Local Structure around In Atoms in InGaN Single-quantum-well by XAFS

$In_xGa_{1-x}N$ is a key material in high-brightness blue/green light-emitting diodes (Fig. 1) and purplish-blue laser diodes [1]. Although such devices have very high densities of threading dislocations, they show a high quantum efficiency in contrast to conventional III-V and II-VI semiconductor-based devices [2]. In mole fluctuation in InGaN active layers is proposed as its origin [3]. In the model, injected carriers are localized into fluctuation-induced potential minima and can efficiently contribute to radiative recombination before captured by dislocation-activated non-radiative recombination centers, which is considered to lead to the high quantum efficiency. Therefore, in order to make the emission mechanism clear in InGaN-based light-emitting devices, it is important to clarify local structures around In atoms in InGaN.

Extended X-ray Absorption Fine Structure (EXAFS) is a powerful tool to investigate local structures in thin layers composed of two or more elements. There are some reports on local structures around In atoms in InGaN by EXAFS [4-6]. The value, however, varies widely even for atomic distances mainly due to the quality of samples. In this work, EXAFS measurements around an In *K*-edge were carried out for a high quality InGaN single-quantum-well (SQW) green light emitting diode.

The sample is an $In_{0.45}Ga_{0.55}N$ SQW of 3 nm thickness, which was grown by metallorganic chemical vapor deposition (MOCVD) on a sapphire (0 0 0 1) substrate. It consists of a sapphire substrate, GaN buffer layer, n-GaN:Si barrier layer (4000 nm), $In_{0.45}Ga_{0.55}N$ SQW (3 nm), p-$Al_{0.2}Ga_{0.8}N$:Mg barrier layer (100 nm), and p-GaN layer (500 nm) (Fig. 2). The XAFS measurements were made at beamline **BL01B1** and the XAFS data were collected with a double-crystal monochromator using Si (111) crystals [7]. The beam was focused on the sample surface. In $K\alpha$-fluorescence emission was measured using a 19 elements Ge detector. The angle between the incident X-ray beam and the sample plane was 2 degrees. The sample was rotated in-plane to remove the Bragg diffraction.

In order to analyze the experimental EXAFS data, XANADU and FEFF6.0 code were used.

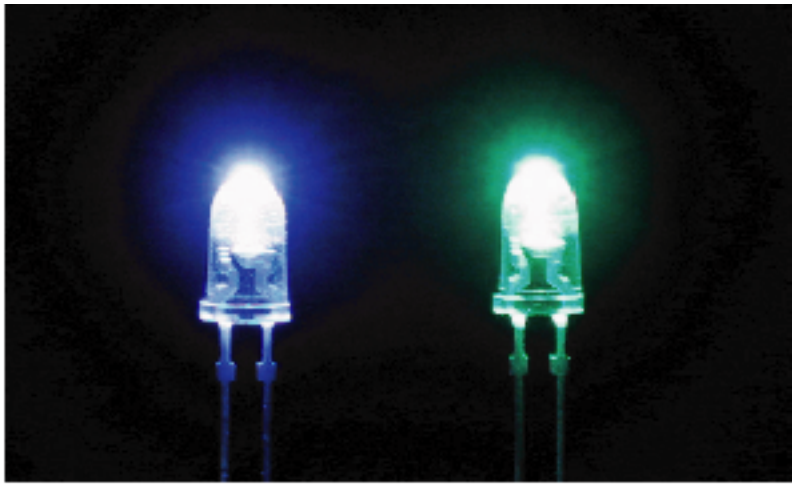

Fig. 1. High-brightness InGaN blue and green LED.

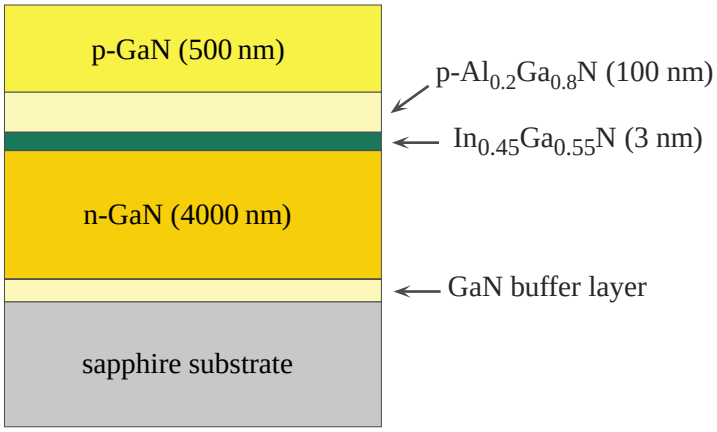

Fig. 2. A schematic view of the structure of the green LED.

