

Abstract Submitted  
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**First-principles study of the thermodynamics of InGaN alloys** C.K. GAN, Institute of High Performance Computing, Singapore, D.J. SROLOVITZ, Physics Department, Yeshiva University — We present the most rigorous density-functional study [1] to date of the thermodynamics of  $\text{In}_x\text{Ga}_{1-x}\text{N}$  alloys. These systems have attracted considerable theoretical and experimental attention due to its enormous potential for high-power, high-frequency, and high-temperature optoelectronic applications. Theoretical calculations of the pseudo-binary phase diagram require an accurate description of the interactions between the constituent atoms, a good representation of a random alloy, the inclusion of the effect of lattice vibrations, and a consideration of the configurational entropy. We have used accurate density-functional theory to calculate the heat of formation of the alloy (represented by special quasi-random structures), as well as the phonon spectra for the lattice vibrational contribution to the free energy. We find that the wurtzite structure is always more stable than the zinc-blende structure for all temperatures and compositions investigated, in agreement with experiment. We find that the lattice vibrations lead to a reduction of the critical temperature by more than 20%, leading to a temperature of 1654 K and 1771 K for the wurtzite and zinc-blende structures, respectively. The lattice vibrations also change the shape of the binodal and spinodal curves. This result suggests that quaternary alloy additions may increase the vibrational contribution to the stability of the disordered phase. Our predicted phase diagrams have been used to interpret several key experiment measurements on MOCVD  $\text{In}_x\text{Ga}_{1-x}\text{N}$  films. The importance of  $\text{In}_x\text{Ga}_{1-x}\text{N}$  alloys has also prompted the study of the surface thermodynamics of InN [2]. New results will be presented.

[1] C. K. Gan, Y. P. Feng, and D. J. Srolovitz, Phys. Rev. B, **73** 235214 (2006).

[2] C. K. Gan and D. J. Srolovitz, Phys. Rev. B., **74** 115319 (2006).

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