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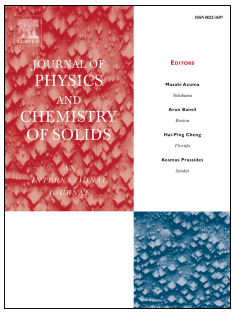


Structural, electronic, optical, thermodynamic and elastic properties of the zinc-blende $Al_xIn_{1-x}N$ ternary alloys: A first principles calculations

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# Structural, electronic, optical, thermodynamic and elastic properties of the zinc-blende $Al_xIn_{1-x}N$ ternary alloys: A first principles calculations

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**Abstract:** The structural, electronic, optical and thermodynamic properties of the $Al_xIn_{1-x}N$ ($x$ = 0, 0.25, 0.50, 0.75 and 1) ternary alloys were investigated using the full potential linearized augmented plane wave (FP-LAPW) method in the framework of density functional theory (DFT). Optimized lattice parameter, bulk modulus and its pressure derivative were determined from suitable fit of the total energy versus volume with Murnaghan equation of state (EOS) for all considered alloys. Variations of the lattice parameter and bulk modulus with the Al concentration ($x$) deviate from Vegard's law. Electronic band structure, dielectric function and refractive indices were investigated and computed for the considered alloys. It is found that the variations of the band gap, the static dielectric constant and static refractive index versus the Aluminum Al concentration obey to a quadratic polynomial. Temperature and pressure dependencies of the Gibbs free energy $G$, isochoric heat capacity $C_V$, entropy $S$ and Debye temperature $\theta_D$ were investigated via the Debye quasi-harmonic model for the $Al_{0.5}In_{0.5}N$ ternary alloy. Furthermore, the elastic constants $C_{ij}$, the bulk modulus B, Shear modulus $G$ with Young modulus $E$ and the Poison's ratio $v$ with the compressibility $B/G$ were carried out in the cubic phase. Deduced results agree well with the available theoretical and experimental results.

**Keywords:** FP-LAPW, DFT, $Al_xIn_{1-x}N$, Ternary alloys, Semiconductors, Thermodynamic
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