第一原理計算による GaN(0001)成長表面のステップ構造とエネルギー論

First-principle study of structures and energetics of atomic steps on GaN(0001) surface

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Gallium Nitride (GaN) is emerging as a candidate for the next generation of power switching applications owing to the material's superior properties. One of the advantages of GaN is its wide band-gap which make GaN more efficient in energy saving with consequent decrease of the excess of heat produced and with a higher yield in both emitted light and generated power. For a massive production of GaN devices, high-quality epitaxial GaN films with atomically smooth, damage-free surfaces are required. Metalorganic vapor phase epitaxy (MOVPE) is well-known to be the best method for a mass production of high quality GaN epitaxial films [1]. In MOVPE, trimethylgallium (TMG) and ammonia are the typical gas-phase precursors carried to the growth section by a carrier gas, H_2 or N_2. Kusaba *et al.* [2] reported that the growing surface under N_2 carrier gas condition is the Ga rich surface.

In this presentation, based on first-principles calculations as implemented in our real space density functional theory (RSDFT) package [3], we have systematically investigated the structural stability of mono-bilayer atomic steps on the Ga rich GaN (0001) surface toward both $[1\bar{1}00]$ and $[11\bar{2}0]$ direction. For steps toward $[1\bar{1}00]$, the edge atoms are classified into 4 types depending on their chemical species and the number of dangling bonds before structural reconstruction: i.e., Ga2, Ga3, N1 and N2. In our periodic-array slab models, due to the characteristics of wurtzite structure, 4 distinct pairs among the 4 step edges explained above appear, being labeled as Ga2Ga3, Ga2N1, N2N1, and N2Ga3. For example, the crystal structure of Ga2Ga3 is shown in Fig.1a. For steps toward $[11\bar{2}0]$, only one step structure type exists called Ga2N1-Ga3N2, as shown in Fig. 1b.

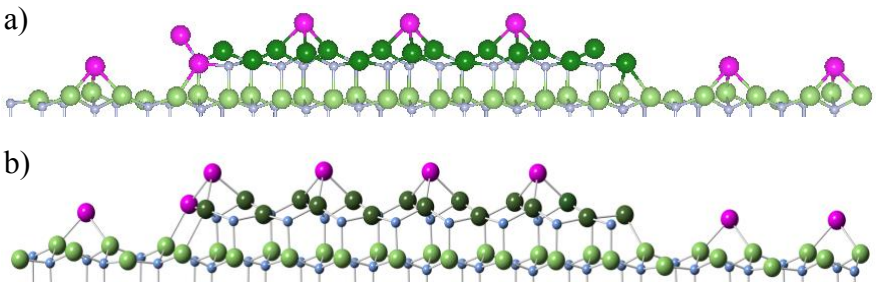

Figure 1: *Atomic structure of step structure of a) Ga2Ga3 along [$1\bar{1}00$] and b) Ga2N1-Ga3N2 along [$11\bar{2}0$] direction. N atoms are colored in blue. Ga atoms on lower terrace, upper terrace, and adatom are shown in light green, dark green, and pink, respectively.*

We have generally found that the more Ga-Ga bond is formed at the step edge, the more stable that system is. For steps toward $[1\bar{1}00]$, the most stable step edge is Ga2Ga3 in which Ga on upper terrace (UT) makes the Ga-Ga weak bond with Ga on lower terrace (LT) on both Ga2 and Ga3 side. For steps toward $[11\bar{2}0]$, the most stable step edge is the structure in which there are Ga adatoms located near the Ga2N1 side on both UT and LT, and the Ga adatom on UT and LT is on the same side. Our previous calculation shows that the Ga-Ga weak bonds is the hotspot for the N incorporation [4], thus the step edge in which there are Ga-Ga weak bonds may promote N incorporation, or in another word, enhance GaN thin film growth, in accordance with the generally observed step-flow epitaxy.

References:

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