Computational study on thermochemical processes of adatoms on the GaN (0001) surface during GaN MOCVD

원용선*
삼성전기
(yongsun.won@samsung.com*)

A computational study on thermochemical processes – adsorption, diffusion, and dissociation – of various reactant species on the GaN (0001) surface was performed using DFT calculations combined with a GaN (0001) surface cluster. The energetics including transition state search of NH3(ad) dissociation through N(ad) proposed that the dissociation of NH3(ad) to NH(ad) occur fast with less kinetic barriers. An analysis including surface diffusion of adatoms demonstrated that Ga(ad) and NH(ad) become primary reactant species for 2D film growth, while the N(ad) develops rather into a nucleation center. It was thus suggested that Ga-rich condition and the control of the dissociation of NH3(ad) are necessary to improve epitaxial film quality. In addition, the H(ad) resulted from NH3(ad) dissociation was found to adsorb stably on the surface and contribute the etching of GaN(s). An experimental study with NH3(g) gradually substituted by H2(g) during GaN growth was consistent with computational propositions.