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Effect of Phase Purity on Dislocation Density of PR-MOVPE-Grown InN

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1. Introduction

Due to a small bandgap of about 0.7 eV, and its thermal stability, InN is regarded as a promising material for optoelectronic devices. However, improvement of the crystal quality is difficult due to a narrow growth window from high nitrogen equilibrium vapor pressure. To overcome the high equilibrium vapor pressure of nitrogen, we have developed a pressurized-reactor metalorganic vapor phase epitaxy (PR-MOVPE). By using this method we have reported the enlargement of the growth window [1]. However, there are inclusion of twinned metastable zincblende (ZB) phases in the stable wurtzite (WZ) phase which were detected by Raman scattering measurement [2], and X-ray diffraction pole figure measurement [3]. Especially pole figure revealed the orientation relationship between WZ and ZB InN as WZ(0001)//ZB(111) along the growth direction, and WZ($10\bar{1}0$)//ZB($11\bar{2}$) in plane. Obtaining pure WZ-InN is an important issue for further improvement of crystal quality of InN grown by PR-MOVPE. Understanding the nature of ZB-InN inclusion by investigating its effect on crystal quality is still needed to achieve this goal.

In this paper, the effect of ZB inclusion on the threading dislocation densities (TDDs) has been studied. X-Ray diffraction (XRD) rocking curve measurements on symmetric and asymmetric planes are used to derive screw and edge component of the TDDs.

2. Experiments

InN films were grown by PR-MOVPE directly on nitrided *c*-plane sapphire substrate at 1600 Torr. The growth was performed for 4 hours after the thermal cleaning and nitridation. Trimethylindium flow rate was set to 15 μmol/min, and NH_3 flow rate was set to 0.38 mol/min. Growth temperature (T_g) was varied from 500 to 700°C with 25°C intervals. Thicknesses of the films were 100~200 nm.

XRD measurements were performed using high-resolution X-ray diffractometer (Bruker-AXS, D8 Discover). Pole figures of WZ-InN ($10\bar{1}1$) plane and ZB-InN (111) plane were measured to estimate the volume fraction and orientation of ZB InN [3]. In determining the volume fraction from each diffraction intensity, structural factors, scattering factors and Lorentz's polarization factors for both crystallographic phases were taking into accounts. Full-width half-maximum (FWHM) of rocking curve was used to derive the TDDs. Rocking curve was measured on symmetric plane (0002) and asymmetric plane ($10\bar{1}1$) to investigate the crystal quality. As an asymmetric plane, ($10\bar{1}1$) was chosen instead of usual ($11\bar{2}0$), because films were very thin. Actually, ($10\bar{1}1$) diffraction involves the two contributions from the tilts of (0002) and ($10\bar{1}0$) planes which were normal to each other. Even in this case, the broadening of the ($10\bar{1}1$) peak can be deconvoluted to the above two components using

$$\Gamma = \sqrt{(\Gamma_c \cos(\chi))^2 + (\Gamma_a \sin(\chi))^2}\ , \qquad (1)$$

where Γ is FWHM of ($10\bar{1}1$) rocking curve, Γ_c is FWHM of (0002), Γ_a is FWHM of ($10\bar{1}0$), and χ is an inclination angle of the ($10\bar{1}1$) Bragg plane from (0002).

3. Results and Discussion

Fig. 1 shows the result of 2θ-ω scan. The diffraction peak of $2\theta \approx 31.3^o$ is a peak from WZ-InN (0002) and/or ZB-InN (101). These peaks have a small difference of 0.03 arcdegree on 2θ, so it is difficult to distinguish with each other. Additional diffraction peak at $2\theta \approx 32.9^o$ was observed at T_g of 600~675°C. This peak appears to be the diffraction from metallic indium (101). The precipitation of metallic indium indicates the nitrogen desorption from InN films due to the high T_g. Rocking curve of this peak shows a clear evidence of *c*-axis-oriented behavior. However, there will be no in-plane epitaxial relationship between this domain and sapphire, since any asymmetric diffraction peak of metallic indium was not observed.

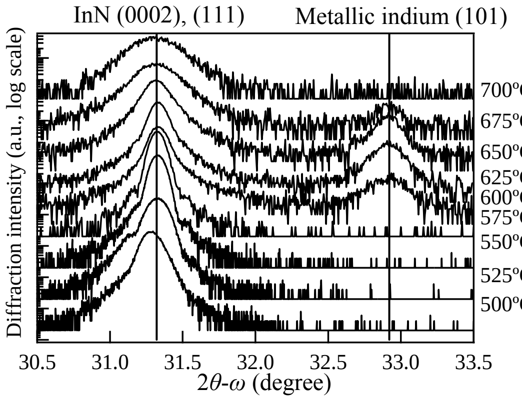

Figure 1 2θ-ω scan profiles of InN films. T_g are shown on right hand side of the figure.

