

# PEIERLS STRUCTURAL PHASE TRANSITION IN QUASI-ONE-DIMENSIONAL ORGANIC CRYSTALS

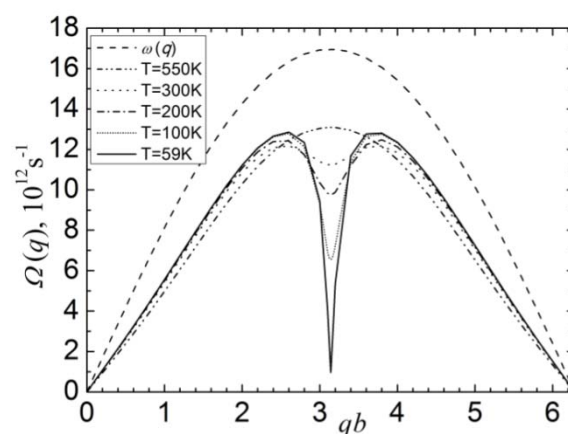
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The Peierls transition represents a structural phase transition of a quasi-one-dimensional (Q1D) lattice of ions with conduction electrons from metallic type with uniformly displaced ions at high temperatures to a dielectric state with not uniformly displaced ions when the temperature diminishes. Due to interaction of charge carriers with periodic lattice potential and with lattice vibrations the energy of carriers' subsystem is diminished when the lattice is deformed and at some temperature this diminution prevails on the increase of lattice deformation energy. For entire system this lattice distortion becomes energetically favorable. But this leads to creation of an energy gap exactly upper the Fermi energy: the Q1D system which at high temperature was metallic passes with the temperature decreasing into a dielectric state. The temperature at which this transition takes place is named Peierls critical temperature  $T_p$ . The Peierls transition in electronic Q1D systems, both organic and inorganic, has been investigated in many papers.

The aim of this paper is to study the Peierls transition in Q1D organic crystals of TTF-TCNQ (tetrathiofulvalinium-tetracyanoquinodimethane) and  $\text{TTT}_2\text{I}_3$  (tetrathiotetracene iodide). The first crystal has the conduction band filled at half, but the second has a band filled by one quarter. Unlike the previous papers, we apply for Q1D organic crystals a more compel physical model than so far. Two electron-phonon interactions are considered. The first is similar to that of deformation potential and is connected with the fluctuations due to lattice vibrations of the transfer energy of an electron from one molecule to the nearest one along the molecular chains. Usually, only this interaction was considered earlier in Q1D organic crystals. But the compounds studied here are formed from big molecules. Their polarizability is large. The energy of polarization of molecules surrounding the conduction electron is great and the variation of this energy due to lattice vibrations is important too. Thus, the second interaction is similar to that of polaron with induced polarization. The ratio of amplitudes of these two interactions determines the crystal parameter  $\gamma$ .



*Fig.1. Spectrul renormat al fononilor pentru  $\gamma = 1.5$  și diferite temperaturi.*

In order to find the renormalized phonon spectrum the retarded Green function was calculated in the random phase approximation. From the terms of perturbation theory for phonon Green function the series of diagrams with close loops of two electronic Green functions were summed up. The renormalized phonon spectrum is calculated as the pole of Fourier component of Green function. The results for TTF-TCNQ are presented in Fig.1 for  $\gamma = 1.5$  and different temperatures. The dashed curve corresponds to phonon spectrum calculated in the absence of electrons. It is seen that electron-phonon interaction modifies considerably the spectrum. The maximum frequency is diminished from  $17 \times 10^{12} \text{s}^{-1}$  up to  $12.7 \times 10^{12} \text{s}^{-1}$ . This means that due to electron-phonon interaction, the elastic force of interaction between the molecules is diminished in a large interval of wave numbers  $q$ . For  $q$  in the proximity of  $\pi/b$  ( $b$  is the lattice constant) the phonons are softened with decreasing temperature and at  $T$  near 59 K the Peierls transition takes place. The sound velocity is diminished by 1.7 times. The calculations for other parameters are also presented and analyzed.