FRENKEL EXCITONS AND THE ENERGY BANDS STRUCTURE IN CRYSTALS PbGa₂S₄

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On the basis of lead tiogalat (PbGa2S4) was created the active elements for lasers which allow to control the generation spectroscopic properties of lasers and parameters of the laser radiation [1]. In these crystals were found Frenkel excitons with large oscillator strength (292meV) at room temperature. At a temperature of 10 K was observed the Wannier-Mott exciton [2]. The contours of the exciton reflection spectra of Frenkel and Wannier-Mott excitons, for PbGa₂S₄ crystals, was calculated on the basis of dispersion relations [3], Figure 1. It allow to determine the value of the splitting due to crystal field (Δ_{sp}), spin-orbit (Δ_{so})interaction of the upper valence bands in the center of the Brillouin zone in PbGa₂S₄ crystals. At the minimum of interband gap the exciton series A is formed by pair of bands (V₁-C₁) with $\Gamma_5^{\pm} - \Gamma_5^{\mp}$ symmetry, the B series is formed by pair of zones (V₂-C₂) with $\Gamma_5^{\pm} - \Gamma_5^{\mp}$ symmetry. In this model, both exciton series is formed in the center of the Brillouin zone, at same value of the wave vector \vec{k}_0 . Zones C1 and C2 are degenerate in the center of the Brillouin zone. The values of band gap for the polarizations $E \perp c$ and $E \parallel c$, obtained from calculations of the exciton spectra coincede.



Fig.1. Experimental and calculated contours of reflection spectra of Wannier-Mott (A-eks.) and Frenkel (B-eks.) excitons in PbGa₂S₄ crystals

In the energy range 3-6eV was measured reflection spectra at temperatures of 14, 77 and 300 K for the polarization $E \perp c$ with $E \parallel c$. The experimental spectra are calculated by the Kramers-Kronig relations and determined the optical constants n, k, ε_1 and ε_2 . The observed transitions for PbGa₂S₄ crystals, is discussed in the theoretical calculations of the energy band structure of tiogalat crystals. On the basis of PbGa₂S₄ possible to predict the creation of optoelectronic devices, operating at room temperature, the action is based on physical principles of interaction of light with excitons.

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[2] N.N. Syrbu, V.I. Parvan, V.V. Ursaki, Optical Materials 34 (2012) 691.