Structural analysis in real space of Indium atom incorporated into $In_xGa_{1-x}N$ single quantum wells by coaxial-impact collision ion scattering spectroscopy

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The high-quality $In_xGa_{1-x}N$ single quantum wells (SQWs) for ultraviolet, blue, and green-light emitting devices were investigated by coaxial-impact collision ion scattering spectroscopy (CAICISS) for the first time. Indium atoms incorporated into $In_xGa_{1-x}N$ SQW were found to occupy the substitutional Ga site and have Ga-face (+c) polarity. From the CAICISS analyses, the structural disordering of In was suggested for the InGaN SQW with smaller In content.

KEYWORD: $In_xGa_{1-x}N$ single quantum wells (SQWs), CAICISS, polarity, InN mole fraction

1. Introduction

$In_xGa_{1-x}N$ ternary alloys are exclusively used as an active layer of the column III-nitride ultraviolet, blue, and green light-emitting diodes and blue laser diodes [1,2]. These devices are built on the polar surface, and the characteristics depend on whether the GaN film is Ga (+c) or N- (-c) face polarity[3]. Observation of the GaN have been reported using CAICISS[4,5], and the influence of GaN polar direction during the growth on both the growth mode[6] and the impurity incorporation[7] have been also reported. The mechanism of the intense electroluminescence or photoluminescence from $In_xGa_{1-x}N$ in spite of large threading dislocation density up to $10^9 cm^{-3}$ has been intensively studied[8]. Therefore, structural analysis of $In_xGa_{1-x}N$ single quantum wells (SQWs) are required both for improving the device performance and understanding the optical properties of InGaN alloys. In this letter, the device quality $In_xGa_{1-x}N$ SQWs on a 3μm-thick GaN layer are investigated by CAICISS with respect to the substitutional structure of In incorporated into the SQWs.

2. Experiment

Samples were 3-nm-thick undoped $In_xGa_{1-x}N$ (x=0.05, 0.2 and 0.5) SQWs grown on a 3μm-thick Si-doped (~$5x10^{18} cm^{-3}$) GaN layer on the c-plane sapphire substrate using a low-temperature GaN buffer layer by the two-flow metalorganic chemical vapor deposition (MOCVD). The InN mole fraction of the wells was nominally estimated from the results of X-ray diffraction (XRD) measurements on thicker $In_xGa_{1-x}N$ layers, assuming that the films were perfectly relaxed. In CAICISS analysis the dependence of both Ga and In signal intensities on azimuth angle was investigated when the glancing angle was fixed at 36° and 60°. And then, the dependence of Ga and In signal intensities on the glancing angle at the [11$\bar{2}$0] azimuth was measured to determine the polarity.

3. Results and Discussion

Time-of-flight of He back-scattered due to collision with In and Ga were theoretically calculated to be 6417nsec and 6550nsec, respectively. The positions of two sharp peaks assigned to In and Ga signal could be detected in CAICISS analysis. Figure 1 shows the glancing angle dependence of Ga and In intensities at the [11$\bar{2}$0] azimuth for $In_{0.5}Ga_{0.5}N$ SQW. It is confirmed from comparison with the data for Ga (+c)- and N (-c)-face GaN epitaxial films in Ref. 4 that the alloyed In has Ga-face (+c) polarity as well as the variation of Ga signal exhibits also +c polarity. The same polarity (+c) was ascertained for the other SQWs.

Figure 2 illustrates the dependence of In and Ga signal intensity on azimuth angle for $In_xGa_{1-x}N$ SQWs under the condition that glancing angle was fixed at 60°. The intensity variations can be explained taking the shadowing and focusing effect of ion scattering into account[11,12]. The peaks and dip of In or Ga signal intensity at 60° of glancing angle in Fig. 2 take place due to the atomic configuration of only III-group atoms of wurtzite structure. These signals for SQWs reflect that the shadow cone of He ion due to scattering with Ga (or In) atom at the top layer collides with Ga (or In) atoms at the second and third layers. As shown in Figs. 2(a)-2(c), Indium signal intensity exhibits three-fold symmetry due to the hexagonal structure of $In_xGa_{1-x}N$. With increase of Indium content, this symmetric behavior is likely to be clearer. Compared with Ga signal variation in Fig. 2 (d), the positions of both peak and dip in the In signal variation for $In_{0.5}Ga_{0.5}N$ SQW are consistent with those in Ga signal variation. The variations for Ga and In signals were also found to be synchronized for the other SQWs.

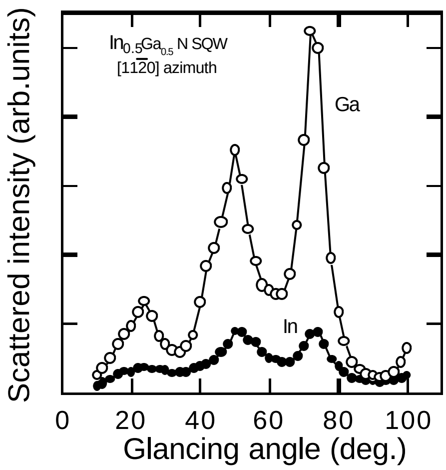

Fig.1. Glancing angle dependence of Ga and In signal intensity at the [11$\bar{2}$0] azimuth for $In_{0.5}Ga_{0.5}N$ SQW. The variation of both Ga and In signal indicates +c polarity.

