DSCM O8 EXCITONIC STATES AND ELECTRON TRANSITIONS IN $HgGa_2Se_4$ SINGLE CRYSTALS

V.V. Zalamai*, N.N. Syrbu, A.V. Tiron
Technical University of Moldova, Chisinau, Moldova
*E-mail: zalamai@yahoo.com

$HgGa_2Se_4$ crystals belong to the $HgGa_2X_4$ (X = S, Se, Te) compounds and crystallize in a classical chalcopyrite structure. An investigation of such materials as $HgGa_2Se_4$ is of interest since they possess linear and nonlinear optical properties and a wide band gap (2.2 - 2.6 eV) [1]. The active elements and different devices whose properties based on nonlinear optical effects are developed basing on $HgGa_2Se_4$ crystals. $HgGa_2Se_4$ single-crystals are direct-band semiconductors as $ZnAl_2Se_4$. The $HgGa_2Se_4$ compound crystallizes in tetrahedral lattice with S_4^2 space group. The band structure of these crystals is split taking into account a pseudopotential configuration of Hg ($5d^{10}6s^2$), Ga ($3d^{10}4s^24p^1$) and Se ($3d^{10}4s^24p^4$) atoms [2].

The $HgGa_2Se_4$ crystals were grown by gas-transport method in ampoules and were plates with mirrored surfaces ~ 5x7 mm and 2 - 6 mm thickness. The plate's surfaces were parallel with ***c*** axis and could be recognized visually. Low-temperature spectra of crystals deposed in closed helium LTS-22 C 330 optical cryogenic system were measured on MDR-2 spectrometer with optical efficiency 1:2 and linear dispersion 7 Å/mm. The measurements of resonance Raman scattering and photoluminescence were carried out by help of spectrometer DFS-32 with optical efficiency 1:5 and linear dispersion 5 Å/mm.

The ground and excited states of excitonic series A, B, C and D were discovered in $HgGa_2Se_4$ crystals in Brillouin zone center in the region of band gap. The Γ_4 excitons (A series) and the Γ_5 excitons (B and C series) are allowed in E||c and in E⊥c polarizations, respectively. The Γ_4 symmetry excitons are formed by electrons of conduction band C_1 of Γ_6 symmetry and holes of valence band V_1 of Γ_7 symmetry. The effective mass of electrons m_c is equal to $0.26m_0$ and holes masses m_{v1}, m_{v2} and m_{v3} are equal to $2.48m_0$, $2.68m_0$ and $1.06m_0$, respectively in Γ point of Brillouin zone. The splitting of valence bands in Brillouin zone center by crystal field (Δ_{cf} = 70 meV) and spin-orbital interaction (Δ_{so} = 250 meV) were estimated.

When excited by the 5145Å Ar^+ laser line of $HgGa_2Se_4$ crystals at 10 K, emission lines shifted to the long-wave side from the exciting line to an energy equal to one, two, three, etc. LO are phonons are observed. The lines are due to resonant Raman scattering which are superimposed on the luminescence spectra from the ground states of excitons. For lines located near the exciton resonance, an increase in intensity is observed.

Direct transitions revealed in reflection (R) and wavelength modulated reflection ($\Delta R/\Delta\lambda$) spectra were discussed and identified in all actual points of Brillouin zone in framework of recent theoretical calculations of band structure of $HgGa_2Se_4$ crystals. The optical constants (n, ε_1 and ε_2) for E||c and E⊥c polarizations in energy interval 2 - 6 eV were calculated from measured reflection spectra by Kramers-Kronig relations.

[1] S.I. Radautsan et al. *Sov. Phys. Semicond.*, (1977), **11**(1), 38.
[2] X. Jiang and W.R.L. Lambrecht, *Physical Review B*, (2004), **69**, 035201