Thermodynamic Analysis of Oxide Vapor Phase Epitaxy of GaN

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Introduction Gallium nitride (GaN) has superior physical properties compared to Si, and using GaN makes it possible to fabricate energy-saving and high-performance devices. For spread of GaN devices, cost reduction of wafer is necessary, and we are studying on the Oxide Vapor Phase Epitaxy (OVPE) which uses Ga_2O as a Ga precursor to manufacturing low-cost and high-quality GaN [1]. In OVPE and other vapor phase epitaxy (VPE) methods, there are many parameters for crystal growth, such as reactor geometry, total pressure, temperature, partial pressure of gases, flow velocity, total flow rate, and so on. Therefore, performing a thermodynamic analysis before the experiment to predict the effect of each parameter on crystal growth allows the experiment to proceed efficiently. In fact, detailed studies have been done on effect of each parameter on crystal growth in various VPE methods such as Metalorganic Vapor Phase Epitaxy (MOVPE), Hydride Vapor Phase Epitaxy (HVPE), etc. [2, 3]. On the other hand, in OVPE, there has been no study on the effect of each parameter on crystal growth by thermodynamic analysis. In this study, we performed thermodynamic analysis of OVPE to investigate how each parameter contributes to GaN growth in OVPE. In addition, we performed actual crystal growth and investigated whether the trends obtained by the thermodynamic analysis were consistent with the experimental results.

Results Before the experiment, we constructed a thermodynamic model. Six gas species were considered: Ga_2O, H_2O, NH_3, H_2, Ga, and inert gas (IG). The total pressure, $\sum P_i$, was fixed at 1.0 atm, the mole fraction of decomposed NH_3, α, was fixed at 0.30, the conversion ratio (Cr) of H_2O to Ga_2O in source zone was fixed at 0.60. The growth temperature, T, and the input partial pressures of Ga_2O, NH_3, and H_2, $P^{o}_{Ga_2O}$, $P^{o}_{NH_3}$, and $P^{o}_{H_2}$, were used as growth parameters. Fig. 1 (a) shows the equilibrium partial pressure of each gases as a function of the input H_2 partial pressure. The increase in the Ga_2O partial pressure indicates a decrease in the number of Ga atoms absorbed from the gas phase to the solid phase as GaN. Therefore, it is thermodynamically predicted that GaN is less likely to be generated as the increase in the input H_2 partial pressure. Fig. 1 (b) shows the growth rate as a function of the input H_2 partial pressure. The growth rate decreases with increasing input H_2 partial pressure. This result is consistent with the results predicted by the thermodynamic analysis. For other parameters, the results of thermodynamic analysis were also consistent with that of experiments. These results will be reported on the day of conference.

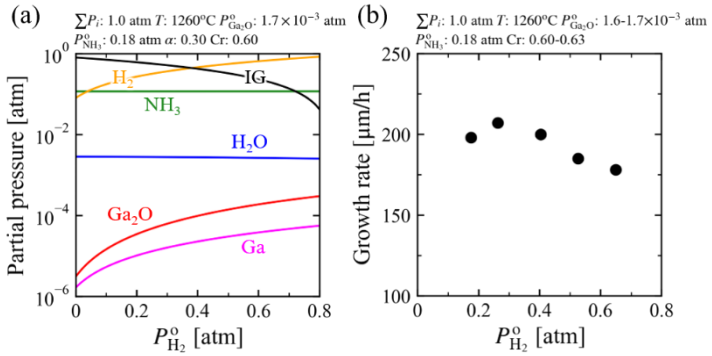

Fig. 1 (a) Calculated equilibrium partial pressures and (b) experimental growth rate as a function of the input partial pressure of H_2.

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