Microcavity effects in GaN epitaxial films and in Ag/GaN/sapphire structures

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Luminescence spectra of GaN epitaxial layers grown on sapphire display a strong intensity modulation of the below-band gap transitions and on the low-energy side of the near-band gap transition. The intensity modulation is attributed to a microcavity formed by the semiconductor–air and semiconductor–substrate interface. The microcavity effect is enhanced by using metallic reflectors which increase the cavity finesse. It is shown that microcavity effects can be used to determine the refractive index of the microcavity active material. Using this method, the GaN refractive index is determined and expressed analytically by a Sellmeir fit. © *1997 American Institute of Physics.* [S0003-6951(97)00421-X]

Microcavity effects in semiconductor optoelectronic devices have attracted much attention due to the potential of high-efficiency light-emitting diodes (LED), and low threshold lasers.[1] The enhancement of the spontaneous emission by microcavity effects has been demonstrated for resonant-cavity LEDs in organic[2] as well as semiconducting[3] material systems. High-finesse GaN microcavities with distributed Bragg reflectors were recently realized by Redwing *et al.*[4]

In the present study, the microcavity effects occurring in GaN epitaxial layers are analyzed and used for refractive index determination. Due to the refractive index step at the substrate–epilayer interface, the cavity effects are observed in GaN layers with a sufficiently small surface roughness.[5] By using metallic silver reflectors instead of the weakly reflecting semiconductor–air interface, the microcavity effects can be strongly enhanced. It is shown that the *near-band gap* transition of GaN is modulated on the low-energy shoulder only. In contrast, the entire band of *below-band gap* transitions are modulated. A new method is developed to determine the refractive index of the optically active material of microcavity structures. The usefulness of this method is demonstrated for GaN and the refractive index of GaN is expressed in analytic form by the Sellmeir equation.

The GaN epitaxial layers were grown on (0001) oriented sapphire in an Emcore metal-organic vapor phase epitaxy (MOVPE) system. An initial 200-Å-thick GaN buffer layer was grown at 500 °C after nitridation of the substrate. A homogenous 3-μm-thick Si-doped GaN epitaxial layer ($n = 2\times 10^{18}$ cm^{-3}) was grown at 1050 °C. After growth, the substrate was polished to allow for transmittance measurements. These measurements were performed using a broadband xenon light source. A polished sapphire substrate was used for reference measurements. The photoluminescence measurements were performed at room temperature with excitation by the 325 nm line of a HeCd laser. The very high luminescence intensity of the samples demonstrates the excellent quality and high radiative efficiency of the GaN epitaxial films. An excitation power density of 10 W/cm^2 on the sample surface was used. The luminescence was dispersed in a 0.75 nm monochromator and detected by a GaAs photomultiplier connected to phase-sensitive amplifier. The 2500-Å-thick silver (Ag) films were deposited on the GaN samples in a thermal evaporator.

The room temperature photoluminescence spectra of a sapphire/GaN/air cavity and a sapphire/GaN/Ag cavity are shown in Fig. 1. The spectra[6] show that the GaN emits light over a broad range of energies (1.8–3.6 eV). Inspection of the spectra reveals a strong near-band gap luminescence line at 3.4 eV. An additional emission band in the yellow spectral region is centered at 2.3 eV (Ref. 7) and a third weak band is centered 2.9 eV. The yellow emission band was recently proposed to be due to Ga vacancies.[8] The emission at 2.9 eV is probably caused by acceptor (Mg or Cd) impurities.[9]

Comparison of the room temperature photoluminescence (PL) spectra of the uncoated [curve (a) in Fig. 1] and the Ag-coated [curve (b) in Fig. 1] sample shows a more pronounced intensity modulation for the Ag-coated sample. The strong modulation is displayed in Fig. 2 which shows the luminescence spectra on a linear scale. This result is expected since the reflectivity of the GaN-air reflector, and thus the cavity finesse, is increased by the metallic reflector.

