Journal of Engineering Science *Vol. XXX, no. 3 (2023), pp. 7 - 15*
Fascicle *Industrial Engineering* *ISSN 2587-3474*
Topic *Materials Science and New Technologies* *eISSN 2587-3482*

https://doi.org/10.52326/jes.utm.2023.30(3).01
UDC 536.784:539.21

ANALYSIS OF PHONONS BEHAVIOR IN QUASI-ONE-DIMENSIONAL CRYSTALS OF TTT(TCNQ)$_2$ NEAR THE PEIERLS STRUCTURAL TRANSITION IN A 3D APPROXIMATION

Silvia Andronic*, ORCID 0000-0002-7092-6867,
Ionel Sanduleac, ORCID: 0000-0001-7532-1288

Technical University of Moldova, 168 Stefan cel Mare Blvd., Chisinau, Republic of Moldova
*Corresponding author: Silvia Andronic, *silvia.andronic@mt.utm.md*

Received: 08. 12. 2023
Accepted: 09. 05. 2023

Abstract. This research paper focuses on investigating the metal-insulator transition occurring in quasi-one-dimensional organic crystals of TTT(TCNQ)$_2$. The study utilizes a 3D approximation approach and introduces a physical model that incorporates two essential electron-phonon interactions. The first interaction is akin to the deformation potential, while the second interaction follows a polaron type behavior. By employing the random phase approximation, the renormalized phonon spectrum is calculated across different temperatures and various values of the dimensionless Fermi momentum k_F. The findings indicate that the transition exhibits characteristics of the Peierls type, and the critical temperature associated with the Peierls transition is determined. Furthermore, an interesting observation is made that the Peierls critical temperature experiences a notable decrease with an increase in carrier concentration.

Keywords: *Metal-insulator transition; organic materials; quasi-one-dimensional organic crystals; renormalized phonon spectrum; Peierls critical temperature.*

Rezumat. Articolul se concentrează pe investigarea tranziției metal-dielectric care are loc în cristalele organice quasi-unidimensionale de TTT(TCNQ)$_2$. Studiul utilizează o abordare de aproximare 3D și introduce un model fizic care încorporează două interacțiuni esențiale electron-fonon. Prima interacțiune este asemănătoare cu potențialul de deformare, în timp ce a doua interacțiune urmează un comportament de tip polaron. Utilizînd aproximația fazelor aleatorii, spectrul renormat al fononilor este calculat la diferite temperaturi și diferite valori ale impulsului adimensional Fermi k_F. Constatările indică faptul că tranziția prezintă caracteristici de tip Peierls, iar temperatura critică asociată cu tranziția Peierls este determinată. Mai mult, se face o observație interesantă că temperatura critică Peierls înregistrează o scădere notabilă cu o creștere a concentrației purtătorilor.

Cuvinte cheie: *traziție metal-dielectric; materiale organice; cristale organice quasi-unidimensionale; spectrul renormat al fononilor; temperatura critică Peierls.*

1. Introduction

Over the past few years, there has been an increasing focus on studying organic crystals with quasi-one-dimensional (Q1D) properties, driven by their distinct and varied characteristics. These materials have garnered significant interest as they hold potential for application in electronic devices. Theoretical studies [1-4] have demonstrated that, by optimizing certain parameters, these crystals can exhibit significantly improved thermoelectric properties compared to currently known inorganic materials. The utilization of these materials offers several advantages, such as low cost, ecological safety, and relatively inexpensive manufacturing processes. Consequently, they have become a subject of special interest in research. Also, the increased interest in certain Q1D organic materials is due to their high electrical conductivity. For most of the compounds in these categories, it is characteristic that the metallic state manifests itself at temperatures of the order of T = 300 K. Another interesting aspect is the presence of the phase transition, specifically a transition from a metal to an insulator at low temperatures, typically occurring around several tens of degrees K. Quasi-one-dimensional systems also exhibit distinctive features such as the periodic arrangement of charge and spin density.