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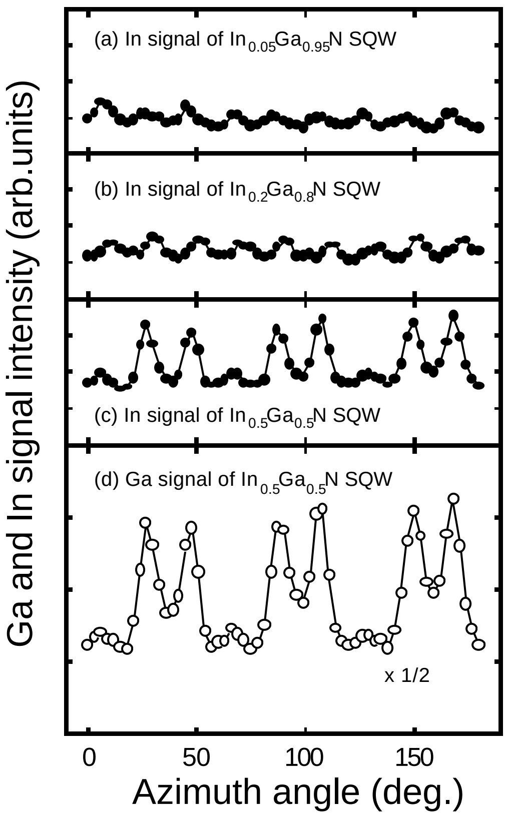

Fig.2. Azimuth angle dependence of In and Ga signal intensity at 60° of glancing angle. In signal for (a) $In_{0.05}Ga_{0.95}N$, (b) $In_{0.2}Ga_{0.8}N$, and (c) $In_{0.5}Ga_{0.5}N$ SQWs. (d) Ga signal for $In_{0.5}Ga_{0.5}N$ SQW. Horizontal lines represent zero-intensity level.

Furthermore, similar results were obtained in the azimuth dependences which were taken at 36° of glancing for all SQWs. These indicate that In atoms incorporated occupy the precise site of Ga atom substitutionally in SQWs.

Since the signal peaks in Fig.2 come from focusing effect of ion beam between adjacent atoms, it might reflect more sensitively the information on atomic arrangement inside the SQW. It is known that higher ratio of peak to dip intensity ($R_{p/d}$) implies better crystalline quality. Figure 3 shows average $R_{p/d}$ values of In and Ga signals evaluated from three-fold symmetric azimuth angles in Fig. 2. Although the $R_{p/d}$ values of Ga for SQWs are lower than that for the GaN film due to lower crystalline quality, they are nearly constant for all SQWs. This indicates that the position of Ga in the crystal structure is hardly shifted by In-incorporation. It is noted that the $R_{p/d}$ values of In decreases with decreasing InN mole fraction, which suggests that the degree of disorder in In atomic arrangements for the sample with low InN mole fraction is larger than that with higher InN mole fraction. This distorted atomicarrangement of In is possibly caused by In-N bond length (displacement of In) and/or In compositional fluctuation[9-11]. The enhanced disordering of In for the SQW with smaller In content is consistent as well with the theoretical calculation by Bellaiche *et.al.*[12].

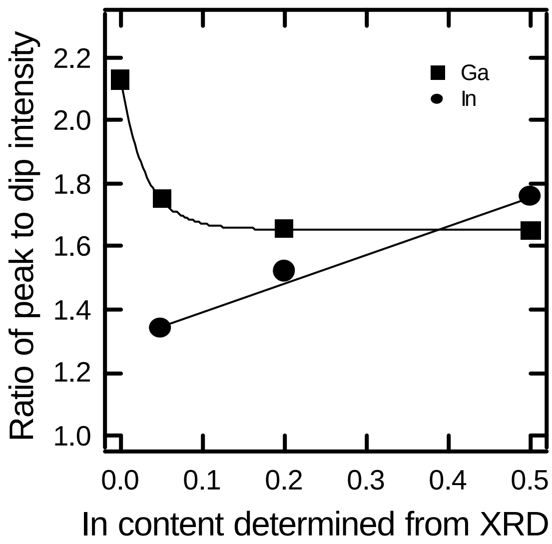

Fig.3. Relationship between the ratio of peak to dip intensity evaluated from azimuth angles in Fig.2 and In content determined by XRD. Closed square and circle represent Ga and In, respectively.

4. Conclusion

The structures of $In_xGa_{1-x}N$ SQWs on 3µm-thick GaN layer for the ultraviolet, blue and green light-emitting devices were investigated by CAICISS. The possibility that CAICISS could analyze structural fluctuation of the ternary system like $In_xGa_{1-x}N$ was demonstrated. It was found that In incorporated into InGaN SQWs occupied the substitutional site of Ga atom having +c polarity.

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