# Optical properties of wurtzite structure GaN on sapphire around fundamental absorption edge (0.78–4.77 eV) by spectroscopic ellipsometry and the optical transmission method

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Spectroscopic ellipsometry (SE) together with the optical transmission method is successfully used to determine the refractive index $n$ and absorption coefficient $\alpha$ of undoped gallium nitride film over the spectral range of 0.78–4.77 eV of photon energy. The SE measurement is carried out at angle of incidence of 60° over the 1.5–4.77 eV energy range and optical transmission measurement over the 0.78–3.55 eV energy range. The refractive index $n$ and absorption coefficient $\alpha$ obtained by both methods show unique results in the overlap wavelength region. Refractive index $n$ is found to follow the Sellmeir dispersion relationship $n^2(\lambda)=2.27^2+304.7^2/(\lambda^2-294.0^2)$ below the fundamental band edge. A free excitonic structure at the band is clearly observed at room temperature, with the transmission energy of free exciton at 3.44 eV, which is in reasonable agreement with the reported results. © *1997 American Institute of Physics.* [S0003-6951(97)04424-0]

Gallium nitride (GaN) is one of the most promising wide-band-gap semiconductors for the fabrication of blue and UV light-emitting diodes and lasers. Light-emitting diodes based on InGaN/AlGaN heterostructures have achieved practical level,[1,2] and very recently, electrical pumping III–V nitride lasers have been reported.[3] However, some of the essential parameters for the design and fabrication of light-emitting devices, such as the optical constants, have not yet been investigated in detail.

The optical transmission, which is an effective and accurate method to determine the optical constants below the fundamental absorption edge, has been used to study GaN by several authors.[3,4] The accuracy of refractive index $n$ in the transmission method is mainly determined by the accuracy of the thickness measurements.[3] Spectroscopic ellipsometry (SE) has widely been used as a nondestructive technique to investigate the optical response of semiconductors. In particular, the film thickness can be determined very accurately by fitting SE data $(\Delta,\Psi)$ in the interference part of the spectrum using a suitable model.[5] Adachi *et al.* also proposed that the overall precision in the index value was 0.02 using the three-phase model analysis for $(Al_xGa_{1-x})_{0.5}In_{0.5}P$ quaternary alloys on GaAs in the interference part of spectrum.[6]

In this letter, we describe the results of SE and optical transmission measurements on a 1.3 $\mu$m thick GaN film on a sapphire substrate over the energy range of 0.78–4.77 eV. We show that the excellent fitting of SE measurement data $(\Delta,\Psi)$ can be obtained using the Sellmier dispersion equation, provided the fitted data set is limited to the interference part of the spectrum. Also, the determination of optical constants by both the SE and transmission methods lead to the same results in the overlap wavelength region.

An undoped GaN epitaxial layer was grown on one side of a polished sapphire (0001) substrate by metal–organic chemical-vapor deposition, using ammonia ($NH_3$) as the nitrogen source. Details of the growth procedure will be published elsewhere. The uncoated backside of the substrate was rough and was mirror polished before the optical transmission measurement. The SE measurement was carried out at an incident angle of 60° over the 260–830 nm wavelength range, and optical transmission measurement over the 370–1600 nm wavelength range. Both of the measurements were performed at room temperature.

The measured SE data, $\Delta$ and $\Psi$, of the GaN film in the interference part of spectrum are shown in Fig. 1 (dotted lines). We analyze these experimental data using a Sellmeir-type dispersion relationship[7]

$$n(\lambda)^2=A_0^2+\frac{A_1^2}{\lambda^2-A_2^2}, \quad k=0, \tag{1}$$

where $A_0$, $A_1$, and $A_2$ are the fitting parameters, and $\lambda$ is the wavelength of light (in micrometers). The fitted $\Delta$ and $\Psi$ spectra, simulated with the best-fit model parameters, which are summarized in Table I, are shown by solid lines in Fig. 1. The thickness (1.25 $\mu$m) of the GaN film matches closely with that obtained by scanning electron microscope cross-sectional thickness measurement (1.3 $\mu$m). The fit was done

