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FP-LMTO method to calculate the structural, thermodynamic and optoelectronic properties of SixGe1-xC alloys

Abstract

The structural and electronic properties of the ternary Si xGe1-xC alloys have been calculated using the full-potential linear muffin-tin-orbital (FP-LMTO) method based on density functional theory within both local density approximation (LDA) and generalised gradient approximation (GGA). The calculated equilibrium lattice constants and bulk moduli are compared with previous results. The concentration dependence of the electronic band structure and the direct and indirect band gaps are investigated. Using the approach of Zunger and co-workers, the microscopic origins of the band gap bowing are investigated also. Moreover, the refractive index and the optical dielectric constant for SixGe1-xC are studied. The thermodynamic stability of the alloys of interest is investigated by means of the miscibility. This is the first quantitative theoretical prediction to investigate the effective masses, optical and thermodynamic properties for SixGe1-xC alloy, and still awaits experimental confirmations

Keywords

Alloys; Bowing parameter; FP-LMTO; GeC; SiC