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Electronic and optical properties of HgIn_2S_4 thiospinels

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Abstract

Photoluminescence (PL), transmission (T), reflection (R), wavelength modulated transmission ($\Delta T/\Delta\lambda$) and reflection ($\Delta R/\Delta\lambda$) spectra of thiospinel HgIn_2S_4 crystals were investigated in temperature interval from 10 to 300 K. The band gap 1.64 eV (300 K) and 1.666 eV (10 K) are formed by electron transitions from L to Γ points of Brillouin zone. The edge temperature shift coefficient β ($\Delta E_g/\Delta T$) is equal to $4.3 \cdot 10^{-3} \text{ eV K}^{-1}$. The direct energy gap in Γ point (E_g^{dir}) corresponds to 1.748 eV. The top valence bands in $k = 0$ are split by the crystal field on 25 meV. Direct electron transitions a1–a7, observed in energy range 1–6 eV, were interpreted conform the theoretically calculated band structure. The optical functions (n , k , ε_1 and ε_2) were determined by Kramers-Kronig analysis.