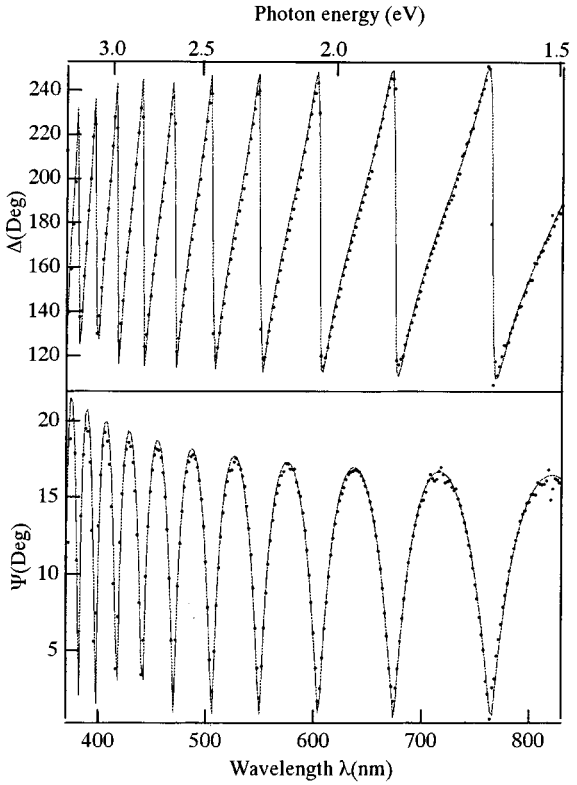


FIG. 1. Measured (dotted line) and calculated (solid line) $\Delta$ and $\Psi$ spectra of GaN on a sapphire substrate in the interference part of the spectrum.

by minimizing the mean-square error $\delta^2$ (unbiased).[8] The excellent fit is found in the wavelength range larger than 400 nm, and the deviations of the fit from the experimental data above 3.4 eV are due to the absorption of light because of the interband transitions.

An optical transmission spectrum of the same sample is shown in Fig. 2. Transmission of the bare sapphire substrate, $T_s$, is also shown in Fig. 2 as the dotted line, which is calculated by using the expression[9]

$$T_s = \frac{2n_s}{n_s^2+1}, \tag{2}$$

where $n_s$ is the refractive index of sapphire, taken from Ref. 10. As can be seen from Fig. 2, the lowest energy maximum (fourth order) of the interference fringes coincides with $T_s$. Two conclusions can be made from this: first, the absorption coefficient is zero near this wavelength region, second, the roughness of the surfaces on both sides of the sample can be ignored.

The film thickness, $d$, obtained by fitting to the SE data, together with the order $m$ of the interference fringes, is then used to obtain refined values of refractive indices from the relationship[9]

TABLE I. Best-fit parameters of GaN on a sapphire substrate determined by SE measurements. The 90% confidence limits are given with (±).

| $A_0$ | $A_1$ ($nm^2$) | $A_2$ ($nm^2$) | Thickness $d$ (nm) | $\delta$ |
|---|---|---|---|---|
| 2.27±0.02 | 304.7±7.8 | 294.0±4.5 | 1250.2±16 | 6.2 |

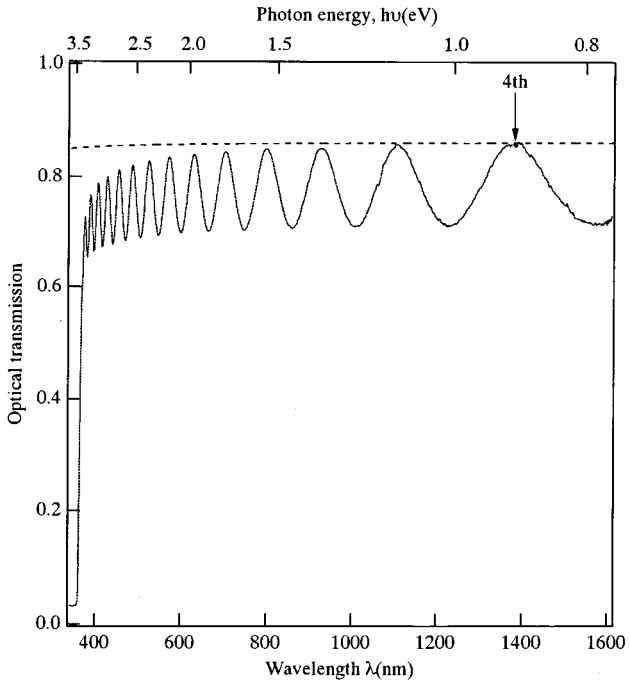


FIG. 2. Optical transmission spectrum of GaN on a sapphire substrate.

