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Photoluminescence of cubic InN films on MgO (001) substrates

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We have studied photoluminescence from cubic InN films grown on MgO substrates with a cubic GaN underlayer by RF N_2 plasma molecular beam epitaxy. A single PL peak was observed at 0.47 eV. By analyzing the reflectance spectra of cubic InN films, we could derive the refractive index and extinction coefficient, and found the band gap energy of cubic InN is 0.48 eV, indicating that the PL peak observed at 0.47 eV is due to the interband transition of cubic InN. The difference in the PL peak energy between hexagonal and cubic InN is in good agreement with that predicted by ab-initio calculations.

1 Introduction

Although III nitride semiconductors have usually hexagonal structure, cubic III nitride semiconductors can be grown as a metastable structure. Cubic III nitride semiconductors have several advantages for electronic and optoelectronic device applications compared with hexagonal ones [1], for instance, no piezoelectric nor spontaneous polarization-induced electric fields, which exist in hexagonal III nitride semiconductors and lead to the lowering of optical transition probability. Although a number of papers have reported the growth and characterization of cubic GaN (c-GaN), AlN and their alloy [2, 3], the growth of cubic InN (c-InN) has been less reported [4-6]. Furthermore, little has been reported on the physical properties, such as band gap energy of c-InN. In our previous study [6], we successfully obtained c-InN films with high phase-purity and a smooth surface by optimizing the growth conditions, and clarified the longitudinal and transverse optical phonon energies of c-InN based on Raman scattering measurements for the high-quality films. In the present study, we report on the photoluminescence (PL) from c-InN films grown on MgO (001) substrates with c-GaN underlayers by RF-N_2 molecular beam epitaxy (MBE) and discuss the band gap energy of c-InN.

2 Experimental

The samples used in this study were c-InN films grown on MgO (001) substrates by MBE with an RF-N_2 plasma source. Prior to the growth of c-InN epilayers, c-GaN underlayers were grown on MgO at 700 °C. The hexagonal phase content in the GaN underlayers was less than 1%, and the surface of the c-GaN underlayers was very smooth. Following the growth of c-GaN underlayers, c-InN films with a thickness of 1.2 μm were grown at 480 °C. The crystal quality was investigated by x-ray diffraction (XRD). The hexagonal phase content in the GaN and InN layers was estimated from the relative XRD intensity [5, 7]. We have carried out PL measurements at 13 K using a diode-pumped solid state laser (532 nm) and an InSb photovoltaic device as the excitation source and the detector, respectively. We have filled the light path with dry N_2 gas in order to eliminate the optical absorption due to the moisture in the air. Furthermore, we have measured reflectance spectra of the c-InN films at room temperature using a Fourier-transform infrared spectrometer (JASCO Irtron IRT-30).

3 Results and discussion

Figure 1 shows the XRD θ-2θ scan profile for a c-InN film grown at 480 °C on MgO substrate with a c-GaN underlayer. The peaks observed at 35.8°, 39.8° and 42.9° correspond to c-InN (002), c-GaN (002) and MgO (002), respectively. The phase purity and full width at half maximum of (002) XRD of the c-InN film were 96% and 32 arcmin, respectively.

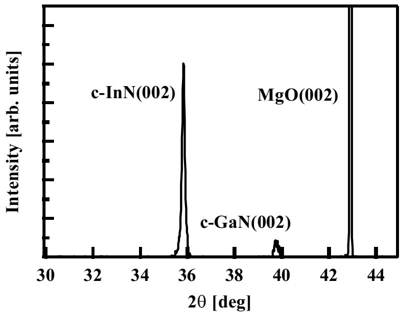

Figure 1 XRD θ-2θ scan profile for a c-InN film grown on MgO with a c-GaN underlayer.

Figure 2 shows a typical PL spectrum from a c-InN film measured at 13 K. Two PL peaks were observed at 0.47 eV and 0.69 eV. The weaker PL peak observed at 0.47 eV can be attributed to the emission from the c-InN phase, as will be discussed below. It should be noted that the PL peak at 0.47 eV was not observed for our hexagonal InN (h-InN) films [8]. On the other hand, the stronger PL peak at 0.69 eV corresponds to the emission from the h-InN phase slightly included in the film. The weak emission at 0.47 eV indicates that the crystal quality of c-InN is considerably low in comparison with h-InN obtained in this study. We found the intensity of the PL peak at 0.69 eV of this sample was ~1/20 of that of the PL peak of a h-InN film [8], which is reasonable taking into consideration the volume fraction.

