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Novel approach for Growth Mechanism of Atomic Layer Epitaxy of GaAs and AlAs

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Abstract

In the GaAs and AlAs atomic-layer epitaxy (ALE), it has been experimentally found that AlAs layer is deposited by two mono layers (2 MLs) per one ALE cycle while GaAs layer is deposited by one mono layer (1 ML). We successfully explain this growth mechanism by the first-principles total energy calculation based on the density functional theory (DFT), which reveals that 2 MLs Al more stably absorbed on the As-terminated GaAs than 2 MLs Ga.

1. Introduction

In order to satisfy recent semiconductor device specifications, it is crucial for semiconductor production processes to develop thin film crystalline deposition technology [1]. Thus, atomic layer epitaxy (ALE) has been attracted because of its controllability of the atomic layer deposition due to the self-limiting deposition mechanism [2, 3]. In the GaAs and AlAs ALE, it has been experimentally found that AlAs layer is deposited by 2 MLs per one ALE cycle while GaAs layer is deposited by 1 ML [4, 5]. However, these growth mechanisms are not necessarily clear even though several hypotheses have been proposed.

In this study, we compare the stability of Ga and Al atoms on the As surface of GaAs substrate using first-principles total energy calculations. As a result, it is revealed that Al atoms were more stably adsorbed with two mono layers on the As-terminated GaAs substrate than Ga atoms, which suggests that 2 MLs deposition is favorable than 1 ML deposition for the AlAs ALE while 1 ML deposition is favorable for the GaAs.

2. Experimental

ALE Gas pulse sequence and apparatus configuration

We used trimethylaluminum (TMA), trimethylgallium (TMG), and AsH_3 for Al, Ga and As source gases, respectively. Figure 1 shows the gas pulse sequence. The gas pulses of TMA or TMG and AsH_3 were separately supply to the growth chamber purged by H_2 before each source gas supply. One ALE cycle is defined as shown in Fig. 1. ALE Growth was carried out in a low-pressure reactor designed for pulsed jet deposition as shown in Fig. 2[6].

Computational method

The PHASE code was used to evaluate the adsorption energies of the system [7]. The PHASE code is a program package for performing first-principles total energy calculations based on the density functional theory (DFT), and the ultra soft pseudo-potential scheme. We adopt a five-layered GaAs (001) 4 × 4 slab model as a substrate. The back surface (As-polar) is terminated with pseud hydrogens with +0.75*e*.

We define the adsorption energy (E_{ad}) :

$$E_{ad} = (E_{total} - E_{sub})/N - E_{atom} \qquad (1)$$

Where E_{total}, E_{sub}, E_{atom}, and N are total energy of the system, total energy of the substrate, total energy of a single adsorbed atom, and number of adsorbed atoms, respectively.

3. Result and discussion

Figure 3 shows the growth rate per cycle with respect to the supply time of TMG and TMA at 500℃. The self-limiting system of the ALE are clearly occurred with 1ML for GaAs and 2 MLs for AlAs. Figure 4 shows the results of the adsorption energy, which is physically calculated for Ga and Al on a stable As-terminated GaAs (100). We obtained the E_{ad}'s of -3.34 eV for 1 ML Ga, -3.13 eV for 2 MLs Ga, -3.78 eV for 1 ML Al, and -3.72 eV for 2 MLs Al, respectively.

At the growth temperature of 500℃, the E_{ad} of 2 MLs Ga is higher than that of 1 ML Ga by 0.21 eV, so it is difficult for 2 MLs Ga to be adsorbed on As-terminated GaAs. On the other hand, 2 MLs Al easily adsorbs because its E_{ad} is lower than that of 1 ML Al by only 0.06 eV.

From these results, we consider that the self-limiting mechanism of the GaAs ALE works with 1 ML Ga adsorbed on the As-terminated surface after TMG supply, and one GaAs atomic layer grows by following AsH_3 supply [Fig. 5]. On the other hand, the self-limiting does not occur until 2 MLs for the Al deposition, resulting in the AlAs two atomic layer growth after AsHs supply. [Fig. 6].

3. Conclusions

We compared the adsorption energy of Ga and Al on GaAs (100) surface using first-principles total energy calculations. Al atoms were found to adsorb more stably 2 MLs

on GaAs surface than Ga atoms. These results well explain that the 2 MLs growth AlAs per one ALE cycle.

