

Spectroscopic Ellipsometry Study on the Electronic Structure near the Absorption Edge of GaAsN Alloys

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Spectroscopic ellipsometry has been used to investigate the electronic structure near the fundamental absorption edge of GaAsN alloys grown by metalorganic vapor phase epitaxy. The fundamental absorption edge is clearly observed in the imaginary part of the dielectric function and shifts to lower energies with increasing N concentration. In addition, the absorption structure is observed near the E_0 gap energy of GaAs even in GaAsN alloys. This unequivocally shows that the fundamental absorption edge of GaAsN is not shifted from the E_0 gap of GaAs but newly formed by the N incorporation. Thus, the formation of the narrowest band gap of GaAsN alloys is found to be completely different from that of conventional compound semiconductor alloys, such as AlGaAs and GaAsP.

Introduction Recently, III–V–N alloys are intensively studied since these semiconductor alloys have promising potential for optoelectronic device applications due to their unique electronic and optical properties, such as a huge band gap bowing [1–6], anomalous increase in the refractive index [7], and so on. Particularly, (In)GaAsN is expected as a material for long-wavelength semiconductor lasers used in the optical fiber communications, because their large conduction band offset to (Al)GaAs realizes the sufficient electron confinement and leads to high characteristic temperature of the semiconductor lasers. Although a lot of studies have been made to clarify the mechanism of the huge band gap bowing, one of the most interesting properties of III–V–N alloys, it has not yet been clarified. Previously, we have measured complex dielectric functions of GaAsN alloys using spectroscopic ellipsometry to investigate higher-energy band gaps [8], and have found that the optical transition probability at the E_1 gap decreases with increasing N concentration and that the lowest conduction band is formed by contribution of the L-point state. In the present study, we have focused our attention on the electronic structure near the fundamental absorption edge.

Experimental The samples used in this study were GaAs_{1-x}N_x alloys ($x = 0, 1.0\%$, and 2.3%) grown on GaAs (001) substrates by metalorganic vapor phase epitaxy. Tri-

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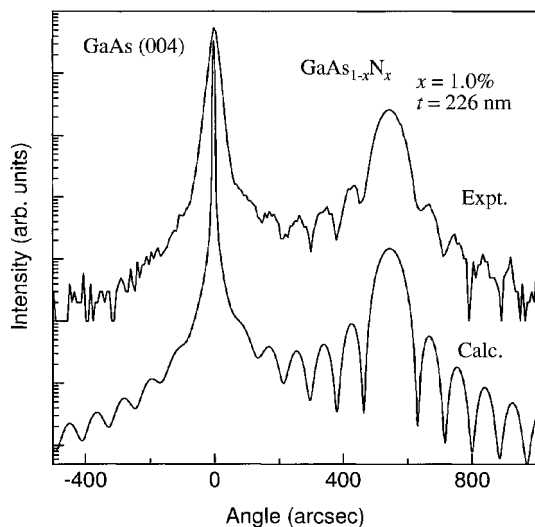


Fig. 1. (004) X-ray diffraction curve of $\text{GaAs}_{1-x}\text{N}_x$ alloy

methylgallium, arsine and 1,1-dimethylhydrazine were used as Ga, As, and N sources, respectively. The N concentration and layer thickness of GaAsN alloys were determined using X-ray diffraction.

Figure 1 shows an example of results of the (004) X-ray diffraction curve of GaAsN alloy taken using $\text{Cu K}\alpha_1$ radiation. Upper and lower curves represent the experimental and calculated diffraction curves, respectively. The lower diffraction curve was calculated based on dynamical X-ray diffraction theory [9]. From this X-ray diffraction measurement the N concentration and the layer thickness were estimated to be 1.0% and 226 nm, respectively. The spectroscopic ellipsometry measurements (Sopra, model GESP-5) were carried out in the wavelength range of 700–1200 nm at room temperature. The light was incident at 75° on the samples. For a GaAs epitaxial layer grown simultaneously with GaAsN layers, the thickness of the native oxide layer was 3 nm. Thus, we assumed the same thickness as on GaAs. The complex dielectric functions, $\epsilon_1 + i\epsilon_2$, of GaAsN alloys were numerically determined using the Newton-Raphson method for the sample structure determined from the X-ray diffraction measurements. We have also measured photoluminescence at room temperature using an Ar ion laser as the excitation source to compare with the results of spectroscopic ellipsometry.

Results and Discussion Figure 2 shows the complex dielectric functions, ϵ_1 and ϵ_2 of $\text{GaAs}_{1-x}\text{N}_x$ alloys ($x = 0\%, 1.0\%, 2.3\%$). The real part of the dielectrics functions, ϵ_1 , is shifted by +0.5 and +1.0 for $x = 1.0\%$ and 2.3% , respectively.