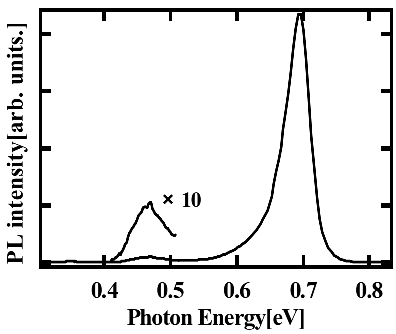

Figure 2 PL specrum observed from a c-InN film at 13 K.

Figure 3(a) shows the reflectance spectrum of the c-InN film measured at room temperature. We have used the following expression to analyze the reflectance spectrum.

$$\varepsilon(\omega) = \varepsilon_\infty \left(\frac{\omega_L^2 - \omega^2 - i\Gamma_L \omega}{\omega_T^2 - \omega^2 - i\Gamma_T \omega} \right) + \frac{A_0}{E_0^{1.5}} \times \frac{1 - \sqrt{1+\chi_0} - \sqrt{1-\chi_0}}{\chi_0^2},$$

where

$$\chi_0 = \frac{\hbar\omega + i\Gamma}{E_0}.$$

This expression for dielectric function is the sum of contributions from optical phonon and 3-dimensional M_0 interband transition [9]. For the contribution from optical phonon, ε_∞ is the high frequency dielectric constant, ω_T and ω_L are the TO and LO phonon frequency, Γ_T and Γ_L are the TO and LO phonon damping constants, respectively. We adopted the values for c-InN ω_T = 467 cm^{-1}, ω_L = 596 cm^{-1} [6]. For the contribution from interband transition, A_0 is the parameter for optical transition probability, E_0 is the band gap energy, and Γ is the broadening parameter. We have constructed three-layer (c-InN/c-GaN/MgO) model and fitted the above expression to the measured reflectance spectrum. The fitted result is shown in Fig. 3(a). The fit is in good agreement with the reflectance spectrum in the energy range of 0.3-0.7 eV. Some discrepancy in the reflectance spectrum at lower energies may be due to the coupling between plasmon and LO phonon. From the fitting to the reflectance spectrum, we could derive the refractive index and extinction coefficient as a function of photon energy, as shown in Fig. 3(b). We also found that the band gap energy E_0 = 0.48 eV. This value agrees well with the PL peak energy of 0.47 eV, showing that this emission can be identified as the interband transition of c-InN. Our experimental results indicate that the band gap energy of c-InN is 0.22 eV smaller than that of h-InN based on the difference in the PL peak energy.

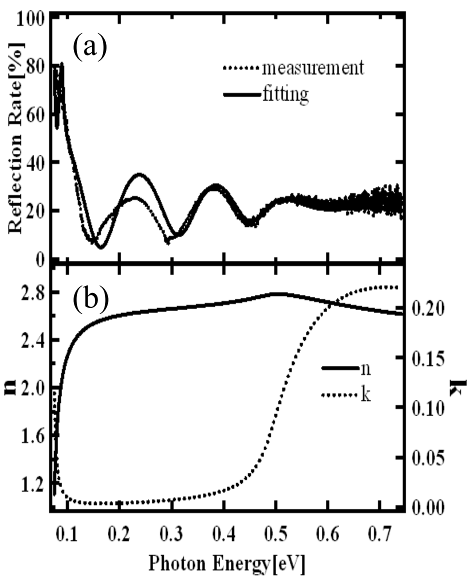

Figure 3 (a) Reflectance spectrum of a c-InN film measured at room temperature, and (b) refractive index and extinction coefficient of c-InN.

Ab initio calculations predict the band gap energy of c-InN is 0.58 eV [10] or 0.53 eV [11]. Although these values are a little larger than our experimental value of 0.48 eV, the difference in the band gap energy between h-InN and c-InN predicted by the theoretical calculations (0.23 eV [10] or 0.19 eV [11]) is close to our result of 0.22 eV. This suggests that the band gap energy of c-InN is smaller than 0.5 eV and supports our experimental result, because a large number of papers have reported the band gap energy of h-InN is smaller than 0.7 eV.

4 Conclusion

We observed a PL peak at 0.47 eV from c-InN films grown on MgO substrates with c-GaN underlayers by RF-N_2 plasma MBE. Reflectance spectrum of the c-InN film was also measured at room temperature. Analyzing the reflectance spectrum, we could derive the refractive index and extinction coefficient of c-InN, and found the band gap energy of c-InN is 0.48 eV. This good agreement with the PL peak energy indicates that the PL peak is due to the band edge emission of c-InN. Our experimental result is consistent with the difference in the band gap energy between h-InN and c-InN predicted by ab initio calculations.

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