References

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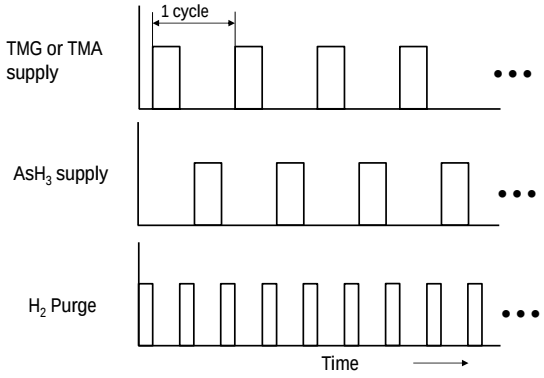

Fig.1 Gas pulse sequence for AlAs and GaAs ALE.

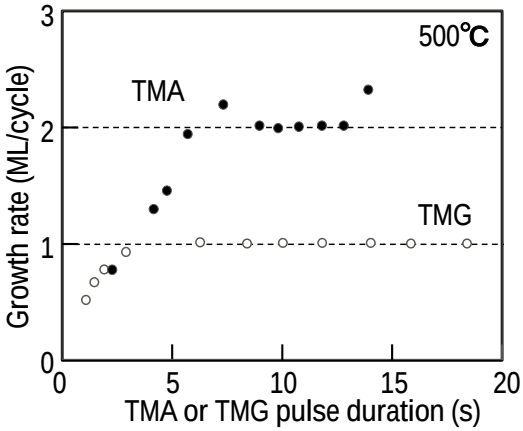

Fig. 3 Growth rate dependence of AlAs and GaAs as a function of TMA and TMG pulse duration at 500℃.

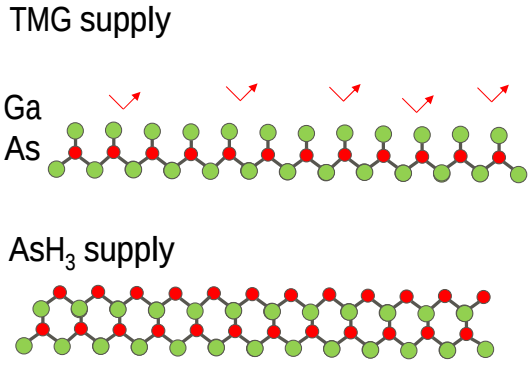

Fig. 5 Growth model for GaAs ALE.

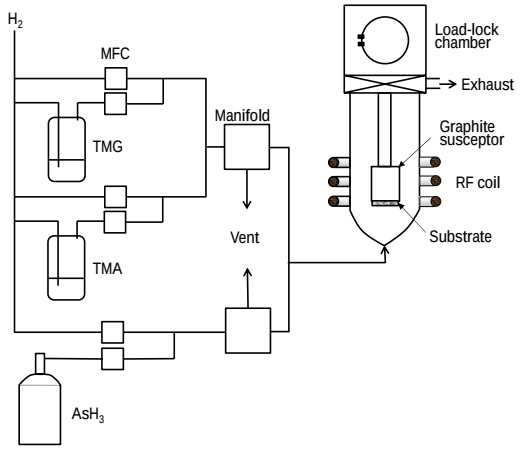

Fig. 2 Schematic diagram of the growth system for ALE.

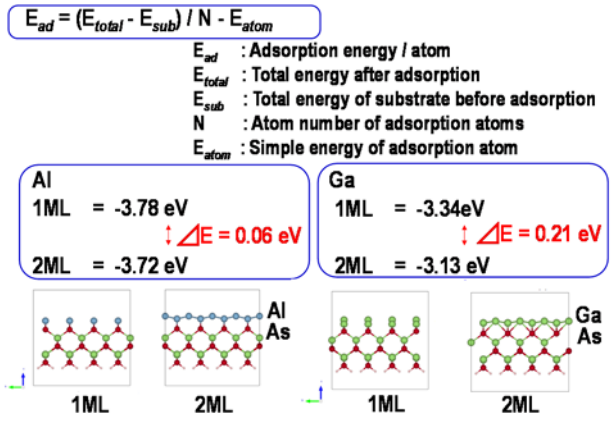

Fig. 4 Al and Ga atom adsorption energy on GaAs (001).

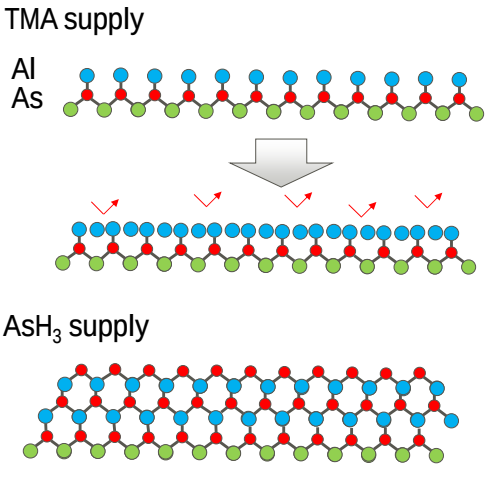

Fig. 6 Growth model for AlAs ALE.