

Ordering phenomena and formation of nanostructures in  $\text{In}_x\text{Ga}_{1-x}\text{N}$  layers coherently grown on GaN(0001)

이상현<sup>†</sup>, Christoph Freysoldt<sup>1</sup>, Joerg Neugebauer<sup>1</sup>

KIST 연료전지연구센터; <sup>1</sup>Max-Planck-Institut fuer Eisenforschung GmbH  
(sang@kist.re.kr<sup>†</sup>)

We study the impact that local strain effects have on the spatial distribution of In in coherent  $\text{In}_x\text{Ga}_{1-x}\text{N}$  grown epitaxially on GaN(0001) using an effective crystal growth modeling technique that combines a semi-grand-canonical Monte Carlo simulation with an ab initio parameterized empirical force field. [Physical Review B 90, 245301(2014)] Our calculations show that  $\text{In}_x\text{Ga}_{1-x}\text{N}$  epitaxial layers exhibit a strong tendency towards ordering, as highlighted by the formation of a vertical stack of the  $\sqrt{3}\times\sqrt{3}$  patterned layers along the direction. The ordering phenomena are identified as a key factor that determines lateral phase separation in  $\text{In}_x\text{Ga}_{1-x}\text{N}$  epitaxial layers at the nanometer scale. Consequences of this nanophase separation for the enhanced radiative emission through carrier localization in  $\text{In}_x\text{Ga}_{1-x}\text{N}$  of  $x < 1/3$  are discussed.