EFFECT OF PEIERLS TRANSITION ON THE PHONON SPECTRUM IN ORGANIC CRYSTALS OF TTT_2I_3 FOR DIFFERENT VALUES OF CARRIER CONCENTRATION

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The metal-insulator transition of Peierls type and its effect on the phonon spectrum in quasi-one-dimensional organic crystals of TTT_2I_3 for different values of carrier concentration is studied in 2D approximation. In the frame of the physical model, two electron-phonon interaction mechanism are taken into account. The first mechanism is of deformation potential type and the second one is of polaron type. The ratio of amplitudes of polaron-type interaction to the deformation potential one in x and y directions is characterized by parameters γ_1 and γ_2. The interaction of carriers with structural defects is also considered. It was demonstrated that this interaction is very important to explain the behavior of Peierls transition. The renormalized phonon spectrum is calculated in the random phase approximation. The method of retarded temperature dependent Green function is applied.

Computer modellings for 2D physical model of the crystal were performed for different values of carrier concentration. The numerical calculations for renormalized phonon spectrum, $\Omega(q_x)$ as function of q_x, for different temperatures are presented in two cases: 1) when the interaction between transversal chains is neglected ($q_y = 0$) and 2) when the interaction between the adjacent chains is considered ($q_y \neq 0$). It is shown that in the second case when the interaction between adjacent chains is considered, the Peierls transition occurs at a lower temperature compared to the case when the interaction between transversal chains is neglected, for the same value of carrier concentration. Furthermore, it is shown that the Peierls structural transition strongly depends on iodine concentration. It was observed that with an increase in carrier concentration the Peierls critical temperature decreases.

Keywords: *Peierls transition, quasi-one-dimensional organic crystals, renormalized phonons, Peierls critical temperature, interchain interaction.*

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