Simulation Study For Rf-MBE Of Gan(0001) Using The First Principles Calculation And The Kinetic Monte Carlo Method.

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We investigate the dynamics for Ga and N adatoms on the GaN(0001)-(2 ×2) surface as a typical local structure for the Ga-rich growth condition using the first principle's calculation. We found that presumably, the nitrogen atom sit on the H3 site which is at the midpoint of the three Ga atoms in the topmost layer. The H3-N is most stable also for truncated GaN(0001) surface[1]. The additional Ga adatom comes to the ontop site of the H3-nitrogen. It will cause reversal polarity of Ga and N.

Therefore, the first principles calculation suggests us that Ga-rich condition is required for MBE growth of GaN(0001) with atomic nitrogen supply[2-4]. In order to check the theoretical prediction, we perform the kinetic Monte Carlo simulation with parameters for migration barrier energies of Ga and N which are determined by the first principles calculation. In the simulation, Ga can take the temporally site of T4 and N can take the temporally site of H3. Using the simulation program, we can choose temperature, supplied beam intensities, Ga/N ratio, beam flux modulation, and initial surface reconstruction.

After our results[2,3], we can obtain a guideline for the epitaxial growth of GaN(0001) surface . The key is to introduce gallium atoms before nitrogen supply. We never cut Ga beam supply during growth to prevent nitrogen adatom sit on the H3 site. The similar idea has been already presented in experimental trial[4]. The Ga-rich condition is also essential: it is necessary to keep a nitrogen adatom having two gallium adatom to occupy the two dangling bonds. The most stable atomic configuration for two gallium adatoms with one nitrogen adatom is that the nitrogen adatom takes the position similar to the Wurtzite structure. For the similar reason, using NH2 as a source of nitrogen work well, because the two bonds of the nitrogen is occupied by the two hydrogen atom.

Development of similar simulations for heteroepitaxial growth on sapphire and SiC substrates are now going on based on the first-principles calculation for these substrate[6,7].

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Figure Result of kMC simulation.
Left : rough surface case. (III/V ratio is 2, 800ºC).
Right: smooth surface case (III/V ratio is 1.2. 1000 ºC)