Excitonic spectra and band structure of CdGa$_2$Se$_4$ birefractive crystals

**N. N. Syrbu, I. G. Stamov, V. I. Parvan,
V. V. Zalamai, I. M. Tiginyanu**

Abstract

We report on the intersection of spectral dependences of refractive indices no and ne at the wavelengths 546nm (λ_o) and 450nm (λ_{o1}) in CdGa$_2$Se$_4$ single crystals. The value of difference $\Delta n = n_e - n_o$ is equal to zero at the wavelengths involved. When placed between two crossed polarizers, the crystals of CdGa$_2$Se$_4$ exhibit a transmission band at the wavelength of λ_o=546nm (300K). The ground and excited states of three excitonic series (A, B and C) were found out at 13K in CdGa$_2$Se$_4$ crystals, and other parameters of excitons and bands were determined. In the Γ point of Brillouin zone the effective mass of electrons mc is equal to 0.14m$_o$, and the effective masses of holes m$_{v2}$ and m$_{v3}$ are equal to 0.76m$_o$ and 0.94m$_o$, respectively. The hole mass mv1 depends upon the direction of wave vector k: at polarization E∥c, k∥a the mass m$_{v1}$=1.15m$_o$, and at polarization E∥c, k∥b m$_{v1}$=0.84m$_o$. The values of valence bands splitting in the center of Brillouin zone by the crystal field (Δ_{cf}=49meV) and spin−orbital interaction (Δ_{so}=351meV) were determined. The optical functions n, k, ε_1 and ε_2 in polarizations E⊥c and E∥c for the energy diapason from 3 to 6eV were calculated from the reflectivity spectra by Kramers−Kronig analysis. The evidenced features are discussed on the basis of recent theoretical calculations of the band structure of CdGa$_2$Se$_4$ crystals.