Research on organic conductors marked an intense development since the 1960s, when TCNQ (tetracyanoquinodimethane) molecules were discovered [5]. Then in 1970 TTF (tetrathifulvalene) molecules were discovered [6]. In 1973, the first quasi-one-dimensional organic metal stable at room temperature was synthesized, TTF-TCNQ (tetrathiofulvalinium-tetracyanoquinodimethane) with a partially full conduction band [7, 8]. It was sought to achieve the transition in the superconducting state when the temperature decreased, but the transition in the dielectric state was obtained. This groundbreaking result provided initial experimental evidence of the Peierls transition, a widely observed phenomenon in quasi-one-dimensional systems.

Peierls transition was theoretically predicted in 1955 by the scientist Rudolf Peierls and today this phenomenon bears his name [9]. Peierl's theory suggests that at certain reduced temperatures, a one-dimensional metallic crystal with a conduction band that is half-filled must undergo a transition to a dielectric state where the crystal lattice becomes dimerized. This critical temperature at which this transition occurs is known as the Peierls critical temperature.

The Peierls structural transition has received significant attention in Q1D crystals, as evidenced by numerous studies [10-16]. In the case of TTF-TCNQ crystals, intriguing observations have been made regarding this transition. Specifically, it has been noted that the transition manifests at 54 K in TCNQ stacks and at 38 K in TTF stacks. These transitions coincide with the emergence of band gaps in the electronic spectrum above the Fermi energy and a notable reduction in electrical conductivity. As the temperature decreases, distinct alterations in the phonon spectrum become apparent. Eventually, at a critical temperature, the renormalized phonon frequency reaches zero for a specific phonon wave vector value. This critical temperature corresponds to the occurrence of the Peierls transition [15, 16].

In our research, we have conducted a complete investigation of the transition occurring in TCNQ stacks using a more comprehensive physical model [17]. Our findings indicate that the Peierls transition begins at approximately 59.7 K in isolated TCNQ chains, resulting in a significant decrease in electrical conductivity. However, due to the interchain interactions, the transition is completed at a slightly lower temperature of approximately 54 K. Our study has demonstrated the pivotal role of electron-phonon interaction in this process.

Specifically, it causes a reduction in the renormalized phonon spectrum compared to the initial frequency of free phonons, leading to a decrease in sound velocity across a broad temperature range.

The investigation presented in [18] delved into the Peierls transition occuring in Q1D crystals of TTT_2I_3 type, employing a 2D physical model. The primary focus of the research was to analyze how lattice distortion affects the dispersion of renormalized acoustic phonons. The results revealed that the Peierls transition commences at approximately 35 K in TTT chains. Furthermore, due to the interchain interaction, the transition is finalized at a lower temperature of around 19 K.

The study also demonstrated that the interaction between holes and phonons, along with interactions with the structural defects, contribute to a reduction in the renormalized phonon spectrum and a decrease in the sound velocity over a considerable temperature range.

This paper focuses on studying the behavior of phonons in the vicinity of the Peierls structural transition in quasi-one-dimensional crystals of TTT(TCNQ)$_2$, using a 3D approximation. In Section II we present a comprehensive physical model of the crystal and provide a description of it. Section III is dedicated for examining the renormalized phonon spectrum. Finally, the paper concludes with a summary of findings and conclusions.

2. A 3D approximation of the physical model

The crystals of TTT(TCNQ)$_2$ exhibit a dark - violet needles – like morphology with lengths ranging from 3 to 6 mm. These crystals possess a pronounced quasi-one-dimensional internal structure, consisting of isolated chains of TTT anions and chains of TCNQ cations. The lattice constants for the *x*, *y*, and *z* directions are measured as follows: c = 3.75 Å, b = 12.97 Å and a =19.15 Å [19]. The *x* – axis aligns parallel to the TCNQ chains along the ***b*** - direction. This compound functions as a charge transfer complex, with the main charge transport occurring through the TCNQ chains. The electron transfer energy between adjacent TCNQ molecules in the *x* direction is represented as w_1 = 0.125 eV. In the perpendicular directions, w_2 and w_3 are relatively small, and transport primarily relies on the hopping mechanism. The stoichiometric concentration of electrons in TTT(TCNQ)$_2$ crystals is estimated to be $n = 1.1 \cdot 10^{21}$ cm^{-3}. In crystals with this stoichiometric concentration, the electrical conductivity ranges from 20 to 160 Ω^{-1}cm^{-1} [19], depending on the purity of the crystal. It has been theoretically demonstrated that there is the possibility of optimizing the thermoelectric properties by increasing the concentration of electrons and by purifying the crystal.

