Electron-deformational Phase Transitions in a $TlGaSe_2$ Layered Crystal

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Recently, a ternary layered $TlGaSe_2$ crystal has attracted considerable interest due to its ferroelectric and semiconducting properties. Based on experimental investigations, it has been shown that $TlGaSe_2$ besides of the sequences of phase transitions, possesses unusual electrical and optical characteristics [1-3]. It has been suggested [3] that an anomalous behavior of the physical parameters in the temperature interval quite far from the known phase transition temperatures can be related to the non-equilibrium electron phase transitions. However, a theoretical description of these transitions for $TlGaSe_2$ is still absent.

According to a theory, the electron phase transition takes the place in the multi-valley semiconductors [4], or in the initial inhomogeneous single-valley ones with the fluctuating concentrations of charge carriers [5], as a consequence of the collective interactions. In our opinion, the observed nonlinear effects in the $TlGaSe_2$ monoclinic crystal, similar to those in the In_4Se_3 crystal [5], can be caused by the instability of the electron subsystem due to the electron-phonon interaction.

In this report, we present an investigation of the self-consistent localized electron states, which are connected with charge carrier inhomogeneities in the $TlGaSe_2$ crystal. For this purpose, we use the developed deformational theory of phase transitions [4,5], where the interaction between the electrons and phonons is taken into account within the deformational potential. In the framework of the continuum and the deformational potential approaches, by utilizing the variational procedure and a nonstandard dispersion law for charge carriers which follows from the *ab initio* band structure calculation of the $TlGaSe_2$ crystal [6], we obtain the energy dependence of a localized electron on the variational parameter. This dependence is characterized by the presence of two minima with different energy depth. This feature indicates a possibility for the formation of stable localized states (polaron or condenson type), with different bond energy, which are separated by the potential barrier, and which can be responsible for realization of the deformational phase transition in the presence of the non-equilibrium charge carriers in $TlGaSe_2$.

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