of the refractive index of 5.18 μm thick GaN at 21, 251, and 515 °C for the wavelength range from 367 to 1000 nm. Figure 1(b) shows the curves of 9.23 μm thick AlN for the wavelength range from 217 to 1000 nm. At room temperature, the measured curves for both GaN and AlN agreed with the reported dispersion curves of GaN (Refs. 10 and 11) and AlN,[12] respectively. In Fig. 1, the solid lines are curve fits using the second-order Sellmeier equation,[13]

$$n_o(\lambda)^2 = A_0 + \frac{A_1\lambda^2}{\lambda^2 - B_1^2} + \frac{A_2\lambda^2}{\lambda^2 - B_2^2}, \tag{1}$$

where A_0, A_1, A_2, B_1, and B_2 are the fitting parameters, and λ is the wavelength of light. Since a good fitting for the entire wavelength region was not obtained by the first-order Sellmeier equation, the second-order equation, Eq. (1), was used to express the refractive index dispersion.

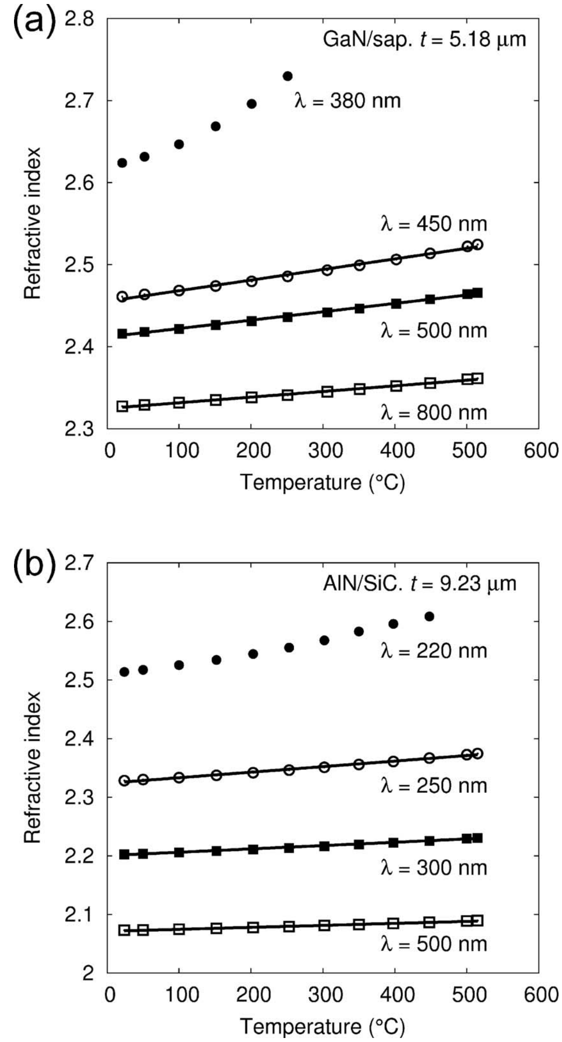

FIG. 2. The refractive indices of (a) GaN for 380, 450, 500, and 800 nm and (b) AlN for 220, 250, 300, and 500 nm as a function of temperature. Solid lines are linear fits.

The refractive indices of 5.18 μm thick GaN for 380, 450, 500, and 800 nm are plotted in Fig. 2(a) as a function of temperature. Figure 2(b) shows the refractive indices of 9.23 μm thick AlN for 220, 250, 300, and 500 nm. The refractive index increases almost linearly with increasing temperature up to 500 °C except for the near band-gap region (below 420 nm for GaN, 230 nm for AlN). Figure 3 shows the calculated thermo-optic coefficients for GaN and AlN. Since the thermo-optic coefficient is an inherent property of the material, the results should not be affected by the thickness of the sample. The good agreement (within 5% error) between the 10.6 μm thick GaN and 5.18 μm thick GaN implies an accurate and precise determination of the thermo-optic coefficient.

