Abstract Submitted
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First-Principles epitaxial phase-diagram, short-range order, microstructure and electronic properties of (In,Ga)N zincblende alloys on GaN[1] ZHE LIU, PAULO PIQUINI, ALEX ZUNGER, National Renewable Energy Lab., Golden, CO 80401 — A first-principle total energy cluster expansion method is developed to study thermodynamic properties of epitaxial semiconductor alloys coherent to substrate (i.e., $<$ critical thickness h_c), in which coherent strain energy as a function of atomic configuration is explicitly described. The search for epitaxial ground state structures of (In, Ga)N alloy grown on GaN (001) substrate concludes that epitaxial strain suppresses phase separation, which is normally observed for bulk (In,Ga)N alloy and relaxed films. Two (102) superlattices: $(InN)_2/(GaN)_2$ and $(InN)_4/(GaN)_1$ are determined to be the epitaxial ground state structures. Composition-temperature phase diagram calculated by Monte Carlo method shows that homogeneous solid solution phase is thermodynamic stable at typical growth temperature of blue and green LED by MBE and MOCVD (x(In)$\sim 0.20 - 0.30$ and $h_c \sim 10 - 30$nm). Such calculated phase diagram can be used to understand the controversy regarding atomic microstructures in (In,Ga)N quantum well devices. Short-range-ordering of the solid solution phase and its influence on the electronic properties are also discussed.

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