Temperature and composition dependence of the refractive index of AlGaN

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The wide band-gap III-V nitrides find application in visible to UV laser diodes, which can be operated at roo temperature (RT) without cooling. Under operating conditions, the temperature of the active layers and waveguides of these lasers is well above room temperature. Theref ore knowledge about the temperature dependence of the optical constants for the III-V nitrides is crucial for the optimization of laser implementation. GaN and AlGaN are the major components of such laser structures. A typical GaN based laser diode, lasing at 3eV, might incorporate a GaN waveguide, embedded into $Al_xGa_{1-x}N$ cladding layers. Hence, the refractive indices of GaN and AlGaN and their relative changes with temperature are of great technological importance. In this work, the temperature dependence *above room temperature* of the refractive indices of GaN and $Al_xGa_{1-x}N$ in the transparent spectral region is determined by spectroscopic ellipsometry (SE). The measured refractive index is presented as an analytical function of composition x and temperature T, for $0 \leq x \leq 0.65$ and $20^oC \leq T \leq 300^oC$.
Measurements have been conducted on nominally undoped hexagonal GaN and $Al_xGa_{1-x}N$ layers, deposited on c-plane sapphire by metal organic vapor phase epitaxy (MOVPE). The Al molar fraction x varied between 0 and 0.65. The c emical composition of the AlGaN samples was determined by energy dispersion spectroscopy (EDS) and the incorporation of the aluminum into the crystal lattice was confirmed by high resolution x -ray measurements. The band-gap of the AlGaN samples at RT was derived from optical transmission measurements and described by a phenomenological quadratic function of x. The temperature dependence of the GaN band-gap between RT and 300°C was investigated by photoluminescence (PL) measurements. In accordance with Brunner et al.[1] we assumed the same temperature dependence for AlGaN, and hence $E_g(x,T)$ could be obtained in closed analytical form as an independent input parameter for the analysis of the SE data. The root mean square surface roughness was determined by atomic force microscopy (AFM) and was found to be between 2 and 18 nm. SE measurements have been conducted in air over a spectral range from 1.5 eV up to just beyond the respective band gaps (3.42 eV 4.7 eV). In order to increase the reliability of our data, measurements have been taken at 2 - 3 angles of incidence. For all AlGaN samples, SE measurements were taken between RT and 307^{o}C at approximately equi-distant steps. Fig. 1 shows the ellipsometric spectra for GaN measured at temperatures between RT and 307^{o}C, at an angle of incidence of 72 °. The shift of the fundamental band edge towards lower energies can clearly be observed. Pronounced changes of the oscillation period can be observed in the vicinity of the band -gap, whereas in the region below 2 eV the periodicity is nearly unchanged. This is understood, since the strongest temperature dispersion of the refractive index is expected in the vicinity of the band gap. Qualitatively similar temperature shifts of the SE spectra have been observed for all AlGaN compositions. From the multi-angle SE data, the index of refraction for the transparent region has been derived using a four-layer model (substrate, buffer layer, AlGaN main layer and the surface roughness-overlayer). The temperature dependent dielectric function of $Al_xGa_{1-x}N$ below the fundamental band gap was described as:

$$\varepsilon(E,x,T) = C(x,T) + \frac{A(x,T)}{E_g^{1.5}(x,T)} \cdot \frac{2-\sqrt{1+y}-\sqrt{1-y}}{y^2} \qquad \text{wit } y = (E+i\Gamma)/E_g(x,T) \qquad (1)$$

$A(x,T)$ and Γ are the transition strength parameter the broadening of the fundamental transition respectively, and $C(x,T)$ takes into account the contributions from higher energy transitions. A regression analysis was applied to vary C, A, Γ, and layer thickness simultaneously until the measured values of the ellipsometric parameters matched the calculated ones as accurately as possible. For all AlGaN samples, excellent coincidence between measured and calculated ellipsometric spectra could be achieved. From the set of values for C and A for different compositions x and temperatures T we obtained simple polynomial expressions $C(x,T)$ and $A(x,T)$. Wit $C(x,T)$, $A(x,T)$ and $E_g(x,T)$, it is now possible to calculate the refractive index $n(E,x,T)$ of AlGaN as a simple function of photon energy, composition and temperature according to Eq. 1. Our analytical model for $n(E,x,T)$ can be used to predict reliably the refractive index in the transparent region for any $Al_xGa_{1-x}N$ composition between $x = 0$ and $x = 0.65$,

[1]D. Brunner, H. Angerer, B. Bustarret, F. Freudenberg, R. Hopler, R. Dimitrov, O. Ambacher and M. Stutzman; J. Appl. Phys. 82, p. 5090 (1997).

within a temperature range between RT and 307^{o}C. The proposed model is most reliable in the vicinity of the band gap, where the strongest thermal dispersion of the refractive index occurs.
On the basis of the proposed model, Fig. 2 illustrates simultaneously the influence of composition and temperature on the refractive index. For all compositions, the *n* increases with temperature and in accordance with the *T*-shift of the SE spectra, the changes become more pronounced in the vicinity of the band gap. On the other hand, the refractive index decreases with increase in the Al molar fraction *x*. These general trends agree with the expected physical behavior. The effect of compositional changes is much stronger than the T- shifts.

