

Influence of biaxial strain on thermodynamic, structural and electronic properties of $\text{In}_x\text{Ga}_{1-x}\text{N}$ alloys

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The optical properties of $\text{In}_x\text{Ga}_{1-x}\text{N}$ layers and their performance in optoelectronic devices are strongly influenced by tendencies of phase separation and the composition dependence of the fundamental energy gap. There are strong indications for a miscibility gap independent of the wurtzite or zinc-blende polytype of the compound [1]. The deviations $-bx(1-x)$ from a linear composition dependence of the energy gap can be remarkable. Thereby, the magnitude of the bowing parameter seems to vary with the method of determination. Extreme values of $b = 1.0$ eV [2] or $b = 3.8$ eV [3] are discussed in the literature. A common feature of the epitaxy of $\text{In}_x\text{Ga}_{1-x}\text{N}$ layers is the strain influence. There is an internal strain due to the differences in the equilibrium lattice constants of GaN and InN. In addition, an external biaxial strain due to lattice mismatch with the substrate and the difference in the thermal expansion coefficients between the ternary compound and substrate may occur.

In this work we present a theoretical study of thermodynamic, structural and electronic properties of strained $\text{In}_x\text{Ga}_{1-x}\text{N}$ alloys. The interplay of composition fluctuations, miscibility gap and strain influence is studied. The cubic polytype is considered as a model system but changes due to the wurtzite structure are also discussed. The calculations are based on first-principles methods [4] and a combination of generalized quasichemical approximation (GQCA) and cluster-expansion method [5]. The macroscopic alloy is divided into clusters. Each cluster with a certain number of In and Ga atoms is realized with a certain probability. The structure of each cluster is optimized with respect to two lattice constants a_{\perp} and a_{\parallel} . Fixing the in-plane lattice constant the effect of biaxial strain is modelled. The total-energy and electronic-structure calculations for each cluster are performed using a pseudopotential-plane-wave code. According to the fact that a cluster takes its own equilibrium volume, the biaxial strain in each cluster should be different. An inhomogeneous strain distribution occurs on a length scale of the cluster sizes.

In the strain-free limit we find a phase diagram that indicates a wide miscibility gap. The structural properties of the $\text{In}_x\text{Ga}_{1-x}\text{N}$ alloys, in particular the bond lengths and second-nearest-neighbor distances, are in good agreement with recent measurements [6]. We predict a remarkable influence of the composition fluctuations in a given random alloy. They are accompanied by gap fluctuations which allow the definition of a minimum gap and an average gap of the alloy. The bowing of both gaps are completely different and, hence, may explain seemingly contradicting experimental

findings from different measurement techniques.

The influence of biaxial strain is extremely important. We find a remarkable suppression of phase-separation tendencies in $\text{In}_x\text{Ga}_{1-x}\text{N}$. For extreme biaxial strains corresponding to pseudomorphic growth with the lattice constants of GaN or InN we calculate a vanishing critical temperature. This can be seen in Fig.1 where is depicted the mixing free energy ΔF of inhomogeneously strained $\text{In}_x\text{Ga}_{1-x}\text{N}$ alloys versus x for two different temperatures $T=700$ and $T=950$ K. In Fig.2 we show the average energy gap E_g versus composition (a) and the accompanying gap fluctuation (*rms* deviation) ΔE_g (b) for $\text{In}_x\text{Ga}_{1-x}\text{N}$ grown on substrates with lattice constants a_{GaN} and a_{InN} . The bowing of the gap is generally reduced in the presence of strain. This holds not only for the average gap. Strain also reduces drastically the gap fluctuations. This gives rise to a reduction also of the bowing in the minimum gap.

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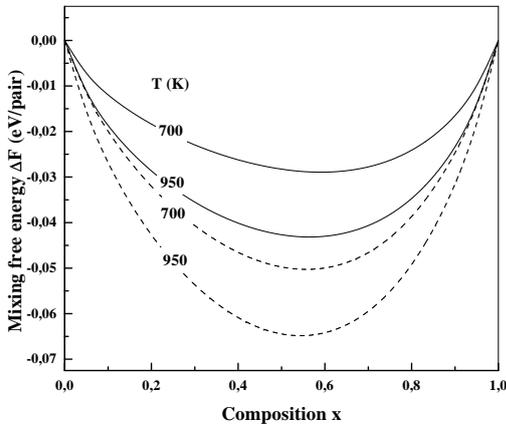


FIG. 1: Mixing free energy of strained $\text{In}_x\text{Ga}_{1-x}\text{N}$ versus x for two temperatures $T=700$ and 950 K. The biaxial strain is defined by $a_{||} = a_{\text{GaN}}$ (solid line) and $a_{||} = a_{\text{InN}}$ (dashed line).

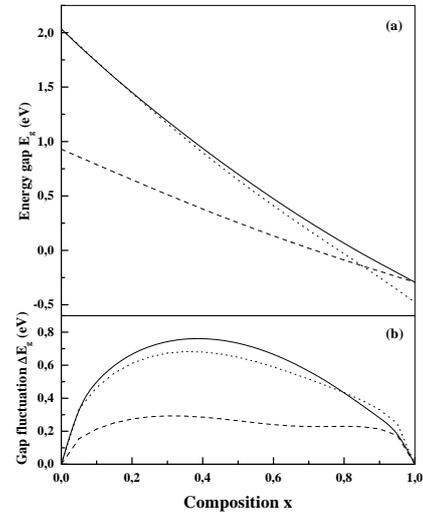


FIG. 2: Average energy gap E_g (a) and gap fluctuation ΔE_g (b) versus composition for $\text{In}_x\text{Ga}_{1-x}\text{N}$; unstrained (solid line), $a_{||} = a_{\text{GaN}}$ (dotted line), $a_{||} = a_{\text{InN}}$ (dashed line).