According to [19], the electrical conductivity measured using the microwave method, at a frequency of 10^{10} Hz, varies within the range of 20 $\Omega^{-1}\cdot$cm^{-1} to 160 $\Omega^{-1}\cdot$cm^{-1} at room temperature.

However, when measured using contact in pressed powder, the electrical conductivity ranges from 0.5 $\Omega^{-1}\cdot$cm^{-1} to 1 $\Omega^{-1}\cdot$cm^{-1} [20]. As the temperature decreases, there is an increase in electrical conductivity observed until around T ~ 90 K. However, beyond this point, the metallic behavior diminishes and the crystal undergoes a Peierls transition, transforming into an insulating state at approximately T ~ 35 K in purer crystals [19].

The physical model of the crystal was elaborated in greater detail in [17]. The Hamiltonian of the 3D crystal model was described within the framework of the tight binding and nearest neighbor approximations. It can be represented as folllows:

$$H = \sum_{\boldsymbol{k}} \varepsilon(\boldsymbol{k}) a_{\boldsymbol{k}}^{+} a_{\boldsymbol{k}} + \sum_{\boldsymbol{q}} \hbar \omega_{\boldsymbol{q}} b_{\boldsymbol{q}}^{+} b_{\boldsymbol{q}} + \sum_{\boldsymbol{k},\boldsymbol{q}} A(\boldsymbol{k},\boldsymbol{q}) a_{\boldsymbol{k}}^{+} a_{\boldsymbol{k}-\boldsymbol{q}} (b_{\boldsymbol{q}} + b_{-\boldsymbol{q}}^{+}). \quad (1)$$

In Eq. (1) - $\sum_{\boldsymbol{k}} \varepsilon(\boldsymbol{k}) a_{\boldsymbol{k}}^{+} a_{\boldsymbol{k}}$ corresponds to the energy operator of free electrons in the periodic field of the lattice. This term $\sum_{\boldsymbol{q}} \hbar \omega_{\boldsymbol{q}} b_{\boldsymbol{q}}^{+} b_{\boldsymbol{q}}$ represents the energy operator of longitudinal acoustic phonons, while $\sum_{\boldsymbol{k},\boldsymbol{q}} A(\boldsymbol{k},\boldsymbol{q}) a_{\boldsymbol{k}}^{+} a_{\boldsymbol{k}-\boldsymbol{q}} (b_{\boldsymbol{q}} + b_{-\boldsymbol{q}}^{+})$ describes the two most important electron-phonon interactions. The creation and annihilation operators of the electrons are denoted by $a_{\boldsymbol{k}}^{+}, a_{\boldsymbol{k}}$ with a 3D quasi-wave vector $\boldsymbol{k}$ and projections (k_x, k_y, k_z) onto the respective crystal axes. The energy of the electron $\varepsilon(\boldsymbol{k})$ is measured relative to the top of the energy band and can be expressed in the following form:

$$\varepsilon(\boldsymbol{k}) = 2w_1(1-\cos k_x b) - 2w_2(1-\cos k_y a) - 2w_3(1-\cos k_z c), \quad (2)$$

where w_1 is the transfer energies of a carrier from one molecule to another in *x* direction (along the chain), while w_2 and w_3 also have the same role, only for the *y* and *z* directions (perpendicular to the chain). In Eq. (1), the creation and annihilation operators of an acoustic phonon are denoted by b_q^{+}, b_q. They are characterized by 3D wave vector $\boldsymbol{q}$ and the frequency $\omega_{\boldsymbol{q}}$. In [21], it was demonstrated that the spectrum of acoustic phonons of a simple one-dimensional chain is described by the following expression:

$$\omega_{\boldsymbol{q}}^2 = \omega_1^2 \sin^2(q_x b/2) + \omega_2^2 \sin^2(q_y a/2) + \omega_3^2 \sin^2(q_z c/2). \quad (3)$$

In the given context, ω_1, ω_2 and ω_3 are limit frequencies for oscillations in *x*, *y* and *z* directions, respectively. As mentioned earlier, two most significant mechanisms of electron-phonon interaction are considered: one of the deformation potential type and the other of the polaron type. In the deformation potential interaction, the coupling constants are proportional to derivatives w_1', w_2' and w_3' of w_1, w_2, and w_3 with respect to the intermolecular distances.

