CMT 11P PHONON DISPERSION ABOVE THE PEIERLS STRUCTURAL TRANSITION IN TTF-TCNQ ORGANIC CRYSTALS

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The softening of acoustic phonons above the Peierls structural transition in quasi-one-dimensional (Q1D) TTF-TCNQ organic crystals is studied in the 3D model. Unlike of other papers, a more complete physical model is applied that consider simultaneously two the most important electron–phonon interactions. The first is similar to that of deformation potential and the second one is of polaron type. The analytic expressions for the phonon Green function and for the phonon polarization operator are obtained in the random phase approximation. The effects of interchain interaction on the phonon dispersion and on Peierls critical temperature are analyzed.

In Figures 1 - 2 the dependences of renormalized phonon frequencies $\Omega(q_x)$ on q_x are shown for different temperatures and different values of q_y and q_z, where q_x, q_y, q_z are the projections of the phonon quasi-wave vector on axes x, y, z, $\omega(q_x)$ is the initial phonon frequency.

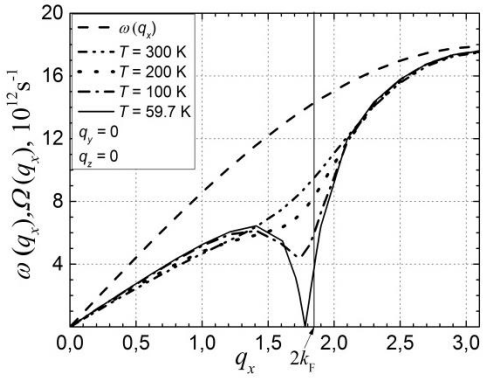

Fig.1. Renormalized phonon spectrum $\Omega(q_x)$ for $\gamma_1 = 1.37$ and different temperatures. The dashed line is for the spectrum of free phonons. $q_y = 0$ and $q_z = 0$.

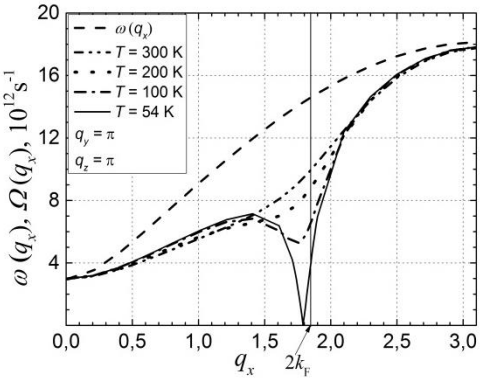

Fig.2. Renormalized phonon spectrum $\Omega(q_x)$ for $\gamma_1 = 1.37$ and different temperatures. The dashed line is for the spectrum of free phonons. $q_y = \pi$, $q_z = \pi$.

From the graphs it is observed that the values of $\Omega(q_x)$ are diminished in comparison with those of frequency $\omega(q_x)$ in the absence of electron-phonon interaction. This means that the electron-phonon interaction diminishes the values of lattice elastic constants. Additionally, it is seen that with a decrease in temperature T the curves change their form. In dependencies $\Omega(q_x)$ a minimum appears that becomes more pronounced at lower temperatures. It was expected that at certain temperature $\Omega(q_x)$ will attains zero for $q_x = 2k_F$. At this temperature, the structural Peierls transition should take place. But our calculations show that renormalized phonon frequencies $\Omega(q_x)$ attain zero for $q_x = 0.58\pi$. This deviation from $q_x = 2k_F$ is caused by deviation of k_F from $\pi/4$, $k_F = 0.59\pi/2$.

Fig. 1 shows the phonon spectrum, when $q_y = 0$ and $q_z = 0$. In this case the interaction between TCNQ chains is not taken into account. The Peierls structural transition occurs in TCNQ chains alone at $T = 59.7$ K (as it is confirmed experimentally by sharp decrease of electrical conductivity). The crystal lattice changes from the initial state with the lattice constant b along TCNQ chains to a new crystalline state with constant $4b$. At this temperature, metal-dielectric phase transition takes place, so as a gap in the carrier spectrum is fully opened just above the Fermi energy.

Fig. 2 shows the dependences of $\Omega(q_x)$ on q_x for $q_y = \pi$, $q_z = \pi$ and different temperatures. It is observed that when the interaction between TCNQ chains is taken into account ($q_y \neq 0$, $q_z \neq 0$), the Peierls critical temperature is diminished and equals $T \sim 54$ K. Note that this value corresponds to the experimental data confirmed by X-ray difraction. It is demonstrated that the electron-phonon interaction diminishes $\Omega(q_x)$ and reduces the sound velocity in a large temperature interval.