FP-APW + lo calculations of the elastic properties in zinc-blende III-P compounds under pressure effects

Abstract

The effect of high-pressures on the structural and elastic properties of XP zinc-blende compounds, with X = B, Al, Ga and In, has been investigated using the full-potential augmented plane wave plus local orbitals method within density functional theory. The bulk properties, including lattice constant, bulk modulus and its pressure derivative are obtained. The elastic constants and their pressure dependence are calculated using total energy variation with strain technique. We derived the bulk modulus, shear modulus, Young's modulus and Poisson's ratio for ideal polycrystalline XP aggregates. We estimated the Debye temperature of XP compounds from the average sound velocity. Our results are in reasonable agreement with the available theoretical and experimental data.

Keywords: III-P compounds; FP-APW + lo; Elastic moduli; Pressure effect