Abstract

The sp3s*d5 empirical tight-binding approach is used to study some properties of the electronic structure in a group of III-V zincblende semiconductors which are of most interest to electronics and optoelectronics. Particularly, it is investigated the influence of [111] uniaxial strain upon these properties. We make use of a formulation based on the elasticity theory to properly derive the relative positions of the nearest neighbors in the lattice and, consequently, write down the set of four basis vectors centered at the anion. Special attention is paid to the inclusion of the internal deformation effect. We present the variation of the L-, X- and L-related energy gaps and conduction band effective masses as functions of the uniaxial strain in the case of AlAs, GaAs, InAs, GaP. Comparison with experimental reports on indirect interband transitions in bulk GaP under compressive strain gives very good agreement between these reports and the calculated variation of X-related energy gap as a function of the strain.

Keywords

Tight-binding, III-V materials, electronic structure, uniaxial strain.