

ABM 9P BAND STRUCTURE OF CdAl₂S₄ CRYSTALS

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Reflection and wavelength modulated reflection spectra were investigated at temperature 10 K in CdAl₂S₄ crystals. Ground and excited states of three excitonic series (A, B and C) were found out. Contours of reflection excitonic spectra were calculated and main parameters of excitons and bands in $k = 0$ were determined. The effective mass of electrons m_c is equal $0.30m_0$ and holes masses m_{v1} , m_{v2} and m_{v3} are equal to $1.55m_0$, $0.90m_0$ and $2.07m_0$, respectively in Γ point of Brillouin zone. Valence bands $V_1 - V_2$ splitting due to crystal field (141 meV) and bands $V_2 - V_3$ splitting by spin-orbital interaction (152 meV) were estimated.

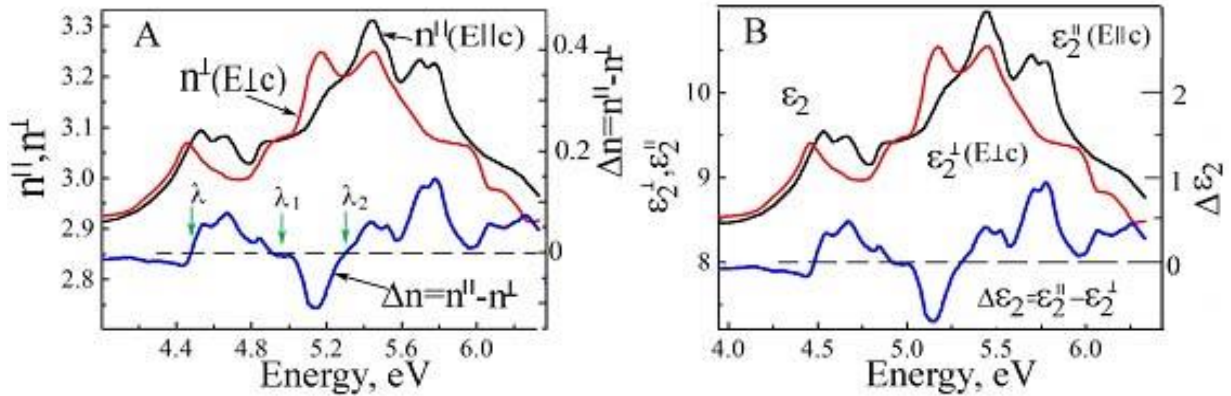


Fig. 1 A - spectral dependencies of refractive indices (n^{\parallel} and n^{\perp}) and its difference ($\Delta n = n^{\parallel} - n^{\perp}$); B - spectra of permittivity imaginary parts ($\varepsilon_2^{\parallel}$ and ε_2^{\perp}) and theirs difference ($\Delta\varepsilon_2 = \varepsilon_2^{\parallel} - \varepsilon_2^{\perp}$) for $E\parallel c$ and $E\perp c$ polarizations and CdAl₂S₄ crystals.

Three groups of maxima were discovered in reflection spectra in intrinsic region. The most long wavelength group was formed in the region of excitonic transitions (A, B and C). The second group of maxima is situated at energies 3.9 – 5.2 eV and the next high energy group at 5.2 – 6.5 eV.

Spectral dependencies of refractive index (n), imaginary part of permittivity (ε_2) and its differences (Δn and $\Delta\varepsilon_2$) were calculated by Kramers-Kronig method from measured reflection spectra, Fig. 1. Also spectral dependencies of extinction coefficients (k^{\perp} and k^{\parallel}), its difference ($\Delta k = k^{\perp} - k^{\parallel}$), phases (φ^{\parallel} and φ^{\perp}) and a phases difference ($\Delta\varphi = \varphi^{\perp} - \varphi^{\parallel}$) were calculated for $E\parallel c$ and $E\perp c$ polarizations at temperature 80 K.

Features for all calculated optical functions have a good correlation with features observed in measured reflection spectra of CdAl₂S₄ crystals. Spectral dependencies of refractive indices n^{\parallel} and n^{\perp} intersect in three energies: 4.474 eV, 4.924 eV and 5.303 eV (marked as λ_0 , λ_1 and λ_2). The difference $\Delta n = n^{\parallel} - n^{\perp}$ crosses the zero axis at the same energies (wavelength), Fig. 1, A. Spectral dependencies of imaginary parts of permittivity in $E\parallel c$ and $E\perp c$ polarizations ($\varepsilon_2^{\parallel}$ and ε_2^{\perp}) and its difference ($\Delta\varepsilon_2 = \varepsilon_2^{\parallel} - \varepsilon_2^{\perp}$) have the same features at the same wavelengths, Fig. 6, B. The intersection of spectral dependencies of refractive indices indicates that the crystal is isotropic and does not recognize the light polarization at these wavelengths. Such regularities show optical activity and take place in a lot of crystals including A^{II}B₂^{III}C₄^{VI} compounds.