# Bandgap Energy and Effective Mass of BGaN

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# **1. Introduction**

Boron gallium nitride (BGaN) is attracting much attention for the application of light emitting devices operating in ultraviolet (UV) spectral region. Because it was estimated using quantum dielectric theory that BGaN ternaries have direct bandgap corresponding to UV spectral region [1]. Furthermore, epitaxial growth of those ternaries has been reported using metalorganic vapor phase epitaxy [1-3]. However, the possibility for the application of light emitting devices has not been discussed based on experimental results. In this paper, we re-estimated the bandgap energies and effective masses of BGaN and discussed those propriety based on photoluminescence spectra.

## 2. Theoretical Estimation

The bandgap energy and effective mass are important parameters for the optical gain. At present, those parameters of w-BN were not reported. Thus those are estimated using Harrison's theory [4]. The parameters of c-BN are adopted in this study because the parameters of w-BN have not been reported. The bandgap energies of B<sub>x</sub>Ga<sub>1-x</sub>N using Harrison's theory and quantum dielectric theory [1,5] are shown in Fig. 2. The estimated results are roughly consistent with those reported previously around the lattice matching composition, x = 0.17 [1]. The estimated effective mass dependence on the boron composition is shown in Fig. 3. The hole's and electron's effective masses of GaN obtained in this study are consistent with the experimental results reported previously [6]. The effective mass of BGaN is somewhat smaller than that of GaN owing to the large bowing. The effective mass affect an acceptor and donor level when we consider the hydrogen approximation. Thus, it indicates that p-type and n-type doping will be possible.

#### **3. Experiments**

Photoluminescence spectra of BGaN ternaries were observed at low temperature (20 K). A 325 nm light from He-Cd laser was used for the excitation light source. Reflection Spectra were also observed using halogen lump as a white light source.

The BGaN layers were grown on (0001) 6H-SiC substrates by metalorganic vapor phase epitaxy (MOVPE) with a horizontal quartz reactor. No buffer layer was used in this study. Growth conditions are summarized in Table II. Triethylboron (TEB), trimethylgallium (TMGa) and ammonia (NH<sub>3</sub>) were used as B, Ga and N sources, respectively. Schematic diagram of growth time sequence is also shown in Fig. 3. Boron composition in a BGaN

layer was estimated using the atomic concentration resulted from Auger electron spectroscopy (AES) and the lattice constant from X-ray diffraction (XRD).

#### 4. Results

Photoluminescence and reflection spectra of GaN and BGaN at low temperature (20 K) are shown in Fig. 4. The emission peaks originated from free-exciton recombination were observed in those layers. The emission peak of a BGaN layer in near-band-edge region shifted high-energy side from that of a GaN layer. That indicates that the bandgap energy of a BGaN layer is larger than that of a GaN layer.

The temperature dependence of the exciton emission also studied. The binding energy of exciton in BGaN was as same as that of GaN. That indicates effective masses of BGaN are almost equal to those of GaN, because the reduced effective mass is in proportion to the binding energy of exciton.

# 5. Discussion

The energy of excitonic emission is plotted in Fig. 1. The energy of emission is consistent with estimated one. Thus the bandgap energies of BGaN ternaries are larger than that of GaN, which correspond to UV spectral region.

In InGaN layers, excitonic emission originating from localized states, which are created by inhomogeneous of indium content [7]. However, in the case of BGaN the exciton peak originating from such a localized state was not observed because the excitonic absorption energy in the reflection spectra agrees with the excitonic emission peak in the photoluminescence spectra. The bandgap energies will have a small bowing parameter depending on boron composition.

#### 6. Summary

In summary, bandgap energies and effective masses of BGaN ternaries were estimated using Harrison's theory. The bandgap energies were larger than that of GaN and located in UV spectral region. The effective masses were almost equal to those of GaN. Reflection and photoluminescence spectra of a BGaN layer grown by metalorganic vapor phase epitaxy were studied at low temperature. The excitonic emission was observed in the BGaN layer. Furthermore, the excitonic emission depending on observed temperature was studied. The results indicate that effective masses of the BGaN layer were almost equal to those of GaN. It is consistent with the estimated effective masses. Thus BGaN ternaries have an advantage for the application of semiconductor lasers operating in ultraviolet spectral region.

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Fig. 1 Bandgap energy of BGaN.



Fig. 2 Effective mass of BGaN.

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Fig. 3 Growth procedure in this study.



Fig. 5 Photoluminescence spectra of GaN (a) and  $B_{0,1}Ga_{0,9}N$  at 20K.