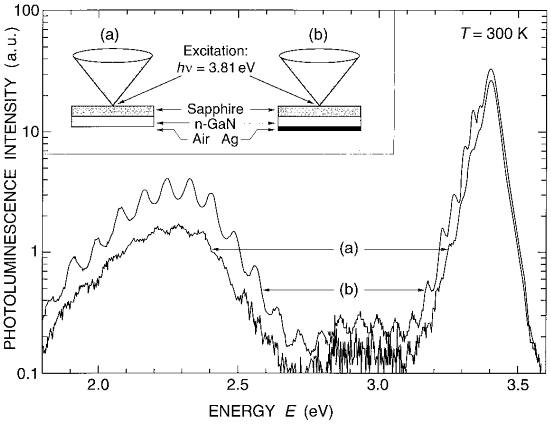

FIG. 1. Room-temperature photoluminescence spectra of epitaxial GaN on sapphire on a logarithmic scale. Spectrum (a) and (b) are for samples without and with silver coating, respectively. The sample geometry for spectrum (a) and (b) is shown in the inset.

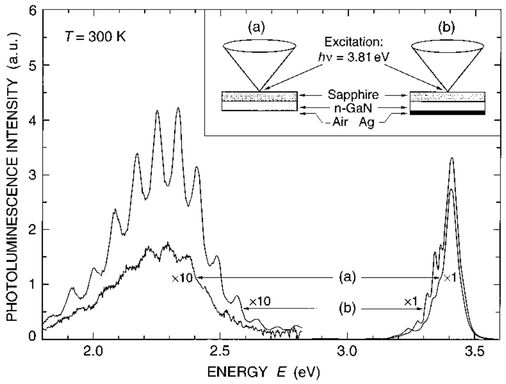

FIG. 2. Room-temperature photoluminescence spectra of epitaxial GaN on sapphire on a linear scale. Spectrum (a) and (b) are for samples without and with silver coating, respectively. The sample geometry for spectrum (a) and (b) are shown in the inset.

Note that the near-band gap photoluminescence exhibits intensity modulation only on the low energy side ($E < 3.35$ eV) but *not* on the high energy side. The lack of intensity modulation on the high energy side is evident from the spectra shown in Fig. 1 and in Fig. 3. Also shown in Fig. 3 is the transmittance spectrum of the sample not coated with the Ag reflector. Comparison of the luminescence peak energy with the transmittance spectrum indicates that the luminescence originates from a range of energies very close to the band gap energy. This further supports that the modulation is a microcavity effect: for higher energies, the absorption of the GaN causes quenching of the cavity finesse and the modulation of the luminescence is suppressed. Next it will be shown that microcavity effects can be used to determine the refractive index of the GaN active material.

Unlike other semiconductor systems, in which the refractive indices of the substrate and the epitaxial layer (n_1 and n_2 respectively) are similar, sapphire and GaN have different refractive indices [sapphire $n_1 = 1.78$ (Ref. 10); GaN $n_2 \approx 2.5$ (Ref. 11); air $n_3 = 1$]. The value of the Fresnel coefficient[12] for the GaN-sapphire and of the GaN/air interface is $|r_{12}| = |(n_1 - n_2)/(n_1 + n_2)| = 0.17$ and $|r_{23}| = 0.43$, respectively, which yields a round-trip reflectivity of $|r_{12}r_{23}| = 0.072$. The modulation amplitude is strongly enhanced throughout the visible and ultraviolet region by coating the GaN with silver. This is caused by the change of refractive index from air to Ag [$n_3 = 0.25 + 3.6i$ (Ref. 13)], which yields a higher cavity round trip reflectivity of $|r_{12}r_{23}| = 0.16$. In the spectral range of 2.25–2.32 eV, where the underlying, unmodulated luminescence band is flattest, the intensity ratio between maximum and adjacent minimum[14] changes from 1.26 to 1.53 for the uncoated and Ag-coated sample, respectively.

