Structural parameters, band-gap bowings and phase diagrams of zinc-blende $Sc_{1-x}In_xP$ ternary alloys: A FP-LAPW study

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Abstract

Using first-principles total-energy calculations, we investigate the structural, electronic and thermodynamic properties of the cubic $Sc_{1-x}In_xP$ semiconducting alloys. The calculations are based on the fullpotential linearized-augmented plane wave (FP-LAPW) method within density functional theory (DFT). The exchange-correlation effect is treated by both local-density approximation (LDA) and generalizedgradient approximation (GGA). In the latter approach, both Perdew-Burke-Ernzerhof (PBE) and EngelVosko (EV) functional of the exchange-correlation energy were used. The effect of atomic composition on structural parameters, band-gap energy, mixing enthalpy and phase diagram was analyzed for x = 0, 0.25, 0.5, 0.75, 1. Lattice constant, bulk modulus, and band-gap energy for zinc-blende $Sc_{1-x}In_xP$ alloys show nonlinear dependence on the aluminium composition x. Deviations of the lattice constant from Vegard's law, and deviations of the bulk modulus and band-gap energy from linear concentration dependence (LCD) were found. The variation of the calculated equilibrium lattice constant versus indium concentration shows a small deviation from Vegard's law with upward bowing parameter of -0.043 Å and -0.058 Å for PBE and LDA, respectively. The bulk modulus as a function of indium composition shows a small deviation from the linear concentration dependence (LCD) with upward bowing equal to -0.790 GPa using PBE, and with net downward bowing of 0.847 GPa using LDA. The results show that the band gap undergoes a direct (X→ X)-to-direct (C→ C) transition at a given indium composition x. The physical origin of the band-gap bowing in zinc-blende $Sc_{1-x}In_xP$ semiconducting alloys was investigated. The calculated excess mixing enthalpy is positive over the entire indium composition range.

Keywords

Density functional calculations; Electronic properties; Structural properties; Thermodynamic properties.