Structural and electronic properties of bulk GaP and AlP and their $(GaP)_n$ / $(AlP)_n$ superlattices

Abstract

The structural and the electronic properties of binary GaP and AlP compounds and their $(GaP)_n$ / $(AlP)_n$ superlattices are investigated using the recent version of the first-principles full potential linear muffin-tin orbitals method (FP-LMTO) (Lmtart 7.0). The structural parameters and the pressures at which these compounds undergo structural phase transition from zinc-blende (B3) to the rocksalt (B1) are determined. From the results of the electronic properties we find that the parent materials (GaP, AlP) have indirect bandgaps. The resemblances between GaP and AlP and their small lattice mismatch led us to perform investigations on zinc-blende/zinc-blende $(GaP)_n$ / $(AlP)_n$ for n = 1, 2 and 3 monolayer. Our calculations performed for band structure and density of state show an indirect band gap superlattices for n = 1 and 2 and a direct band gap for n = 3. Details of the electronic structure of superlattices are discussed. An excellent agreement was found between our results and those of other theoretical predictions and experimental measurements.