Superlattice structure along the phase boundary in alloy phase diagram of InGaN thin film by Monte Carlo simulations

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Semigrand canonical (SGC) Monte Carlo (MC) simulation has been performed for $In_xGa_{1-x}N$ thin film pseudomorphic to the GaN (0001) substrate. In the SGC ensemble the chemical potential differences, $\Delta\mu=\mu_{In}-\mu_{Ga}$, is given. The species identity

changes are attempted in the SGC MC simulation with the total number of particles being fixed. Free energies of Ga-rich and In-rich phases at a temperature T=800K have been calculated by integrating the composition (the mole fraction, $x_{\mathrm{In}}=n_{\mathrm{In}}/(n_{\mathrm{In}}+n_{\mathrm{Ga}})$) by $\Delta\mu$ in this case. Once one obtained a phase equilibrium condition $\Delta\mu(T)$ at T, one can search the phase equilibrium condition at the adjacent temperature $T+\mathrm{d}T$ with the help $\mathrm{d}(\Delta\mu)/\mathrm{d}T = -\Delta h/T\Delta x$, where Δh and Δx are enthalpy difference and the composition difference, respectively. We have applied this method, the Gibbs-Duhem integration technique, to outline the boundary of the $In_xGa_{1-x}N$/GaN alloy phase diagram. We have looked into the detailed structure of the $In_xGa_{1-x}N$/GaN along the Ga-rich boundary and found the superlattice structure.

KYEWORDS

InGaN/GaN, thin film, pseudomorphic, alloy phase diagram, strain, ordering, superlattice, Monte