These derivatives quantify how the electronic energy is affected by changes in the distances between neighboring molecules. On the other hand, in the polaron interaction, the coupling constant is proportional to the average polarizability of the molecule α_0. This interaction is particularly relevant in crystals composed of large molecules such as TCNQ, so as α_0 is roughly proportional to the volume of molecule.

The square module of matrix element $A(\boldsymbol{k},\boldsymbol{q})$ from Equation (1) has the following form:

$$|A(\boldsymbol{k},\boldsymbol{q})|^2 = 2\hbar w_1'^2 (NM\omega_{\boldsymbol{q}}) \Big\{ \Big[\sin(k_x b) - \sin(k_x - q_x, b) + \gamma_1 \sin(q_x b) \Big]^2 + d_1^2 \Big[\sin(k_y a) - \sin(k_y - q_y, a) + \gamma_2 \sin(q_y a) \Big]^2 + d_2^2 \Big[\sin(k_z c) - \sin(k_z - q_z, c) + \gamma_3 \sin(q_z c) \Big]^2 \Big\}. \quad (4)$$

In Eq. (4), *M* represents the mass of TCNQ molecule; *N* describes the number of TCNQ molecules in the basic region of the crystal; $d_1 = w_2 / w_1 = w_2' / w_1'$; $d_2 = w_3 / w_1 = w_3' / w_1'$; parameters γ_1, γ_2, and γ_3 have the sense of the amplitudes ratio of the polaron-type interaction to the deformation potential one in the *x*, *y*, and *z* directions:

$$\gamma_1 = 2e^2\alpha_0 / b^5 w_1'; \ \gamma_2 = 2e^2\alpha_0 / a^5 w_2'; \ \gamma_3 = 2e^2\alpha_0 / c^5 w_3'. \tag{5}$$

The renormalized phonon spectrum $\Omega(\boldsymbol{q})$ is determined by the pole of the Green function. It is obtained by solving the transcendent dispersion equation

$$\Omega(\boldsymbol{q}) = \omega_{\boldsymbol{q}} \left[1 - \bar{\Pi}(\boldsymbol{q}, \Omega)\right]^{1/2}, \tag{6}$$

where the principal value of the dimensionless polarization operator takes the form:

$$\mathrm{Re}\,\bar{\Pi}(\boldsymbol{q}, \Omega) = -\frac{\bar{N}}{2\pi^3 \hbar \omega_{\boldsymbol{q}}} \int_{-\pi}^{\pi} dk_x \int_{-\pi}^{\pi} dk_y \int_{-\pi}^{\pi} dk_z \left| A(\boldsymbol{k}, -\boldsymbol{q}) \right|^2 \times \frac{n_{\boldsymbol{k}} - n_{\boldsymbol{k}+\boldsymbol{q}}}{\varepsilon(\boldsymbol{k}) - \varepsilon(\boldsymbol{k}+\boldsymbol{q}) + \hbar\Omega}. \tag{7}$$

In Eq. (7) $n_{\boldsymbol{k}}$ is the Fermi distribution function, $\hbar$ is the Planck constant and $A(\boldsymbol{k}, \boldsymbol{q})$ is the matrix element of electron-phonon interaction. The integral in Eq. (7) has singularities and must be calculated with a needed accuracy. The Eq. (6) can be solved only numerically. Numerical calculations were performed in the Mathematica package.