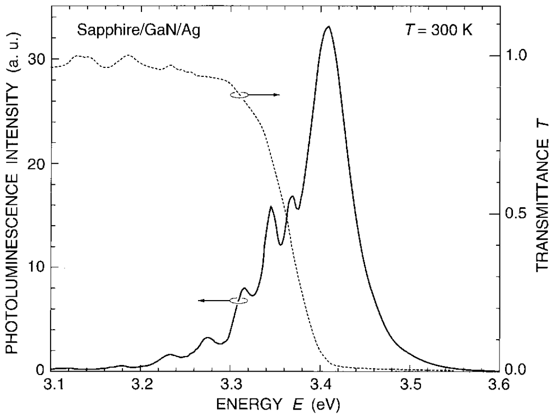

FIG. 3. Room-temperature spectra of the near band gap photoluminescence (solid line) and transmittance (dotted line).

The intensity ratio derived from the extrema in Fig. 1 can be compared quantitatively to the following model: light emitted in the GaN layer normal to the sample surface is partially reflected at each of the cavity interfaces. Summation over all partial waves emitted from one emitter and taking into account that other emitters located along the surface normal emit incoherently, yields the total intensity of cavity-modulated luminescence according to

$$I_{\mathrm{PL}} \propto \{1 + |r_{12}r_{23}|^2 + 2\,\mathrm{Re}[r_{12}r_{23}\exp(i\varphi)]\}^{-1}$$

with

$$\varphi = 4\pi n_2 t_{\mathrm{GaN}}/\lambda, \tag{1}$$

where t_{GaN} and n_2 are the GaN layer thickness and refractive index, respectively, and λ is the wavelength of the luminescence in air. The ratio of the intensities of the extrema is then given by

$$\frac{I_{\mathrm{PL,max}}}{I_{\mathrm{PL,min}}} = \frac{1 + |r_{12}r_{23}|^2 + 2|r_{12}r_{23}|}{1 + |r_{12}r_{23}|^2 - 2|r_{12}r_{23}|}. \tag{2}$$

Using the refractive indices for sapphire and Ag given above and a GaN refractive index of $n_2 = 2.4$, Eq. (2) yields an intensity ratio of 1.75 which is higher than the measured ratio of 1.53. The discrepancy is probably due to (i) the presence of a thickness gradient in the epitaxial layer and (ii) light emerging from the cavity at an off-axis angle thus experiencing a slightly different effective GaN layer thickness. This effect could be accounted for in Eq. (1), if an additional averaging over a small range of t_{GaN} was performed. Instead we can consider the refractive index value of 2.23—which exactly yields the experimental intensity ratio—to be a lower limit for the actual GaN refractive index.

Next the layer thickness and refractive index of GaN are determined self-consistently partially following Swanepoel.[15] For neighboring extrema (occurring at wavelengths λ_a and λ_b) the thickness of GaN layer is calculated using $n_2 = 2.4$ as a first estimate for $n_2(\lambda)$

$$t_{\mathrm{GaN}} = \frac{\lambda_a \lambda_b}{4[\lambda_a n_2(\lambda_b) - \lambda_b n_2(\lambda_a)]}. \tag{3}$$

The GaN refractive index is estimated at $E = 2.3$ eV, thus the thickness calculation is limited to the range of photon energies near 2.3 eV ($2.0\ \mathrm{eV} \leqslant E \leqslant 2.6$ eV). The first estimate of the GaN layer thickness is the average of the calculated thickness values. Then an order is assigned to each extremum. Note that the algorithm[15] designed for materials with a *real* index cannot be applied here since the refractive index of Ag has a large imaginary part. This causes photoluminescence extrema when φ is a noninteger multiple of π in Eq. (1). The extremum closest to $\varphi = 0$ is $\varphi = \varphi_0$:

$$\varphi_0 = -\arg(r_{12}r_{23}) \quad \text{with} \quad |\varphi_0| \pi/2. \tag{4}$$

