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The band structure of birefractive $CdGa_2S_4$ crystals

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Abstract

In this paper, we report on the spectral dependence of $\Delta n=n_o-n_e$ for $CdGa_2S_4$ single crystals for shorter and longer wavelengths than the isotropic wavelength λ_o=485.7nm (300K). It was established that Δn is positive at $\lambda>\lambda o$ and it is negative in the spectral range $\lambda<\lambda_o$. The isotropic wavelength λo exhibits blue spectral shift with temperature decreasing. The ground and excited states of three excitonic series A, B and C with binding energies of 53meV, 52meV and 46meV, respectively, were found out at 10K. The effective masses of electrons for k=0 were derived from the calculation of excitonic spectra: $m_c^{\parallel}$ (E||c)=0.21m_o and $m_c^{\perp}$(E⊥c)=0.19m_o. The holes masses are equal to 0.59m_o and 0.71m_o for E||c and E⊥c, respectively. The value of valence bands splitting, V_1-V_2, by crystalline field equals 24meV, and V_2-V_3 splitting due to the spin–orbital interaction equals to 130meV. The optical functions *n, k,* ε_1 and ε_2 for E⊥c and E∥c polarizations were calculated by means of Kramers–Kronig analyses in the energy interval 3–6eV. The

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evidenced features are discussed taking into account the results of new theoretical calculations of $CdGa_2S_4$ band structure.