25aYB-1

Monte Carlo simulation for alloy phase diagram of InGaN thin film pseudomorphic to GaN (0001) substrate

A. Mori, K. Akasaka, T. Ito,[A]
S. Yanagiya, and T. Inoue

Fac. Eng., Univ. Tokushima
[A]Fac. Eng., Mie Univ.

InGaN materials are used for blue-green light emitting devices. InGaN-based light emitting devices can, in principle, cover the entire visible light region. It was, however, quite recent that InGaN materials with the high indium content was accomplished. We have conjectured the difficulty was due to the existence of miscibility gap at the high In content region.

We have performed semi-grand canonical ($N\Delta\mu PT$-constant) Monte Carlo (MC) simulation;[1] where $\Delta\mu$ denotes $\mu_{InN}-\mu_{GaN}$ with InGaN being treated as stichiometric. Results, which support the above conjecture,[2] have been obtained, though the alloy phase has not been completed yet. Multi stability phenomena have prevented the completion of the phase diagram. It is has been found that the multi valley free energy landscape originates in the superlattice ordering induced by the strain from the substrate.[3]

Previously we tried to calculate the free energy difference between Ga-rich and In-rich phases. Discontinuity, however, made the thermodynamic integral difficult. To overcome this difficulty we rely on the acceptance ratio method.[4]

For the sweep throughout the free energy landscape we employ the exchange MC method.[5] The equation of the principle of detailed balance for swap of tow systems, similar to the usual one[5] has readily been made.

1) D. A. Kofke: Adv. Chem. Phys.105 (1999) 405.
2) A. Mori *et al.*: Mater. Phys. Mech. 6 (2003) 49; Russian J. Phys. Chem. 77 (2003) suppl. 1, S21.
3) A. Mori *et al.*: Phys. Stat. Sol. C 0 (2003) 2486.
4) C. H. Benett: J. Comp. Phys. 22 (1976) 245.
5) K. Fukishima and K. Nemoto: J. Phys. Soc. Jpn. 65 (1996) 1604.