Alloy phase diagram of InGaN/GaN(0001) pseudomorphic thin film and strain-induced superlattice structure: Monte Carlo simulation study

A. Mori*, K.Akasaka*, T. Ito**, S. Yanagiya*, and T. Inoue*
** Department of Optical Science and Technology, Faculty of Engineering, The University of Tokushima, Tokushima 770-8506, Japan*
*** Department of Physics Engineering, Faculty of Engineering, Mie University,1515 Kamihama, Tsu 514-8507, Japan*

Keywords: InGaN/GaN, alloy phase diagram, natural superlattice, Monte Carlo

InGaN materials have been expected to cover the entire visible light region. $In_xGa_{1-x}N$ materials with large x were, however, achieved very recently. We have conjecture that the difficulty is due to miscibility gap at the large x region. To elucidate, we performed semi-grand canonical ($N\Delta\mu PT$-constant) Monte Carlo (MC) simulation [1]; where $\Delta\mu \equiv \mu_{\mathrm{InN}} - \mu_{\mathrm{GaN}}$ with InGaN being stichiometric. Though the alloy phase diagram was incomplete yet, it supports the conjecture [2,3]. The multi valley free energy landscape, which caused the difficulty, was found to originate in the strain-induced superlattice ordering due to the substrate [3,4]. The final goal is construction of the alloy phase diagram with sub-branches of difference superlattice ordering being distinguished.

Due to discontinuity the thermodynamic integrals to calculate the free energy difference were just approximately done [2,3]. We circumvent relying on the acceptance ratio method [5]. We obtain the free energy difference between phases i (i = 1,2) as the difference between C's at two intersecting points between $Y^{(i)}(C) = \left\langle \left[1+\exp\left(\beta U^{\mathrm{ref}} - \beta U + C\right)\right]^{-1} \right\rangle_U^{(i)}$ and $Y_{\mathrm{ref}}(C) = \left\langle \left[1+\exp\left(\beta U - \beta U^{\mathrm{ref}} - C\right)\right]^{-1} \right\rangle_{U^{\mathrm{ref}}}$, where $\beta = \left(k_B T\right)^{-1}$, the subscript under the brackets denotes the interaction potential in MC simulation, the superscript (i) indicates that the sampling is made for phase (i). We note that PV and $N_{\mathrm{In}}\Delta\mu$ contributions cancel if, respectively, βP and $\beta\Delta\mu$ are identical for the system under investigation and the reference. An empirical interatomic potential is used for the system potential U, and a harmonic potential as the reference potential U^{ref}. We have successfully calculated the free energy difference between sub-branches.

1. D. A. Kofke: Adv. Chem. Phys.**105** (1999) 405.
2. A. Mori, B. B. Laird, Y. Kangawa, T. Ito, and A. Koukitu, Mater. Phys. Mech. **6** (2003) 49; Russian J. Phys. Chem. **77** (2003) suppl. 1, S21.
3. A. Mori, T. Ito, and B. B. Laird, Curr. Top. Cryst. Growth Res., in press.
4. A. Mori, T. Ito Y, Kangawa, and A. Koukitu, Phys. Stat. Sol. C **0** (2003) 2486.
5. C. H. Benett, J. Comp. Phys. **22** (1976) 245.

Subject Number: #7, Preference: Poster, E-mail : mori@opt.tokushima-u.ac.jp