Thermodynamic properties of $In_{1-x}B_xP$ semiconducting alloys: A first-principles study

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Abstract

We have carried out first-principles total-energy calculations in order to study the electronic structure and thermodynamic properties of $In_{1-x}B_xP$ semiconducting alloys using the GGA and LDA formalisms within density functional theory (DFT) with a plane-wave ultrasoft pseudopotential scheme. We have also taken into account the correlation effects of the 3d-In orbitals within the LDA+U method to calculate the band-gap energy. We use special quasirandom structures to investigate the effect of the substituent concentration on structural parameter, band gap energy, mixing enthalpy and phase diagram of $In_{1-x}B_xP$ alloys for x = 0, 0.25, 0.50, 0.75 and 1. It is found that the lattice parameters of the $In_{1-x}B_xP$ alloys decrease with B-concentration, showing a negative deviation from Vegard's law, while the bulk modulus increases with composition x, showing a large deviation from the linear concentration dependence (LCD). The calculated band structure presents a similar behavior for any B-composition using LDA, PBE or LDA+U approach. Our results predict that the band-gap shows a x-dependent nonlinear behavior. Calculated band gaps also shows a transition from (Γ→Γ)-direct to (Γ→Δ)- indirect at x = 0.611 and 0.566 for LDA and PBE functionals, respectively. Our calculations predict that the $In_{1-x}B_xP$ alloy to be stable at unusual high temperature for both LDA and PBE potentials.

Keywords

Ab-Initio Calculations; Alloys; Electronic Structure; Thermodynamic Properties.