First-principles calculations of the structural, electronic and optical properties of cubic $B_xGa_{1-x}As$ alloys

Abstract

Density functional calculations are performed to study the structural, electronic and optical properties of technologically important $B_xGa_{1-x}As$ ternary alloys. The calculations are based on the total-energy calculations within the full-potential augmented plane-wave (FP-LAPW) method. For exchange-correlation potential, local density approximation (LDA) and the generalized gradient approximation (GGA) have been used. The structural properties, including lattice constants, bulk modulus and their pressure derivatives, are in very good agreement with the available experimental and theoretical data. The electronic band structure, density of states for the binary compounds and their ternary alloys are given. The dielectric function and the refractive index are also calculated using different models. The obtained results compare very well with previous calculations and experimental measurements.