Temperature Dependence of the Energy Gap of $TlGaSe_2$ Single Crystals

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Layered compounds of the TlMeX26 type (Me = In, Ga; X = S, Se) and alloys based on them are of scientific and practical interest. With knowledge of the composition dependencies of the electrical, photoelectrical and optical properties of TlMeX26 layered compounds, it is possible to control these properties. Upon partial substitution of iron for gallium, the TlGaSe2 crystals acquire magnetic properties. This can be useful in designing materials with characteristics that can be controlled by a magnetic field. The purpose of this work was to investigate the effect of temperature and partial iron substitution for gallium on the photoelectrical properties of TlGaSe2 single crystals. Homogeneous TlGaSe2 <0.5 mole % Fe> samples were obtained by the method of direct synthesis, i.e. by the reaction between the starting components (Tl, Ga, Fe, Se) of high purity degree (no less than 99.99). Single crystals were grown by the Bridgman method. We studied the spectral distribution of the photocurrent for TlGaSe2 and TlGaSe2 at T=115–220 K. The iron doping of the TlGaSe2 single crystals leads to a modification of the photocurrent spectra. The results obtained have demonstrated that partial substitution of iron for gallium lead to a shift in the maximum of the intrinsic photocurrent toward the long-wavelength range of the spectrum. By applying the half-maximum value, we could evaluate the average energy gap for undoped TlGaSe2 and iron-doped single crystals. Temperature dependence of average energy gap Eg has been studied for TlGaSe2 and TlGaSe2 single crystals. The analysis of the experimental results demonstrated that Eg of studied crystals regularly decreases (from 2.03 to 1.97 eV for TlGaSe2 and from 1.90 to 1.83 eV for TlGa0995.Fe0.005Se2) with an increase in the temperature from 115 to 220 K. Thus, upon temperature and partial substitution of iron for gallium in TlGaSe2 it is possible to control the photoelectrical properties of the single crystals studied.