Energetics and electronic properties of GaN nanowires with embedded $In_xGa_{1-x}N$ nanodisks

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In the present work we investigate the influence of strain on the energetics and the electronic properties of nanowires (NWs) consisted of a GaN base part followed by a superlattice part of successive $In_xGa_{1-x}N$ nanodisks (NDs) (x ranging from 3% to 25%) separated by GaN spacers. $In_xGa_{1-x}N$/GaN supercells were modelled and simulations were implemented with the LAMMPS code for Molecular Dynamics, using a bond-order interatomic potential under the III-species environment approach [1], and with AIMPRO for Density Functional Theory calculations.
It has been found by both simulation approaches that among three possible types of strain (biaxial, hydrostatic and uniaxial), the biaxially strained NW superlattice is the one with the lowest excess energy for all indium concentrations. However the energy difference between biaxially and hydrostatically strained states for In concentration below 10% in the NDs is small. It is deduced that up to ~10% of In, the hydrostatic strain state is competitive with the biaxial and above this value the preferable strain model is the biaxial one. Hence, hydrostatic and biaxial strain components should be both considered in the embedded NDs and they are of different physical origin. The biaxial strain originates from growth on lattice mismatched layers, while the hydrostatic strain component originates from the lateral surfaces. Concerning the optoelectronic properties, the strained $In_xGa_{1-x}N$ NDs do not induce states in the bandgap of the NWs. However, a bowing parameter of 4.5 should be taken into account in the quadratic Vegard's equation for the bandgaps in the different concentrations for such $In_xGa_{1-x}N$ ND in GaN NW structure.

References

[1] Kioseoglou et al, pss (b) **245** (2008) pp 1118-1124

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