Infrared Characterization Of GaN Films Grown On Sapphire By MOCVD

Noritaka Kuroda*, Kazuya Saiki*, Hasanudin*, Junji Watanabe*, and Meoungwham Cho†

*Department of Mechanical Engineering and Materials Science, Kumamoto University, Kumamoto, Japan
† LG Electronics Institute of Technology, Seoul, South Korea

Abstract. Reststrahlen reflection and attenuated total reflection due to the surface phonon-polariton waves have been measured for 2 μm-thick films of n-GaN deposited on the (0001) surface of sapphire. It has emerged that the lattice of the top 1 μm-thick portion has a high quality while a large strain remains in the inner half of the films.

A drastic improvement of the electron mobility of n-GaN by the two-flow MOCVD method [1] has accelerated the development of blue LED and LD of group III-V nitrides. Nowadays the similar methods are employed widely. In the present work, by the reststrahl reflection and infrared attenuated-total-reflection techniques we examine the quality of the lattices of the (0001) oriented n-GaN films obtained at the primary stage of fabrication of those diodes. Our concern is the variation of residual strains of the GaN lattice along the thickness of the films.

The thickness of the films studied in this work is in a range of 2.0 to 2.4 μm. Figure 1 shows an example of the reststrahlen spectrum. Since the optical pass of our FTIR spectrometer has the angle of incidence of 10° the *s*-polarization is chosen for this measurement. The spectrum is typical of the composite of two different polar crystals and is almost identical with the one reported previously by Azuhata et al. [2]. Below 500 cm^{-1} since GaN is transparent there appear features due to E_{u1} and E_{u2} modes of sapphire [3,4]. The reststrahlen band of the E_1 mode of GaN manifests itself between 500 and 720 cm^{-1}. Above 720 cm^{-1} the reflection due to the Eu_4 mode of sapphire, of which the low-frequency part is masked by E_1 of GaN, reappears as a prominent hump at 880 cm^{-1}. The oscillatory structure observed beyond 1000 cm^{-1} shows the interference fringes.

It is obvious from the very high reflectivity of the E_1 mode that the quality of the surface lattice of GaN is quite high. However, compared with the reflectivity

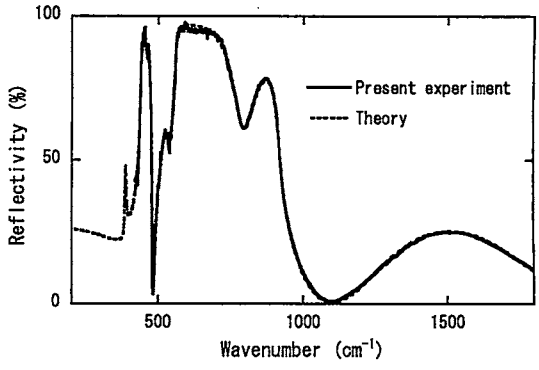

FIGURE 1. Heteroreststrahlen spectrum of GaN/sapphire. Solid and dotted lines are the experimental and theoretical curves, respectively.

due to the E_{u4} mode of sapphire [3], the recovery of reflectivity above 750 cm^{-1} through the hump is insufficient, showing that the GaN lattice is significantly strained inside the film. In fact, as shown in Fig. 1, the calculation of the spectrum by the transfer-matrix method can reproduce the observed spectrum well. In this calculation, as a simple model, we have assumed that the top half and the inner half of the sample have different dielectric functions. The parameters derived from this analysis are summarized in Table 1. Note that the damping constants of TO and LO modes of the inner half of the film are very large.

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Practically, damping constants would be continuously graded inside the film.

TABLE 1. Frequency ω (cm^{-1}) and damping constant γ (cm^{-1}) of E_1(TO) and E_1(LO) modes.

portion	ω_{TO}	γ_{TO}	ω_{LO}	γ_{LO}
Top Half	561	5	748	4
Inner Half	566	19	748	18

If the polarization of the infrared light is changed into *p*-polarization, referring to the oblique incidence reflection demonstrated by Berreman for LiF films deposited on silvered glass slides [5], one may expect to observe the LO phonons propagating along the *c*-axis. As seen in Fig. 2, a clear dip appears at the frequency, 738 cm^{-1}, of the A_1(LO) mode of GaN [6]. Interestingly, the A_{2u}(LO) mode of sapphire [4] also exhibits a dip at its frequency, 882 cm^{-1}.

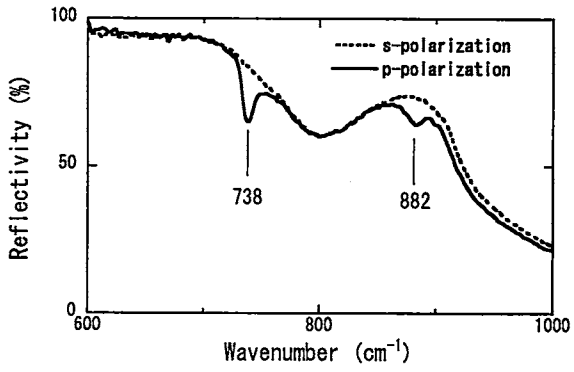

FIGURE 2. Difference in the reflection spectrum between the *p*- and *s*-polarization.

Figure 3 shows the attenuated-total-reflection spectrum. A distinct attenuation due to the surface polariton of the A_1 lattice wave of GaN is observed around 700 cm^{-1}. In our optical configuration the evanescence light of the ZnSe and Ge prisms has the wavevector of 0.81×10^4 cm^{-1} and 1.26×10^4 cm^{-1}, respectively. Consequently, the dispersion of the surface wave causes the resonance frequency to shift from 700 to 706 cm^{-1} upon replacement of ZnSe with Ge. The surface wave propagates in the 1 μm-thick region of the surface of the GaN film. The present observation assures that the lattice quality of the top half of the film is sufficiently high.

The evanescence light penetrates into the GaN film far enough to couple with the A_{2u} surface wave of sapphire, undergoing attenuation at 788 cm^{-1} for the ZnSe prism. The attenuation disappears if the prism is replaced with Ge. The dielectric theory [5] clarifies that the interfacing GaN lattice is highly dispersive and thus the surface wave is damped so strongly that the wavevector can not satisfy the momentum-conservation constraint against the evanescence light of Ge, while the constraint is barely satisfied against the evanescence light of ZnSe. Accordingly, the damping constants of the optical phonons, particularly of A_1(LO), of the inner half portion of the GaN film are suggested to reach 10-20 cm^{-1}. The reflection spectrum shown in Fig.2 supports this implication.

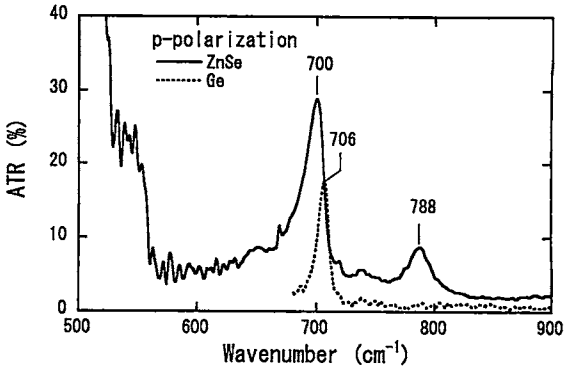

FIGURE 3. Attenuated-total-reflection spectrum obtained with the prism of ZnSe and Ge in the *p*-polarization.

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