What caused the greatest difficulty in the measurement in this system was a quite small photon-counting rate in the detector because the cap on the InGaN SQW (about 600 nm thick, Fig. 2) reduces the incoming photon of In-$K\alpha$. The Fourier transforms (FT) of the present EXAFS are shown in Fig. 3. Since the structure of InGaN is a wurtzite type, the first nearest peak includes the contribution of In-N bond and the second nearest peak includes that of In-Ga and In-In for $In_{0.45}Ga_{0.55}N$. To optimize the values of the structure parameters, these two peaks are individually fitted by the non-linear least square method (curve-fitting) for the *k*-range of 5.0 ~ 12.5 $Å^{-1}$ after the energy shift, the phases and amplitudes are corrected. First, we analyzed the InN powder as a standard sample and obtained reasonably good results ($r_{In\text{-}N}$ = 2.15 Å, $r_{In\text{-}In}$ = 3.53 Å). Then, we applied the empirical parameters from the standard sample to $In_{0.45}Ga_{0.55}N$ SQW. The results for the interatomic distances are as follows: $r_{In\text{-}N}$ is 2.11 Å, $r_{In\text{-}Ga}$ is 3.25 Å, and $r_{In\text{-}In}$ is 3.31 Å. We had good agreement between the theoretical FT by curve-fitting and the experimental one for $In_{0.45}Ga_{0.55}N$ (Fig. 3). The interatomic distances in the $In_{0.45}Ga_{0.55}N$ SQW are shorter in comparison with those in InN. Especially the reduction of In-In distance is prominent. The present EXAFS gives structural information about the horizontal direction of the SQW surface, because the electric vector of the incident X-ray is polarized in the plane of the sample surface. It is possible that $r_{In\text{-}In}$ has been greatly shortened in the horizontal direction affected by the atomic spacing of upper and lower GaN in the $In_{0.45}Ga_{0.55}N$ SQW. Comparison between the measurements of the horizontal and vertical directions to the SQW will be important in the next research project. As for the coordination number (N), $N_{In\text{-}N}$ is 3.2 for the first peak, and $N_{In\text{-}Ga}$ and $N_{In\text{-}In}$ are 11.3 and 1.9 respectively, for the second peak. The EXAFS results suggest that In atoms are homogeneously distributed and may make an ordered phase in the $In_{0.45}Ga_{0.55}N$ SQW [7]. However, there remains a possibility that the actual average concentration of In atom for the present sample is lower ($x \sim 0.2$) than $x = 0.45$ and a more accurate determination of the local structure is in progress.

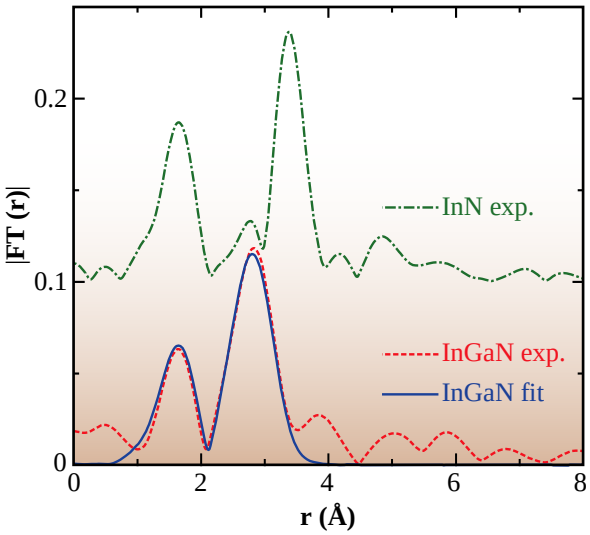

Fig. 3. Fourier transforms of In K-edge EXAFS kχ(k) for InGaN SQW (dashed red line, fluorescence) and InN powder (dash-dotted green line, transmission). Solid blue line is FEFF fit result for InGaN SQW. The energy shift, phases and amplitudes are not corrected in these Fourier transforms.

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