The absorption edge is clearly observed in the imaginary part of the dielectric functions, ϵ_2 , of GaAsN alloys and is found to shift to lower energies with increasing N concentration. The peak corresponding to the absorption edge is also observed in the real part of the dielectric functions. In addition, it is worth noting that the absorption structure was clearly observed near the E_0 gap energy of GaAs even in both the real and imaginary parts of the dielectric functions of GaAsN alloys. This unequivocally shows the fundamental absorption edge of GaAsN alloy is not shifted from the E_0 gap of GaAs but newly formed by the N incorporation. Therefore, the nature of the fundamental absorption edge, or the formation of the narrowest band gap of GaAsN alloys is found to be completely different from that of conventional compound semiconductor alloys, such as AlGaAs and GaAsP, but similar to GaPN [3]. The anomalous increase in the refractive index observed in InGaAsN alloys [7] can be also explained by the fact that the fundamental absorption edge is newly formed by the N incorporation.

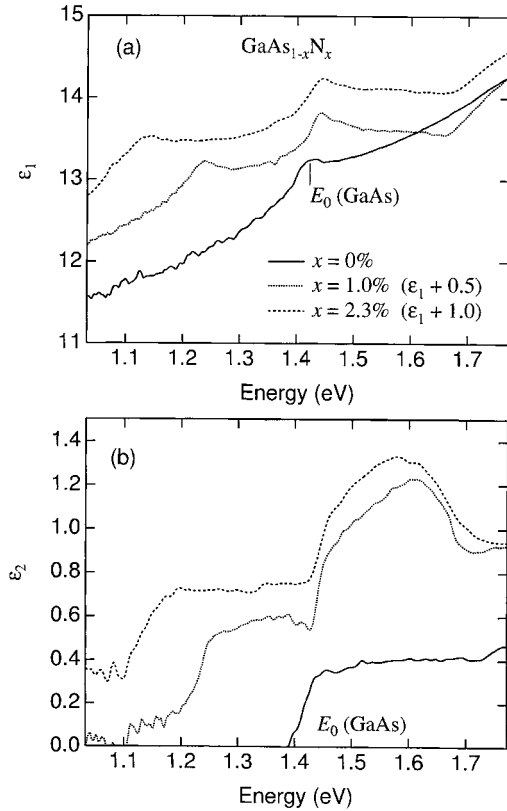


Fig. 2. Complex dielectric functions of GaAsN alloys: a) real part, b) imaginary part

The transition energies of GaAsN alloys were estimated from the complex dielectric functions using model dielectric functions [10]. We treated both fundamental absorption edge and the optical transition near the E_0 gap of GaAs, which we name the “ E_0 ” gap transition hereafter, as three-dimensional M_0 critical points.

Figure 3 shows the fundamental absorption edge energy and the “ E_0 ” gap energy estimated from the analysis using model dielectric functions. The PL peak energy at room temperature is also plotted in this figure.

The fundamental absorption edge energy decreases with increasing N concentration and agrees well with the photoluminescence peak energy at room temperature. This energy shift is also in good agreement with the results

for the absorption measurements [5]. On the other hand, the “ E_0 ” gap energy is almost constant but slightly increases with increasing N concentration. Since the GaAsN layers used in this study were coherently grown on GaAs, the gap energy is affected by the strain.

For example, the E_0 gap energy of GaAs decreases due to its negative volume deformation potential under the tensile strain. However, an increase in the “ E_0 ” gap is found in spite of the tensile strain of the GaAsN layers. This indicates that the energy shift of the “ E_0 ” gap is not due to the strain effect but mainly due to the intrinsic alloy effect.

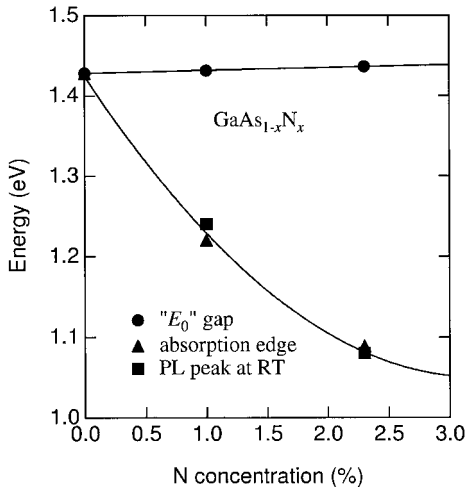


Fig. 3. Absorption edge and the “ E_0 ” gap energies as a function of N concentration

Conclusions The complex dielectric functions near the fundamental absorption edge of GaAsN alloys were studied using spectroscopic ellipsometry. The fundamental absorption edge was clearly observed in the imaginary part of the dielectric functions and the peak corresponding to the absorption edge is also observed in the real part of the dielectric functions. The fundamental absorption edge energy decreases with increasing N concentration and agrees well with the PL peak energy at room temperature. In addition, the absorption structure was clearly observed near the E_0 gap energy of GaAs even in GaAsN alloys. This shows that the fundamental absorption edge of GaAsN is not shifted from the E_0 gap of GaAs but newly formed by the N incorporation.

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