Preferential N-H Bond Direction in GaAsN(001) Grown by Chemical Beam Epitaxy

Kazuma Ikeda, Koushiro Demizu, Nobuaki Kojima, Yoshio Ohshima, and Masafumi Yamaguchi

Toyota Technological Institute
2-12-1 Hisakata, Tenpaku-ku, Nagoya 468-8511, Japan
Phone: +81-52-809-1877 E-mail: kikeda@toyota-ti.ac.jp

Abstract
Bond directions of N-H complexes in (001) plane of GaAsN(001) grown by chemical beam epitaxy were clarified. The N-H stretch modes at 2952 and 3011 cm\(^{-1}\) had maximum (minimum) intensities when the polarization direction of IR was along [1̅10] ([1̅10]). The N-H wag mode at 960 had maximum (minimum) intensities along [1̅10] ([1̅10]). On the other hand, the absorption intensity of the N-H stretch mode at 3098 cm\(^{-1}\) showed small dependence on the IR polarization direction. Therefore, the LVMs at 961, 2952, and 3011 cm\(^{-1}\) have preferential N-H bond directions along [1̅10] in (001), while the LVM at 3098 cm\(^{-1}\) has no preferential N-H bond direction.

1. Introduction

InGaAsN is one of the candidate materials to realize the 4-junction solar cell, InGaN/(In)GaAsN/InGaAsN/Ge, with the conversion efficiency over 50%. However, the electrical properties of InGaAsN have not been enough to achieve such high efficiency of that solar cell. A problem to be resolved in InGaAsN is to clarify the intrinsic defect properties that degrade the electrical properties. N is considered to be related to the defects, because the mobility and lifetime of (In)GaAsN degrades as N composition is increased.

The N-H complex is one of the major defects in (In)GaAsN grown by using organic sources such as the chemical beam epitaxy (CBE) and metal organic chemical vapor deposition (MOCVD), and the molecular beam epitaxy with H-irradiation [1-3]. The N-H complex is considered to affect the carrier density as an unintentional donor or acceptor depending on its structure [4, 5]. However, the structural and electrical properties of N-H complex have been studied. However, the understanding of those properties is still limited.

Local vibration modes of N-H bonds were observed in the CBE-grown GaAsN [1], 3124 and 3101 cm\(^{-1}\) in the MOCVD-grown InGaAsN [2], and 3195, 2967, 1447, 1068, and 957 cm\(^{-1}\) in the H-irradiated MBE-grown GaAsN [3]. At the wavenumbers of 3125, 3098, 2952 and 961 cm\(^{-1}\), the LVMs of GaAsN were observed as unpolarized and linearly polarized spectra [2]. The polarization direction of the incident IR was changed from <1̅10> to <1̅10> in (001) plane. The unpolarized spectrum of GaAsN was normalized by that of a GaAs substrate. On the other hand, the polarized spectra were normalized by the <1̅10> polarized spectrum.

2. Experimental

GaAsN film was grown by CBE method. The detail of the growth procedure is discussed in the previous paper [1]. The semi-insulating GaAs(001) with 2° tilt towards <1̅10> was used as the substrate. The growth pressure was 2×10\(^{-5}\) Pa. The growth temperature was 400 °C. The thickness of the film was around 6 μm. The unpolarized and linear polarized IR absorption spectra of GaAsN film were obtained by Fourier transform infrared spectroscopy (FTIR). The polarization direction of the incident IR was changed from <1̅10> to <1̅10> in (001) plane. The unpolarized spectrum of GaAsN film was normalized by that of a GaAs substrate. On the other hand, the polarized spectra were normalized by the <1̅10> polarized spectrum.

3. Results and Discussion

IR absorptions by N-H LVMs are observed in the unpolarized FT-IR spectrum of GaAsN grown by CBE as shown in Fig. 1. The largest peak of the N-H stretch mode is at 2952 cm\(^{-1}\), followed by 3098, 3011, and 3125 cm\(^{-1}\). Because the absorption coefficients of N-H LVMs are similar, the number densities of N-H defects are expected to be in the same order as the IR absorption intensities.
Comparing linear polarized spectra of GaAsN grown by CBE, it is found that the N-H wag mode at 961 cm\(^{-1}\) has maximum absorption intensities at the polarization direction of \(<1-10>\), while the N-H stretch modes at 2952 and 3011 cm\(^{-1}\) have maximum at \(<110>\). The FT-IR spectrum with polarization direction of incident IR along \(<110>\) subtracted by that along \(<1-10>\) is shown in Fig. 2. The intensity of the N-H wag mode peak at 961 cm\(^{-1}\) is positive, while those of the N-H stretch modes at 2952 and 3011 cm\(^{-1}\) are negative. The result indicates that those N-H bonds prefer to align along \(<1-10>\) in (001) plane. The peak intensities of the N-H stretch modes at 3098 and 3125 cm\(^{-1}\) are below or comparable to the detection limit which is around 5 \times 10^{-5} \text{abs. unit}.

Possible structures of N-H complex with N-H LVMs at 961, 2952, and 3011 cm\(^{-1}\) are the bond center (BC) and anti-bonding (AB) structures. Both structures have the N-H bond directions along [111] which can be detected as \(<1-10>\) or \(<110>\) directions in (001) plane. Those structures have the four-fold rotational symmetry in (001) plane which could not be observed in this measurement. Although the reason is not understood, it is considered to be related to a low polarization degree of the incident IR and the deviation of the N-H bond direction from [111] because of large vibration amplitudes of N-H LVMs.

The difference between the N-H peak intensities in \(<110>\) and \(<1-10>\) polarized IR spectra reflects the non-uniform distribution of the N-H bond direction but the local structure around a N-H defect. The N-H bonds which align along [1-11] or [111] are expected to have different formation energies during the growth process. The chemical reaction at the growing surface can be related to the non-uniformity in the distribution of the N-H bond direction. Further analyses are required.

The order of the original peak intensities in Fig. 1 does not hold in the difference spectrum in Fig. 2. The peak intensity at 3011 cm\(^{-1}\) is larger than that at 3098 cm\(^{-1}\) in the difference spectrum in Fig. 2. This indicates that the non-uniformity of the N-H bond direction depends on the structure of the N-H defect.

4. Conclusions

Bond directions of N-H complexes in (001) plane of GaAsN(001) grown by chemical beam epitaxy were clarified. The N-H stretch modes at 2952 and 3011 cm\(^{-1}\) had maximum (minimum) intensities when the polarization direction of IR was along \([1-10]\) \([110]\). The N-H wag mode at 960 cm\(^{-1}\) had maximum (minimum) intensities along \([110]\) \([1-10]\). On the other hand, the absorption intensity of the N-H stretch mode at 3098 cm\(^{-1}\) showed small dependence on the IR polarization direction. Therefore, the LVMs at 961, 2952, and 3011 cm\(^{-1}\) have preferential N-H bond directions along \([1-10]\) in (001), while the LVM at 3098 cm\(^{-1}\) has no preferential N-H bond direction.

Acknowledgements

This work was supported by the New Energy and Industrial Technology Development Organization (NEDO) under the Ministry of Economy, Trade and Industry (METI), Japan.

References