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Band structure and optical constants of SnS_2 single crystals

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Abstract

Absorption (K), reflection (R) and wavelength modulated transmission ($\Delta T/\Delta\lambda$) spectra in SnS2 crystals of hexagonal phase (space group P63/mmc) were investigated in temperature interval from 300 to 10 K. It was established that indirect band gap (E_g^{ind} - 2.403 eV) is due to unpolarized indirect transitions between Γ and M points of Brillouin zone. A minimal direct band gap (E_g^{dir} - 2.623 eV) in E||b polarization is formed by direct allowed transitions and in E⊥b polarization (2.698 eV) by forbidden transitions in Γ point of Brillouin zone. A magnitude of refractive index (n) changes from 3 to 4 and has a maximum at 2.6 eV. Optical functions (n, k, ε_1 and ε_2) in energy region E > E_g (3–6.5 eV) were calculated from measured reflection spectra by Kramers-Kronig analysis. Features observed in reflection and optical function spectra were assigned to electron transitions. This electron transitions were localized in framework of theoretically calculated band structure.