First principle analysis of ammonia adsorption and desorption on GaN surface

Kieu My Bui[1], Junichi Iwata[2], Yasuteru Shigeta[1]

[1] Center for Computational Sciences, University of Tsukuba, Japan
[2] Graduate School of Engineering, the University of Tokyo, Japan

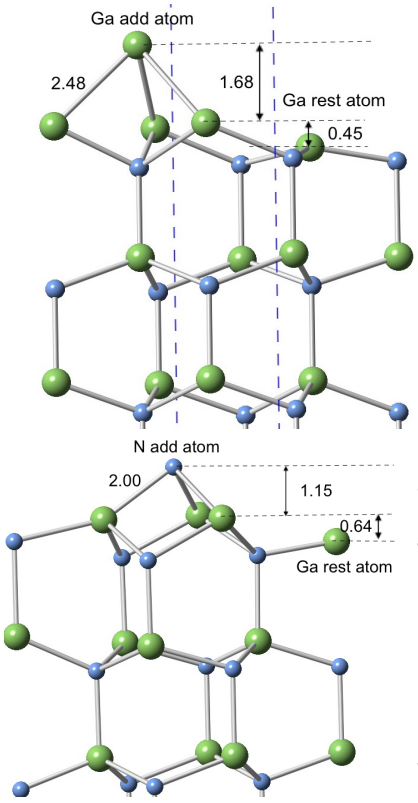

Figure 1: (a) Ga-hcp and (b) N-fcc adatom configurations. All lengths are in Å.

Gallium nitride (GaN), which belongs to the III-V family, is attracting tremendous attention recently. Owing to having a wide band-gap, GaN is used in optoelectronics, photonics, high-power, and high-temperature operation devices. Having well knowledge about the surface adsorption and deposition mechanisms for different precursors is necessary to improve thin-film crystalline quality and growth process requirements. Using density functional theory (DFT) method, as implemented in real-space density functional theory (RSDFT),[1] we aim to theoretically investigate the reaction mechanism of GaN on (0001) surface from ammonia (NH_3) precursor. The calculated lattice parameters (a = 3.2 Å, c = 5.2 Å) are in accordance with experiments.[2] The 2x2 surface reconstruction structure is obtained. We found that, in agreement with previous study by Ranganathan,[3] a Ga adatom is the most favorable to form at hcp site, while a N adatom is at fcc site. The obtained structures for both the Ga and N adatom are shown in Figure 1. More detailed results are presented at the poster.

References

1. Iwata, J., Takahashi, D., Oshiyama, A., Boku, T., Shiraishi, K., Okada, S., Yabana, K., Journal of Computational Physics 2010, **229**, 2339.
2. Schulz, H. and Thiemann, K.. Solid State Commun. 1977, 23, 815–819.
3. Chugh, M. and Ranganathan, M. , J. Phys. Chem. C 2016, **120**, 8076.