3. Results and Discussion

Numerical calculations have been conducted using the following parameters [17, 19]: w_1 = 0.125 eV, w_1' = 0.22 eVÅ^{-1}, c = 3.75 Å, b = 12.97 Å, a =19.15 Å and $M = 3.72 \cdot 10^5\ m_e$ (m_e is the electron rest mass). The sound velocity $v_{s1} \approx 4 \cdot 10^5$ cm/s along chains, in c direction, $v_{s2} \approx 2 \cdot 10^5$ cm/s in b direction and $v_{s3} \approx 1 \cdot 10^5$ cm/s in a direction, d_1 = 0.015, d_2 = 0.01, r = 2 (two molecules in an unit cell), γ_1 = 1.7. The parameters γ_2 and γ_3 are determined from the relation: $\gamma_2 = \gamma_1 2^5 b^5/(a^5 d_1)$ and $\gamma_3 = \gamma_1 2^5 b^5/(c^5 d_2)$. The Fermi momentum varies from the value of $k_F = 0.56\pi/2$ to the value of $k_F = 0.62\pi/2$. These values were chosen in the region of the stoichiometric value of the Fermi momentum for these crystals.

From the information provided, it is evident that the Figures 1-4 depicting the dependence of renormalized phonon frequencies $\Omega(q_x)$ as functions of q_x for various temperatures and different values of q_y and q_z, exhibit several important observations. Firstly, it is observed that the values of $\Omega(q_x)$ are lower (diminished) compared to the frequencies $\omega(q_x)$ in the absence of electron-phonon interaction. This reduction in $\Omega(q_x)$ indicates that the electron-phonon interaction leads to a decrease in the values of the lattice elastic constants.

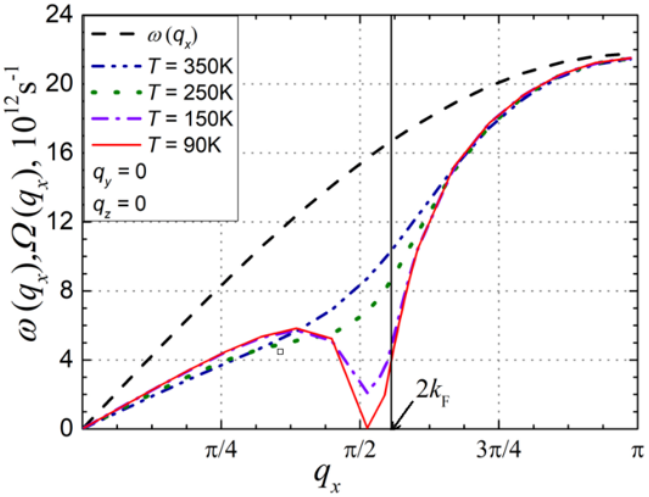

Figure 1. Renormalized phonon spectrum $\Omega(q_x)$ is plotted for various temperatures, with γ_1 = 1.7. The dashed line represents the spectrum of free phonons. The specific value chosen for this plot is: $k_F = 0.56\pi/2$.

This phenomenon arises due to the coupling between electrons and lattice vibrations. Secondly, as the temperature T decreases, the curves representing $\Omega(q_x)$ exhibit changes in their shape. Specifically, a minimum appears in the $\Omega(q_x)$ dependencies, and this minimum becomes more pronounced at lower temperatures. This behavior suggests that there is a critical temperature at which $\Omega(q_x)$ reaches zero. However, contrary to the expectation that $\Omega(q_x)$ will attain zero at $q_x = 2\ k_F$, where k_F represents the Fermi wave vector, the figures indicate that $\Omega(q_x)$ attains zero for a value of $q_x \neq 2\ k_F$. The appearance of a minimum in the $\Omega(q_x)$ dependencies with decreasing temperature suggests the possibility of a structural Peierls transition. However, the deviation of $\Omega(q_x)$ reaching zero from $q_x = 2\ k_F$ is due to the deviation of k_F from the expected value of $\pi/4$ in this particular system.

Figure 1 illustrates a scenario where $q_y = 0$, $q_z = 0$ and $k_F = 0.56\pi/2$. In this particular case, the interaction between TCNQ chains is neglected. When the temperature T reaches 90 K, the transition exclusively occurs within the TCNQ chains. This experimental observation is supported by a significant reduction in electrical conductivity. Moreover, the crystal lattice along the TCNQ chains undergoes a transformation from its initial state with a lattice constant c to a new crystalline state with a constant $4c$, that is four times larger. This temperature marks the occurrence of a metal-dielectric phase transition, accompanied by the complete opening of a gap in the carrier spectrum within the 1D conduction band of TCNQ, positioned just above the Fermi energy.