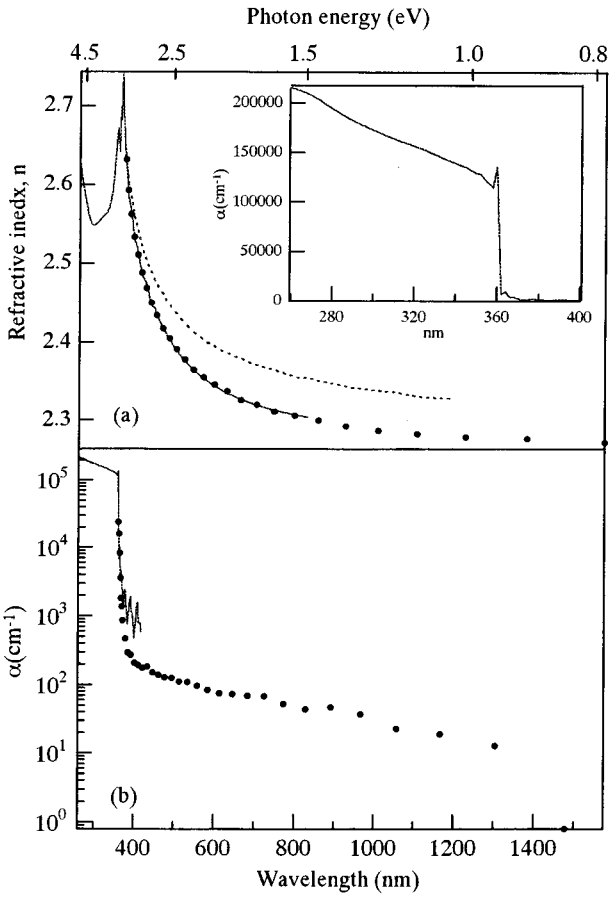


FIG. 3. The optical constants of GaN on sapphire vs wavelength. (a) The refractive indices determined from SE (solid lines) and transmission (data points) compared with data from Ref. 3. (b) The absorption coefficient determined from SE (solid line) and transmission (data points). The expanded figure of the absorption coefficient obtained by SE is shown in the inset.

$$n = \frac{m\lambda}{2d}, \tag{3}$$

and are shown by the solid circles in Fig. 3. Using the same thickness of the film, the refractive index spectrum of GaN has also been obtained from SE measurements and is shown in Fig. 3 by the solid line. For comparison, the refractive index spectrum of GaN, obtained from Ref. 3, is also shown in Fig. 3 as a dashed line. The deviation between these two experimental data is about 2% at 1.0 eV. However, this deviation is within the experimental error of the transmission measurement (2%) (Ref. 3) and SE.

Using the refractive indices obtained from transmission measurement and the thickness in Table I, the absorption coefficient as a function of wavelength are calculated following the formula of the interference-free transmission ($T_\alpha$) details, which are given in Ref. 9. Figure 3(b) shows the plot of the absorption coefficient versus wavelength obtained by both the SE and transmission methods. The absorption coefficient is much smaller than that given in Ref. 4 in the energy range of 0.78–3.0 eV, indicating that the deep level at $\sim$2.0 eV is not observed in our sample. The nonzero absorption coefficient below the fundamental band may be due to the contribution from the deep level at near 1.0 eV. A free-exciton characteristic structure is observed and is shown in the inset of Fig. 3(a). High-temperature free-exciton luminescence in GaN has also been observed by photoluminescence and photoreflectance spectra.[2,11] A simple estimate of transition energy of the exciton based on the Lorentzian line-shape functional form is[12]

$$\frac{d^2\epsilon}{dE^2} = Ae^{i\phi}(E - E_0 + i\Gamma)^{-m}, \tag{4}$$

where $A$ and $\phi$ are the amplitude and phase of the line shape, respectively, and $E_0$ and $\Gamma$ are the energy and empirical broadening parameters of the transition, respectively. The characteristic parameter $m$ is equal to 2, and describes the nature of the interband excitonic transition. From the numerical fitting of the second derivative of the dielectric function $\epsilon$, with respect to the photon energy using Eq. (4), we found the exciton transition energy at room temperature to be 3.44 eV, in reasonable agreement with the reported result of 3.42 eV, obtained from the modulated photoreflectance measurements and photoluminescence spectra.[2,11]

In conclusion, we have shown that using an accurate film thickness, which can be obtained by SE, one can determine optical functions of GaN by both SE and transmission methods leading to the same results in the common wavelength region. The free-exciton absorption in the high-quality GaN sample is evidently observed at room temperature, with the transition energy at about 3.44 eV. However, the deep-level absorption near 2.0 eV is not observed.


[1] S. Nakamura, M. Senoh, and T. Mukai, Jpn. J. Appl. Phys. 2, Lett. **32**, L8 (1993).
[2] S. Nakamura, M. Senoh, S. Nagahama, N. Iwasa, T. Yamada, T. Matsushita, H. Kiyoku, and Y. Sugimoto, Jpn. J. Appl. Phys. 2 **35**, L217 (1996).
[3] E. Ejder, Phys. Status Solidi A **6**, 445 (1971).
[4] L. Galagurov and P. J. Chong, Appl. Phys. Lett. **68**, 43 (1996).
[5] G. E. Jellison, Jr., M. F. Chisholm, and S. M. Gorbatkin, Appl. Phys. Lett. **62**, 3348 (1993).
[6] S. Adachi, H. Kato, A. Moki, and K. Ohtsuka, J. Appl. Phys. **75**, 478 (1994).
[7] E. D. Palik, *Handbook of Optical Constants of Solids* (Academic, Orlando, FL, 1985).
[8] G. E. Jellison, Jr., Appl. Opt. **30**, 3354 (1991).
[9] R. Swanepoel, J. Phys. E **16**, 1214 (1983).
[10] *Handbook of Optical Constant of Solids II*, edited by E. D. Palik (Academic, New York, 1991).
[11] M. Tchounkeu, O. Briot, B. Gil, J. P. Alexis, and R. Aulombard, J. Appl. Phys. **80**, 5352 (1996).
[12] P. Lautenschlager, M. Garriga, L. Viña, and M. Cardona, Phys. Rev. B **36**, 4821 (1987).