Structural and electronic properties of GaN_xAs_{1-x} alloys

Abstract

The structural and electronic properties of cubic GaN_xAs_{1-x} with N-concentration varying between 0.0 and 1.0 with step of 0.25 were investigated using the full potential–linearized augmented plane wave (FP-LAPW) method. We have used the local density approximation (LDA) and the generalized gradient approximation (GGA) for the exchange and correlation potential. In addition the Engel-Vosko generalized gradient approximation (EVGGA) was used for the band-structure calculations. The structural properties of the binary and ternary alloys were investigated. The electronic band structure, total and partial density of states as well as the electron charge density were determined for both the binary and their related ternary alloys. The energy gap of the alloys decreases when we move from x=0.0 to 0.25; then it increases by a factor of about 1.8 when we move from 0.25 to 0.5, 0.75 and 1.0 using EVGGA. For both LDA and GGA moving from x=0.0 to 0.25 causes the band gap to close, showing the metallic nature of the $GaN_{0.25}As_{0.75}$ alloy. When the composition of N moves through x=0.25, 0.5, 0.75 and 1, the band gap increases.