Bismuth in gallium arsenide: Structural and electronic properties of $GaAs_{1-x}Bi_x$ alloys

Abstract

The structural and electronic properties of cubic $GaAs_{1-x}Bi_x$ alloys with bismuth concentration 0.0, 0.25, 0.50, 0.75 and 1.0 are studied using the 'special quasi-random structures' (SQS) approach of Zunger along with the generalized gradient approximation (GGA) and the EngelVosko generalized gradient approximation (EV-GGA). The lattice constant, bulk modulus, derivative of bulk modulus and energy gap vary with bismuth concentration nonlinearly. The present calculations show that the band gap decreases substantially with increasing bismuthconcentration and that spinorbit coupling influences the nature of bonding at high Bi concentrations.