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Excitons and energetic bands structure of ZnP_2-C_{2h}^5 crystals

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Abstract

Reflectivity and transmittance spectra of ZnP_2-C_{2h}^5 crystals in the region of A, B and C excitons and $E>E_g$ had been researched. The spectra had been calculated using dispersion correlations and the Kramers-Kronig correlations. The exciton parameters and optical functions *n, k,* ε_1 and ε_2 had been determined for all excitons. The changes of the damping factor γ, the transversal-longitudinal Δ_{LT} exciton splitting $\Gamma_2^-(z)$, and the exciton mass M in dependence on temperature had been revealed. The effective electron mass $m_c^*=0{,}23m_0$ had been determined. It was shown that the holes mass $m_{V1}^*=4{,}27m_0$ for $E \| c$, $k \| a$ and $E \| b$, $k \| a$ polarizations and $m_{V1}^*=0{,}55m_0$ for $E \| a$, $k \| в$ polarizations. The energies of electronic transitions from V_1, V_2 and V_3 zones into C_1 zone and the symmetry of zones in the Γ point had been determined. The splitting value of V_1-V_2 zones had been determined as being equal 92meV and V_2 - V_3 equals 143.6meV. The singularity of optical functions n, k, ε_1, ε_2, $d^2\varepsilon_1/dE^2$ and $d^2\varepsilon_2/dE^2$ had been determined inside the energy interval 1 – 10eV and were interpreted basing on the theoretical zone calculations.

Keywords

ZnP_2-C_{2h}^5 Crystals, Excitons, Reflectivity and Transmittance Spectra, Optical Functions, Kramers-Kronig Analysis, Band Structure

1. Introduction

ZnP_2 crystals of a monoclinic modification belong to the compounds group A^2B^5, which are crystallizing into a lattice with spatial group C_{2h}^5. The monoclinic ZnP_2-C_{2h}^5 is a direct band of low symmetry, in which several hydrogen-like excitonic series are exciting conditioned as by the electric [1 – 4] as by dipole-forbidden transitions [1, 3 – 5].

Excited states lines up to n=9 are revealed in polarized spectra of excitonic series [1 – 6]. The excitonic spectra in ZnP_2 - (C_{2h}^5) crystals are characterized by a strong exciton polaritonic effect [3 – 8]. A different Raman scattering of excitonic polaritons in the region of transversal-longitudinal exciton splitting is observed in crystals [9 – 12]. A bigger amount of lines are manifesting in transmittance spectra, which are conditioned by opto-excitonic states [13 – 16]. In papers [17 – 20] it was mentioned that an inverse hydrogen-like series (IHS) was present in these crystals in the long wavelength part of excitonic states. In papers [21 – 23] had been studied different influences on optical exciton spectra. A big interest on β-ZnP_2 is, also, the inside condensation phenomena of biexcitonic gas [9] into electron-hole quantum liquid [10]. That is why the monoclinic ZnP_2 represents a model material for studying the Wannier-Mott excitons and their linked phenomena in low symmetry crystals. Active elements and different device structures are developed basing on this crystals, which parameters are researched basing on the anisotropy of optical parameters [23 – 30].

New information on electronic transitions in β-ZnP_2 crystals is obtained in this paper. The optical spectra of β-ZnP_2 crystals are studied in a wide region of energies and temperature values. The absorption and reflectivity spectra