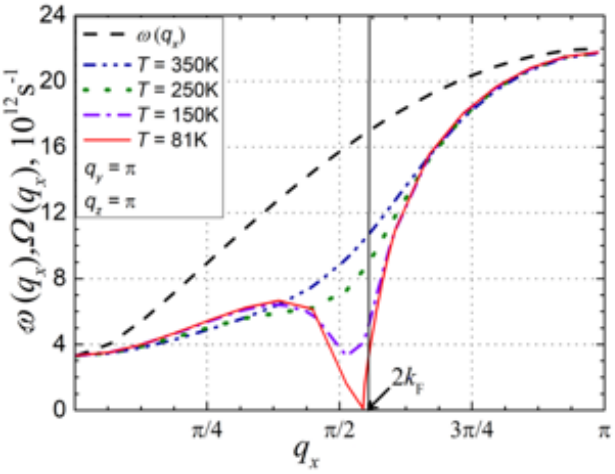

Figure 2. Renormalized phonon spectrum $\Omega(q_x)$ is plotted for various temperatures, with $\gamma_1 = 1.7$. The dashed line represents the spectrum of free phonons. The specific value chosen for this plot is: $k_F = 0.56\pi/2$.

When the interaction between TCNQ chains is considered ($q_y \neq 0$, $q_z \neq 0$), the Peierls critical temperature is reduced. Figures 2 - 4 correspond to 3D physical model with $q_y \neq 0$ and $q_z \neq 0$. These figures illustrate the dependences of $\Omega(q_x)$ on q_x for $q_y = \pi$, $q_z = \pi$, for different values of carrier concentration and different temperatures. Figure 2 represents the case when the Fermi momentum $k_F = 0.56\pi/2$. It is noteworthy that $\Omega(q_x)$ reaches zero at $T = 81$ K, indicating that the transition takes place at this T.

In Figure 3, the renormalized phonon spectrum $\Omega(q_x)$, for the Fermi momentum $k_F = 0.59\pi/2$ and $q_y = \pi$, $q_z = \pi$ can be observed. In this case the interaction between TCNQ chains is taken into account. As a result, the Peierls transition occurs at $T = 57$ K. One can see that with an increase in carrier concentration, the Peierls critical temperature decreases more.

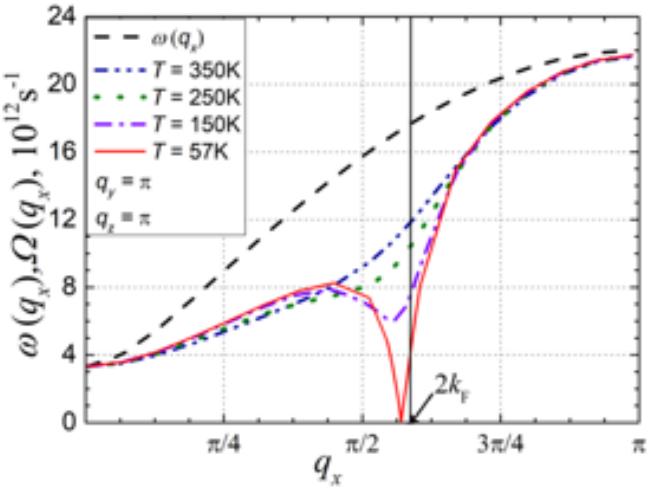

Figure 3. Renormalized phonon spectrum $\Omega(q_x)$ is plotted for various temperatures, with $\gamma_1 = 1.7$. The dashed line represents the spectrum of free phonons. The specific value chosen for this plot is: $k_F = 0.59\pi/2$.

Figure 4 exhibits the identical dependencies of the renormalized phonon spectrum $\Omega(q_x)$ as in the previous figures, but with an increased value of the Fermi momentum $k_F = 0.62\pi/2$, while maintaining $q_y = \pi$, $q_z = \pi$. This figure showcases different temperatures. It can be observed that the transition temperature further decreases and reaches $T = 35.1$ K. This observation indicates that as the carrier concentration increases, the Peierls critical temperature continues to diminish.