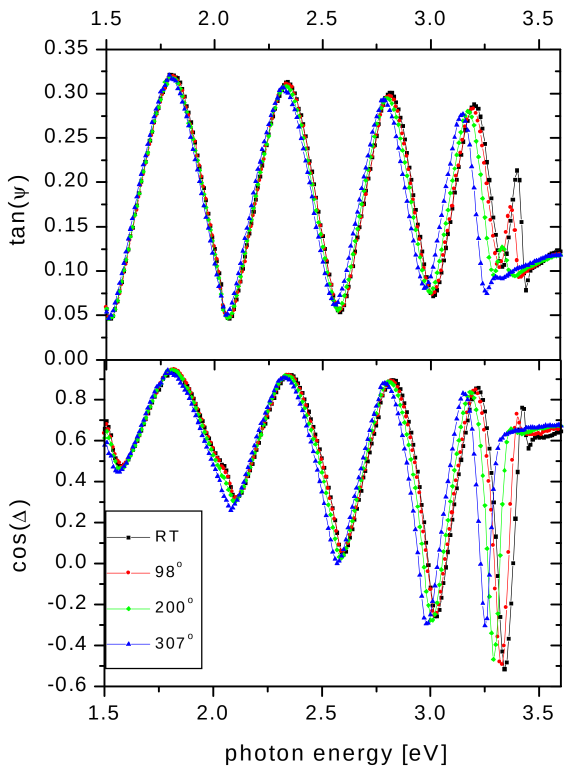

Fig. 1: *Spectra of the ellipsometric parameters tan(ψ) and cos(Δ) for GaN, taken at an angle of incidence of 72 temperatures between RT and 307^{o}C.*

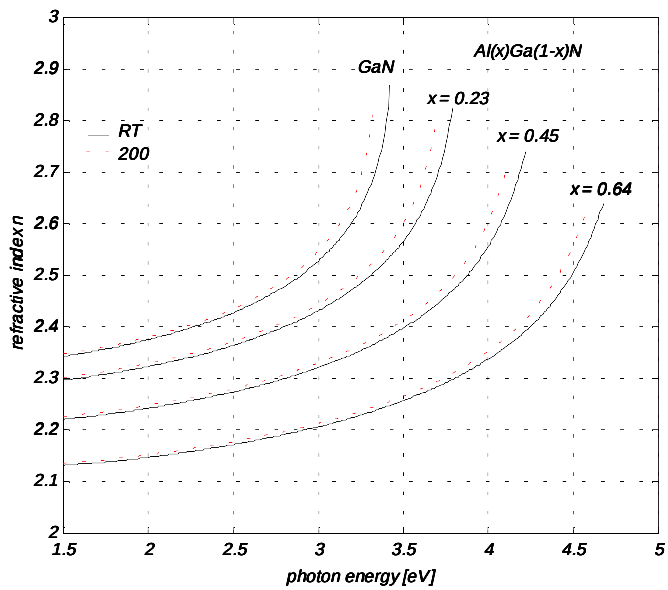

Fig. 2: *Calculated dispersion curves of the refractive index for several AlGaN compositions x at room temperature (solid lines) and at 200^{o}C (dashed lines).*

During operation, the temperature of active layer and waveguide of a typical GaN based laser diode can reach over 100^{o}C. Such temperature changes influence the waveguide properties. The difference between the refractive indices of GaN waveguide core and AlGaN cladding layers, *(n_{core} $n_{cladding}$)*, increases slightly with rising temperature. Thus also the modal volume depends on temperature. Practical examples will be discussed in the talk, in order to illustrate when this effect might be of technological significance. This is especially important for stable single mode performance.
The optical constants of GaN and AlGaN for the transparent region have been obtained with high accuracy by spectroscopic ellipsometry. Temperature and composition dependent dispersion relations were obtained in closed analytic form and enable us to make predictions about the optical properties of GaN based waveguides at elevated temperatures.