Thermodynamic Analysis of 3Ga-H Surface Reaction Process for GaN(0001)

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Clarification of the growth mechanism during GaN MOVPE is crucial for the practical realization of GaN power devices, with which significant energy savings can be achieved. In our previous study, we analyzed the TMG decomposition process based on a calculation of the formation free energy and the activation energy [1]. It has been reported that TMG loses methyl groups one by one which react with H_2 and finally decomposes into GaH in the vapor phase. We concluded that the main reaction gases on the surface of the substrate are GaH and NH_3, which are the gallium and nitrogen sources, respectively. So, we have been investigating the behavior of GaH and NH_3 on the surface of GaN. According to a previous study [2], the reconstructed surface is a 3Ga-H surface, which means the hydrogen terminates 3 out of the 4 top Ga, under the growth conditions of our previous study [1]. Therefore, in this study, we clarify the reactions of GaH and NH_3 and the growth process on a 3Ga-H surface.

In the analysis of the reactions given by GaH and NH_3 at a 3Ga-H surface, we calculated the formation energy of the various surface reactions such as the adsorption reactions of NH_3, NH_2, GaH, and so on. As a result, on a 3Ga-H surface, GaH decomposition occurs, and Ga atom is adsorbed while H2 is desorbed in the vapor phase. Only this reaction can occur at 1300 K, which is the substrate temperature. With this reaction, the surface of the substrate changes from Fig.1 (a) to (b). Moreover, this reaction is repeated. Therefore, at a 3Ga-H surface, GaH decomposes into Ga and H atoms, and the Ga atoms are adsorbed one after another as shown in the following figure; Fig.1 (a) → (b) → (c) → (d). Finally, all 3 H atoms on the surface are desorbed in the vapor phase and 3 Ga atoms are adsorbed onto the GaN surface, forming a Ga-rich layer. This is also considered to correspond to the formation of Ga droplets.

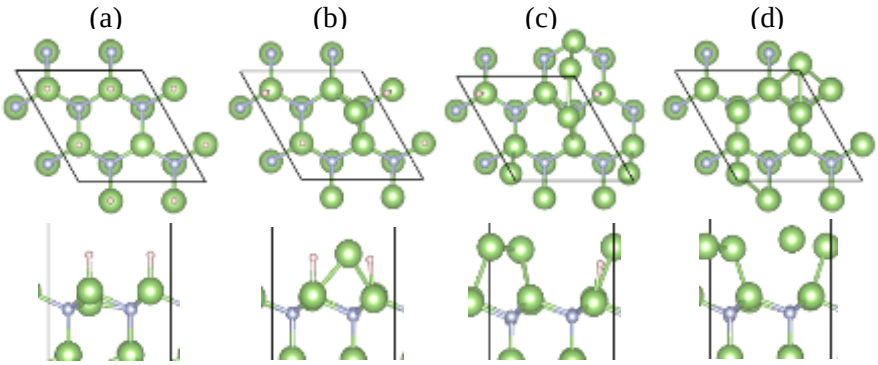

Figure 1. (a)-(d) Surface structure of 3 H, 2 H and 1 Ga, 1H and 2 Ga, and 3Ga adsorptions, respectively. Structure (a) shows the 3Ga-H surface.

[1] K. Sekiguchi et al., Jpn. J. Appl. Phys. **56.4S**, 04CJ04 (2017).

[2] A. Kusaba et al., Jpn. J. Appl. Phys. **56**, 070304 (2017).