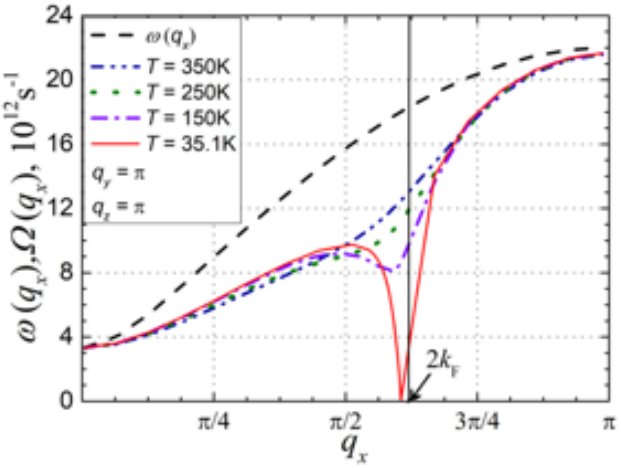

Figure 4. Renormalized phonon spectrum $\Omega(q_x)$ is plotted for various temperatures, with $\gamma_1 = 1.7$. The dashed line represents the spectrum of free phonons. The specific value chosen for this plot is: $k_F = 0.62\pi/2$.

4. Conclusions

We have carried out investigations on phonons near Peierls structural transition in quasi-one-dimensional crystals of TTT(TCNQ)$_2$ in the 3D approximation, using a more comprehensive physical model of the crystal. This model incorporates two most significant electron-phonon interactions. The renormalized phonon spectrum has been computed in the random phase approximation. Numerical calculations of the renormalized phonon spectrum, $\Omega(q_x)$, have been performed for various temperatures and different values of q_y and q_z. Our findigs indicate that when the interaction between TCNQ chains is neglected ($k_F = 0.56\pi/2$, $q_y = 0$, $q_z = 0$), the Peierls transition initiates in the TCNQ chains alone at $T = 90$ K. However, when

the interchain interaction is taken into account ($q_y = \pi$ and $q_z = \pi$), the transition is completed at $T = 81$ K. Moreover, our calculations demonstrate a significant decrease in the Peierls critical temperature with an increase in carrier concentration. So, for $k_F = 0.59\pi/2$, the transition occurs at $T = 57$ K, and for $k_F = 0.62\pi/2$, the transition takes place at $T = 35.1$ K, respectively. These results were obtained for the case when the interchain interaction is considered. We note that the Peierls transition in $TTT(TCNQ)_2$ crystals was studied first time by us. In other *n*-type crystals, such as those of TTF-TCNQ, the Peierls transition has been studied by several authors, both theoretically and experimentally. It has been shown that the transition starts at $T = 59.7$ K in TCNQ chains alone. When the interaction between the adjacent chains are considered the transition is finished at $T = 54$ K. The electron-phonon interaction diminishes renormalized phonon spectrum $\Omega(q_x)$ with respect to initial frequency $\omega(q_x)$.

Acknowledgments: This work was supported by project **20.80009.5007.08** "Study of optoelectronic structures and thermoelectric devices with high efficiency".

Conflicts of Interest: The authors declare no conflict of interest.

