

Empirical Interatomic Potential Calculation for Compositional Instability of III-V nitride alloys in lattice mismatch systems

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GaN-based III-V semiconductor alloys have already been used for optical devices such as high brightness blue and green light-emitting diodes (LEDs) [1]. These optical devices are composed of AlGaIn/InGaIn/GaN double heterostructure. In these materials with heterointerfaces, lattice mismatch between epitaxial layer and bottom layer has a great influence on growth mechanism and film quality. Furthermore, it is known that compositional instability of the InGaIn alloy plays an important role in the self-formation of quantum dots which enhance the lasing characteristic [2]. However, very few calculations for the compositional instability incorporating the contribution of lattice mismatch at heterointerfaces were performed [3]. In this work, we systematically investigated the compositional instability for InGaIn based on excess energy calculations for the bulk InGaIn, InGaIn/(0001)GaIn and InGaIn/(0001)InN. In the calculation procedure, empirical interatomic potentials are used and lattice constraint from bottom layer such as GaIn and InN is incorporated.

Cohesive energies of the semiconductors with wurtzite structure (E_w) is given by

$$E_w = \frac{1}{2} \sum_{i,j} V_{ij} + \Delta E_w . \quad (1)$$

$$V_{ij} = A \exp[-(r_{ij} - R_i)^g] \times [\exp(-q r_{ij}) - B_0 \exp(-l r_{ij}) \frac{G(h)}{Z^a}] . \quad (2)$$

where V_{ij} is the empirical interatomic potential for i and j atoms within the first and second nearest neighbors [4] and ΔE_w the energy contribution beyond short range interactions considered in V_{ij} [5]. Here, r_{ij} is the distance between the atoms, R_i the minimum distance between neighbors, Z the effective coordination number and $G(h)$ the bond bending term for tetrahedrally bonded atom pairs. In the cohesive energy calculations of the epi-layers, the lattice parameters a of basal plane are fixed to be those of GaIn and InN, while another lattice parameters c and displacement of atoms in

the layers are varied to minimize the system energy. The excess energy $\Delta E(x)$ is written in the following equation:

$$\Delta E(x) = E_x - \{x E_{1.0} + (1-x) E_{0.0}\} , \quad (3)$$

where E_x , $E_{1.0}$ and $E_{0.0}$ are the total system energies estimated from the equations (1) and (2) for $\text{In}_x\text{Ga}_{1-x}\text{N}$ alloy, InN and GaN, respectively. Figures 1(a), (b) and (c) show the calculated excess energies for bulk InGaN, InGaN/GaN and InGaN/InN, respectively. In Figs. 1(b) and (c), we found that the asymmetric nature of the excess energy curves is emphasized compared with that for bulk InGaN. Because of the difference, the excess energies for $\text{In}_x\text{Ga}_{1-x}\text{N}$ alloy on GaN layer is larger than that for bulk alloy at $x > 0.65$. The result also indicates that the alloys with a large indium mole fraction are less stable on the GaN layers than bulk state. On the other hand, the excess energy for the alloy on the InN layer is smaller than that for bulk alloy over almost entire composition range. This implies that $\text{In}_x\text{Ga}_{1-x}\text{N}$ becomes more stable on the InN layers than bulk state. These results suggest that incorporating the contribution of lattice constraint is indispensable to predict the compositional instability for InGaN alloy grown on substrates. Systematic examinations for the other III-V nitride alloys are now in progress to obtain the fundamental data applicable to a thermodynamic analysis for vapor phase epitaxial growth [6].

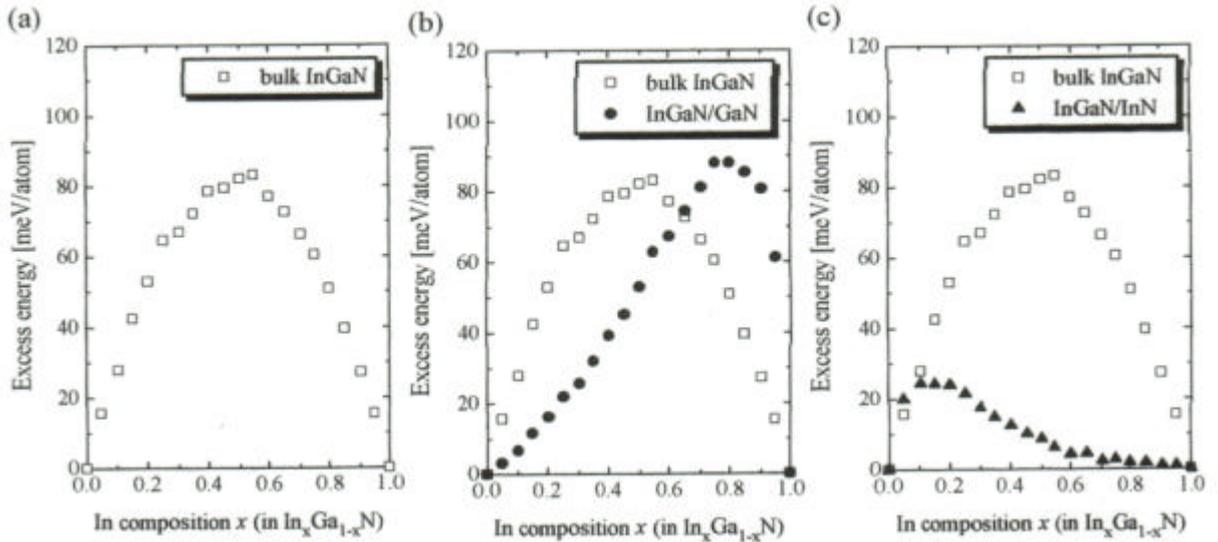


Fig. 1 Calculated change in excess energy with indium composition: (a) bulk InGaN, (b) InGaN on GaN, (c) InGaN on InN.

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