Fig. 2 shows T_g dependence of FWHM of XRD rocking curve. TDDs were derived from FWHM using eq. (2, 3), which has been applied to GaN system by Lee *et al.* [4], and verified for InN by Gallinat *et al.* [5],

$$\rho_s = \Gamma_c^2 / 1.88c^2 , \quad (2)$$

$$\rho_e = \Gamma_a^2 / 1.88a^2 , \quad (3)$$

where ρ_s is a screw component and ρ_e is an edge component of TDDs, and *a, c* are lattice constants of *a*- and *c*-axis of the crystal, respectively. Screw and edge components of TDDs, ZB volume fraction, and integrated diffraction intensity ratio between metallic indium and InN have been plotted in fig. 3. As for the higher T_g regime between 600 and 700°C, the phase is almost pure WZ, however, the metallic indium peak was clearly observed. Both edge and screw components increased monotonically with increasing T_g. We assume that the precipitation of metallic indium affects both edge and screw components of TDDs. On the other hand, at the lower T_g regime between 500 and 575°C, the metallic indium peak was not observed at all, however, the volume of ZB is greater than that of WZ phase. Moreover, the edge component of TDDs dominated, and it is interesting to note that it decreased monotonically with increasing T_g, while the small amount of screw component

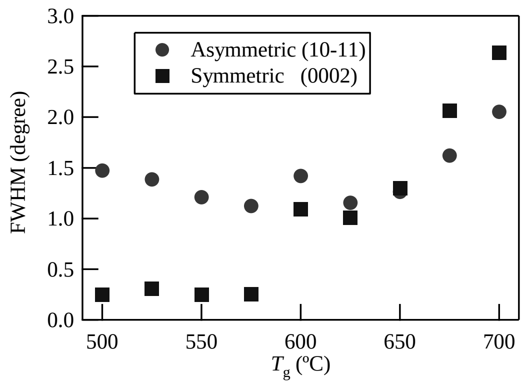

Figure 2 T_g dependence of FWHM of rocking curve.

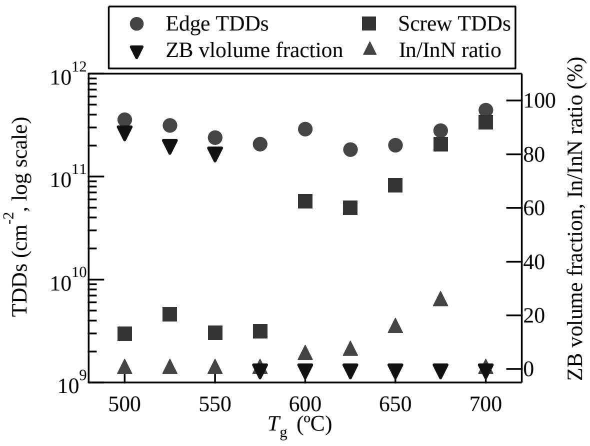

Figure 3 T_g dependence of threading dislocation densities, ZB volume fraction, and In/InN intensity ratio.

shows no clear dependence on T_g. Taking into account the gradual drop of ZB volume fraction when T_g is raised up to the intermediate T_g of 575°C, it is found that the edge component of TDDs shows an apparent correlation with the ZB inclusion.

This result can be explained by a structural model of ZB inclusion. Fig. 4 shows a schematic diagram of structure between WZ and ZB InN, where ZB-InN is formed on a WZ-InN domain by a spontaneous-60°-bond rotation around *c*-axis, as shown in the right-hand side of the figure. Dangling bonds are formed at the boundaries of domains with different phases. This increase of dangling bond density may result in the increase of edge dislocation density. Additionally, it is provable that the screw dislocation will not generated at this boundary since the atomic spacing along *c*-direction should not be varied even in the presence of this stacking faults. Further mechanism will be elucidated by an observation of microstructure using a transmission electron microscopy for proving the explanation proposed here and understanding the mechanism of the growth and ZB inclusion itself.

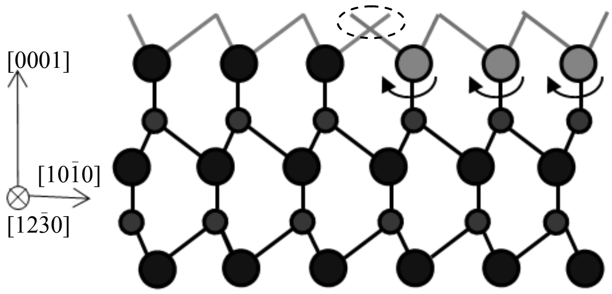

Figure 4 Model of ZB inclusion in WZ. Spontaneous-60°-bond rotation turns WZ-InN into ZB-InN. Dangling bonds form at the boundary between domains with different phases (circled area).

4. Conclusion

TDDs of PR-MOVPE-grown InN films were derived from XRD rocking curve measurements to investigate the effect of ZB inclusion into WZ phase. Results show an apparent correlation between ZB inclusion and edge TDDs.

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