MSC.56P TEMPERATURE DEPENDENCE OF THE OPTICAL GAP $CuGa_5Se_8$

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The investigation of the absorption coefficient spectra below the fundamental edge of ordered vacancy compound $CuGa_5Se_8$ was studied early for samples prepared by Bridgman method [1]. Compositional measurements were carried out by Energy Dispersive X-ray Microanalysis (EDAX). Samples have stoichiometric compositions of Cu:Ga:Se as 7: 35.4: 57.5 atomic percentage, practically equal to 1:5:8.

The optical transmittance spectra in the spectral range 600–900 nm were measured with MDR2 monochromator using halogen lamp as a light source. The transmitted radiation was detected by a Ge photodetector and Unipan amplifier. The temperature interval between 10 and 300K was supplied by close cycle helium Leybold system.

For direct band gap semiconductors $\alpha(h\nu) = A(h\nu - E_g)^{1/2}$ where $h\nu$ is the characteristic energy of a photon, A is a temperature independent constant that depends on the effective mass and the refractive index. Linear dependence near the band edge confirms that $CuGa_5Se_8$ has direct fundamental band gap. From the extrapolation of $(\alpha h\nu)^2$ versus $h\nu$ curves to $(\alpha h\nu)^2 = 0$, the value of E_g is equal to 1.76 at 300 K. Reported value of E_g is about 1.81eV[1] and 1.78 eV[2].

Three-parameter thermodynamic model of O'Donnell and Chen[3], the Einstein model[4] and the Passler model[5] have been employed to describe the temperature variation of the energy gap. By fitting these model to our data of $E_g(T)$, estimated on the base of the linear extrapolation method the following set of parameters was obtained: $E_g(0)$ is the band gap at $T = 0$ K, $\langle E_{ph} \rangle$ is an effective phonon energy, Θ is an effective phonon temperature, S is a dimensionless constant related to the electron–phonon coupling, K is a temperature-independent constant and Ξ is the Einstein temperature.

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