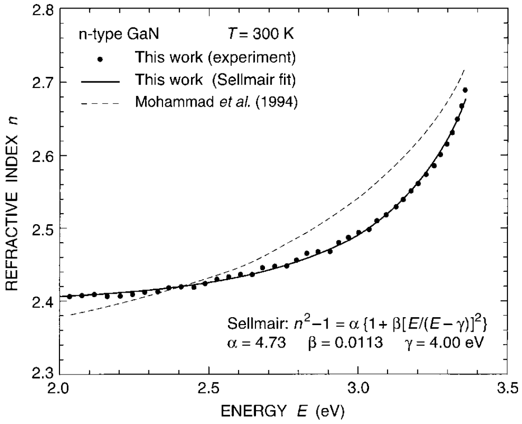

FIG. 4. Refractive index of GaN at room temperature as a function of energy (circles). The solid curve is a fit using Sellmeir's function. Also shown are data reported in Ref. 17 (dotted line).

The extremum given in Eq. (4) is the 0th order extremum $(m=0)$ if the extrema are labeled as

$$\varphi=\varphi_0+m\pi \quad \text{with} \quad m=0,1,2,3,\ldots \tag{5}$$

For real refractive indices, Eqs. (4) and (5) simplify to those used by Swanepoel.[15] The present algorithm is further improved by establishing a relationship between the *parity* of the extremum order and the extremum *type*. For the Ag coated sample, we calculate $\varphi_0=-67°$ and deduce that *minima* correspond to *even* values of m. Solving Eq. (5) for m and taking into account the integer nature of m yields with Eq. (1)

$$m=\mathrm{Int}[(4n_2t_{\mathrm{GaN}}/\lambda)-(\varphi_0/\pi)]. \tag{6}$$

This order assignment can be verified by plotting the phase angle φ as a function of extremum energy E. The extrapolation[16] of the data points with $E<2.6$ eV towards $E=0$ must cross the origin. A new set of values for $n_2(\lambda)$ is obtained by applying

$$n_2(\lambda)=\frac{[m+(\varphi_0/\pi)]\lambda}{4t_{\mathrm{GaN}}}. \tag{7}$$

The algorithm now loops back to Eq. (3).

Figure 4 shows the refractive index of GaN found after few iterations. A Sellmeir function[12]

$$n^2(E)-1=\alpha\left[1+\beta\left(\frac{E^2}{(E-\gamma)^2}\right)\right] \tag{8}$$

is fitted to the data yielding

$$\alpha=4.73, \quad \beta=0.0113, \quad \text{and} \quad \gamma=4.00 \text{ eV}. \tag{9}$$

In addition, the analysis yields a sample thickness of 3 μm in agreement with a thickness of 2.85 μm measured at the edge of the sample by scanning electron microscope. Note that the method presented here is only slightly affected by variation of the refractive index[13] of Ag with wavelength, which causes a wavelength dependence of φ_0. In contrast to the method used by Swanepoel,[15] the new method proposed and demonstrated here is applicable to materials on opaque substrates with a thin (semitransparent) or no metal reflector is used. The data obtained in this study are in reasonable agreement with previously published results[17] on the same material.

In conclusion we have shown that the modulation observed in photoluminescence spectra of GaN thin films grown on sapphire can be enhanced by using metallic reflectors on the GaN surface thereby increasing the finesse of the cavity. From the energies of the luminescence extrema, the refractive index of GaN as a function of energy and the film thickness is deduced self-consistently. The GaN refractive index is expressed analytically by a Sellmeir fit.

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[14] The position of specific extremum is found by drawing tangents between this extremum and the two neighboring extrema of the same kind. This yields a narrow energy range in which the extremum is assumed to be centered. This uncertainty in energy is largest where the unmodulated photoluminescence is curved but never exceeds 0.02 eV at most.

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