Exciton Spectra of $CuAlS_2$ and $CuAlSe_2$ Crystals

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***Abstract* — The reflectivity exciton spectra are researched for $CuAlS_2$ and $CuAlSe_2$ crystals at 10K. The chipping values were calculated caused by the crystal field and spin-orbital interaction of valence zones. There have been estimated the electrons' effective mass (m^*_{c1}) and the holes' effective mass (m^*_{V1}, m^*_{V2}, m^*_{V3}).**

***Index Terms* — anisotropy, exciton, effective mass, reflective spectra, Rydberg constant.**

I. INTRODUCTION

The $CuAlS_2$ and $CuAlSe_2$ materials of I-III-VI_2 group are crystallizing in chalcopyrite structure with spatial group $I^4_{2d} - D^{12}_{2d}$ and are better wideband materials of this group. The lines n = 1 (ω_t = 3.543 eV, ω_L = 3.546 eV) and n = 2 (3.565 eV) of the hydrogen like exciton series Γ_4 are observed in reflectivity spectra of $CuAlS_2$ crystals at 10K and E‖c polarization.

II. EXPERIMENTAL RESULTS

The reflectivity spectra in the region of n=1 line has a view traditional for excitons with a maximum at 3.543 eV and a minimum at 3.546 eV (figure 1). These particularities are conditioned by the presence of longitudinal and transversal excitons. Basing on this data the longitudinal-transversal chipping energy of Γ_4 excitons is estimated, which equals 3 meV. The Rydberg constant which equals 32 meV for the exciton series Γ_4 is determined from the energetic position of the lines n = 1 and n = 2 (figure 1). The continuum energy (E_g, $n = \infty$) equals 3.575 eV. The discussed energy values for the ground (n=1) and excited(n=2) exciton states are correlating with the magnitudes 3.534 and 3.665 eV, obtained at 77K and had been earlier discussed in the work [1].

ε_b (E‖c) equals 7.05 and ε_b (E⊥c) equals 8.14 for $CuAlS_2$ crystals far from the excitonic resonances (v = 4000-3000 cm^{-1}) [3]. The reflective index equals 0.20-0.22 and ε_b changes in the interval 7.1-7.3 for the discussed crystals in the longwave region of excitonic resonances. The medium value of the background dielectric constant not far from excitonic resonance 7.26 was used in calculations.

The derived effective mass of Γ4-excitons is $\mu = \varepsilon_b^2 R/R_H = 0.11 m_0$ at ε_b = 7.26 and the Rydberg constant of Γ_4-exciton R =0.032 eV, where R_{H_2} - the Rydberg energy of the hydrogen atom (13.6 eV).