In the near band-edge region, the thermo-optic coefficients of both GaN and AlN increased sharply due to the redshift in the band gap with increasing temperature. Nepal *et al.*[14] reported the temperature dependence of the band gap for GaN and AlN grown on sapphire substrates. Based on this report, the redshifts from 21 to 515 °C are estimated to be 34 and 18 nm for GaN and AlN, respectively. For GaN, the shift of the dispersion curve of 32 nm, as shown in

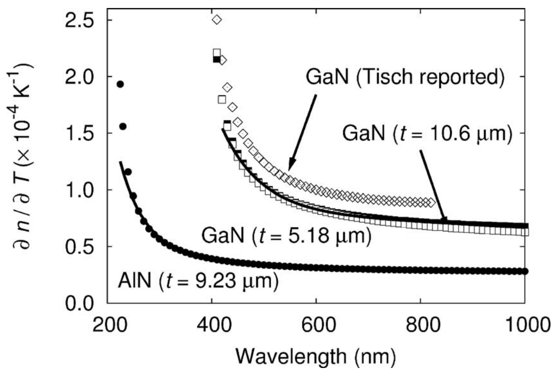

FIG. 3. Thermo-optic coefficients of GaN and AlN compared with reported data from Tisch *et al.* (Ref. 6). Solid lines are polynomial fits of the thermo-optic coefficients of GaN and AlN from Eqs. (2) and (3), respectively.

the inset of Fig. 1(a), is in good agreement with the result of Ref. 14. However, for AlN (12 versus 18 nm shift) the agreement is not as good. The difference may be related to different values of the built-in strain in AlN layers grown on different substrates. The AlN samples used in this study were grown on 6*H*-SiC, while sapphire substrates were used in Ref. 14.

Figure 3 also shows the thermo-optic coefficient of GaN reported by Tisch *et al.*[6] Over the entire wavelength range, their values of GaN are larger than the values determined in this work. The discrepancy might be attributed to the fact that Tisch *et al.*[6] did not separate the ordinary (n_o) and extraordinary (n_e) indices in their measurements, while we evaluated only the ordinary index. Assuming that the data in both reports are accurate, it can be deduced that the thermo-optic coefficient $\partial n_e/\partial T$ is larger than $\partial n_o/\partial T$ in GaN.

For the ranges from 450 to 1000 nm (GaN) and from 250 to 1000 nm (AlN), we obtained experimental polynomial fits of the thermo-optic coefficients as follows:

$$\partial n_o/\partial T(\lambda)_{\mathrm{GaN}} = 4.247 \times 10^4\lambda^{-3} - 1.592 \times 10^2\lambda^{-2} + 2.187 \times 10^{-1}\lambda^{-1} - 3.427 \times 10^{-5}\ (\mathrm{K}^{-1}), \tag{2}$$

$$\partial n_o/\partial T(\lambda)_{\mathrm{AlN}} = 3.486 \times 10^3\lambda^{-3} - 1.689 \times 10^1\lambda^{-2} + 3.245 \times 10^{-2}\lambda^{-1} + 8.361 \times 10^{-6}\ (\mathrm{K}^{-1}), \tag{3}$$

where the wavelength is expressed in nanometers. These formulas can be used for the design of optoelectronic devices in the below band-gap region.

In conclusion, we measured the temperature dependence of the refractive indices of GaN and AlN from room temperature to 515 °C over the spectral range from 1000 nm to wavelengths near the respective band gap of each material. The thermo-optic coefficients for ordinary refractive indices of GaN and AlN were determined over a wide temperature range. In future work, extraordinary index measurements will also be needed for complete characterization of the thermo-optic coefficients. The results obtained thus far are useful for the design of GaN-based optoelectronic devices as well as wavelength-tunable DBRs and photonic crystals actively utilizing the thermo-optic effect.

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