References

1. Casian, A. *Thermoelectric Handbook, Macro to Nano, Ed. by D. M. Rowe, CRC Press*, 2006, cap. 36.
2. Sanduleac, I.; Casian, A.; Pflaum, J. Thermoelectric Properties of Nanostructured Tetrathiotetracene Iodide Crystals in a Two-Dimensional Model. *Journal of Nanoelectronics and Optoelectronics* 2014, 9 (2), pp. 247-252.
3. Jerome, D. Organic Superconductors: When Correlations and Magnetism Walk. *Journal of Superconductivity and Novel Magnetism* 2012, 25, pp. 633-655.
4. Pouget, J. P. Bond and Charge Ordering in Low-Dimensional Organic Conductors. *Physica B* 2012, 407, pp. 1762-1770.
5. Acker, D. S.; Harder, R. J.; Hertler, W. R.; Mahler, W.; Melby, L. R.; Benson, R.; Mochel, W. E. 7,7,8,8-Tetracyanoquinodimethane and its electrically conducting anion-radical derivatives. *Journal of the American Chemical Society* 1960, 82, pp. 6408-6409.
6. Wudl, F.; Smith, G. M.; Hufnagel, E. J. Bis-1,3-dithiolium chloride: an unusually stable organic radial cation. *Chemical Communications* 1970, pp. 1453-1454.
7. Ferraris, J. P.; Cowan, D. O.; Walatka, V.; Perlstein, J. H. Electron transfer in a new highly conducting donor-acceptor complex. *Journal of the American Chemical Society* 1973, 95, pp. 948-949.
8. Coleman, L. B.; Cohen, M. J.; Sandman, D. J.; Yamagishi, F. G; Garito, A. F.; Heeger, A. J. Superconducting fluctuations and the Peierls instability in an organic solid. *Solid State Communications* 1973, 12, pp. 1125-1132.
9. Peierls, R. *Quantum Theory of Solids*. Oxford University Press, London, 1955, pp.108.
10. Jerome, D. Organic Conductors: From Charge Density Wave TTF-TCNQ to Superconducting $(TMTSF)_2PF_6$. *Chemical Reviews* 2004, 104, pp. 5565-5592.
11. Pouget, J. P. The Peierls Instability and Charge Density Wave in One- Dimensional Electronic Conductors. *Comptes Rendus Physique*,2016, 17, pp. 332-356.
12. Streltsov, S. V.; Khomskii, D. I. Orbital-Dependent Singlet Dimers and Orbital-Selective Peierls Transitions in Transition-Metal Compounds. *Physical Review B* 2014, 89 (16), article ID: 161112.
13. Chernenkaya, A.; Medjanik, K.; Nagel, P.; Merz, M.; Schuppler, S.; Canadell, E.; Pouget, J. P.; Schonhense, G. Nature of the Empty States and Signature of the Charge Density Wave Instability and Upper Peierls Transition of TTF-TCNQ by Temperature-Dependent NEXAFS Spectroscopy. *The European Physical Journal B* 2015, 88 (13).
14. Khanna, S. K.; Pouget, J. P.; Comes, R.; Garito, A. F.; Heeger, A. J. X-Ray Studies of $2k_F$ and $4k_F$ Anomalies in Tetrathiafulvalene-Tetracyanoquinodimethane (TTF-TCNQ). *Physical Review B* 1977, 16, 1468.
15. Reitschel, H. The Giant Kohn Anomaly in a Peierls Semiconductor. *Solid State Communications* 1973, 13, 1859.
16. Bulaevskii, L. N. Peierls Structure Transition in Quasi-One-Dimensional Crystals. *Soviet Physics Uspekhi* 1975, 18, pp. 131.
17. Andronic, S.; Casian, A. Phonons near Peierls Structural Transition in Quasi-One-Dimensional in organic crystals of TTF-TCNQ. *Advances in Materials Physics and Chemistry* 2016, 6, pp. 98-104.

18. Andronic, S.; Casian, A. Metal-Insulator Transition of Peierls Type in Quasi-One-Dimensional Crystals of TTT_2I_3. *Advances in Materials Physics and Chemistry* 2017, 7, pp. 212-222.
19. Buravov, L.; Eremenko, O.; Lyubovskii, R.; Rozenberg, L.; Khidekel, M.; Shibaeva, R.; Shchegolev, I.; Yagubskii, E. Structure and electromagnetic properties of a new high conductivity complex $(TTT)^+(TCNQ)_2^-$. *ZhETF Pis. Red.* 1974, 20 (7), pp. 457-461.
20. Shchegolev, I. F.; Yagubskii E. B. Cation-radical salts of tetrathiotetracene and tetraselenotetracene: synthetic aspects and physical properties. *Linear Extendend Chain Compounds* 1982, 2, pp. 385-434. Edited by MILLER, J. S., Plenum Press, New York.
21. Graja, A. Low-dimensional organic conductors. *Word Scientific, Singapore,* 1992.

Citation: Andronic, S.; Sanduleac, I. Analysis of phonons behavior in quasi-one-dimensional crystals of $TTT(TCNQ)_2$ near the Peierls structural transition in a 3D approximation. *Journal of Engineering Science* 2023, 30 (3), pp. 7-15. https://doi.org/10.52326/jes.utm.2023.30(3).01.

Submission of manuscripts: jes@meridian.utm.md