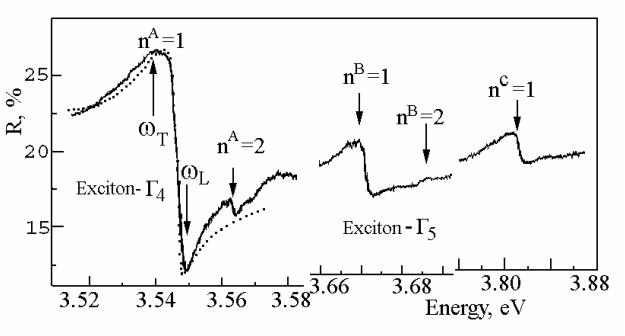

FIG. 1 REFLECTIVITY SPECTRA OF $CuAlS_2$ CRYSTALS

The Bhor radius (a_B) of the *S*-state of Γ_4-exciton equals 0.3×10^{-6} cm. A maximum at 3.668 eV (transversal exciton) and a minimum at 3.670 eV (longitudinal exciton) of the Γ_5 series are observed at E⊥c polarization (figure 1). The longitudinal-transversal chipping of the Γ_5 exciton equals 2.0 meV. The excited state n=2 is revealed at 3.687 eV energy value. The bounding energy of Γ_5 excitons equals 25 meV and the limit of series correlation equals 3.693 eV. The C exciton is revealed at the energy 3.813 eV (n=1) at this polarization. The line 4.39 eV is observed in the energy interval 3.6-4.98 eV at 77K. Other lines were not revealed between the lines 4.39 eV and 3.665 eV at 77K, this is why the line 4.39 eV was earlier described by the authors as being one of the C exciton series [1]. In the spectra described in this work, as it was described earlier, the line 3.813 eV was revealed (figure 1). Taking into account this data we attribute to the ground state of the C exciton the line 3.813 eV. The reflective coefficient for the B-excitonic series at 3.6 eV equals 21% and the dielectric constant εb equals 7.2. The derived effective mass μ equals 0.09mo at a bounding energy of 25 meV. The lines n=1(ω_t = 2.8212 eV, ω_L = 2.8237eV) , п = 2 (2.8390 eV) and a faint line 2.8442 eV of the hydrogen like series of Γ4 exciton are revealed in the reflective spectra of CuAlSe2 crystals at 10K and E‖c, k⊥c polarization (figure 2).

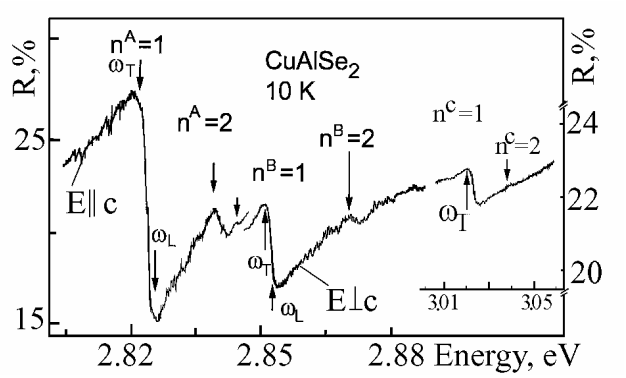

FIG. 2 REFLECTIVITY SPECTRA OF $CuAlSe_2$ CRYSTALS.

The reflective spectra in the region of the line n=1 has a view traditional for excitons with a maximum and minimum. These particularities are caused by the presence of transversal and longitudinal excitons. Basing on this data the energy of transversal-longitudinal chipping of Γ_4 excitons, which equals 25 meV can be estimated. The rydberg constant for the excitonic series Γ_4 can be determined from the energetic position of the $n = 1$ and $n = 2$ lines and equals 24 meV (figure 2). The continuum energy (E_g, $n = \infty$) equals 2.845 eV. The above discussed energy values for the excitonic ground states ($n = 1$) are correlating with the magnitudes 2.737, 2.851 and 3.012 eV, obtained at 77K, for A, B and C–excitons, respectively, discussed in the works [2, 3]. The reflectivity coefficient equals 0.24-0.25 in the region of excitonic resonances, and ε_d changes in the interval. The value of background dielectric constant in the neighborhood of exciton resonance was used in calculations. The derived effective mass of Γ_4-excitons $\mu = \varepsilon_b^2 R/R_H = 0.1 m_0$ at $\varepsilon_d = 7.6$, where R (0.024 eV) – the Rydberg constant of Γ_4-exciton and R_{H_2} - the Rydberg energy of the hydrogen atom (13.6 eV). The Bhor radius (a_B) of *S*-state of Γ_4-exciton equals 0.3×10^{-6} cm. A maximum at 2.851 eV (transversal exciton) and a minimum at 2.853 eV (longitudinal exciton) of the Γ_5 series is observed at E⊥c polarization (figure 1). The transversal-longitudinal chipping of the Γ_5 exciton equals 2.0 meV. The excited state n=2 is revealed at the energy of 2.868 eV. The Γ_5 exciton bounding energy equals 22 meV and the series' correlation limit equals 2.873 eV. The C exciton is revealed at the energy 3.023 eV (n=1) and 3.039eV (n=2) in the same polarization. The line form of the ground state of C exciton is shown in figure 1. The Rydberg constant equals 18 meV and the band-gap equals 3.038 eV.

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