SSNN O10 **TEMPERATURE DEPENDENCES OF THE THERMOELECTRIC POWER FACTOR OF TTT$_2$I$_3$ ORGANIC CRYSTALS**

I. Sanduleac[*], A. Casian

Technical University of Moldova, Chisinau, Rep. of Moldova
*E-mail: sanduleac_ionel@yahoo.com

The organic crystals of p − type of tetrathiotetracene-iodide (TTT$_2$I$_3$) are very prospective for thermoelectric applications. The internal structure consists of segregate linear TTT molecular chains spaced at approximately 0.9 nm one from other. In the chain direction, the distance between the nearest TTT molecules is ~ 0.25 nm, and the overlap of electronic wavefunctions provide a narrow conduction band in this direction. The crystal is a Charge-Transfer complex, with a transfer rate of 0.5 electron per TTT molecule to the iodine chains. The electrical conductivity is highly anisotropic and is mainly provided by TTT chains. Two most important electron-phonon interaction mechanisms are considered: of the deformation potential type and of the polaron type. For a narrow interval of electronic states in the conduction band, the interactions compensate partially each other, diminishing the electron-phonon scattering and leading to a significant increase in the relaxation time of charge carriers. Therefore, the thermoelectric properties can be significantly enhanced by optimizing the structural composition of the crystal.

A two-dimensional physical model of the crystal is applied. The main Hamiltonian consist of the electronic part, calculated by using the approximation of tight-binding electrons, with w_1, w_2 being the transfer energies of an electron from one molecule to the nearest one, along the TTT chains and in transversal direction, respectively. The free phonon part takes into consideration only the acoustic longitudinal vibration branch. The coupling constants of the first interaction mechanism are proportional to the derivatives of transfer energies, w_1', w_2' with respect to the intermolecular distance. The polaron type interaction mechanism is proportional to the mean polarizability of TTT molecule α_0. The scattering of electrons on impurities and defects is also considered.

The kinetic equation of Boltzmann type is obtained in the frame of weak temperature gradient and weak electric field by the method of two-particle retarded Green functions. The power factor is calculated numerically as a function of temperature for different concentrations of charge carriers.

The following parameters of TTT$_2$I$_3$ crystals are considered: $M = 6.5 \cdot 10^5 m_e$ (m_e is the mass of the free electron), $b = 4.96$ Å, $a = 18.35$ Å (lattice constants), $w_1 = 0.16$ eV, $w_1' = 0.26$ eVÅ^{-1} [1], $d_1 = w_2 / w_1 = w_2' / w_1' \approx 0.015$, $v_{s1} = 1.08 \cdot 10^3$ m/s, $E_F = 0.12$ eV. The average value $\alpha_0 = 46$ Å^{-3} was estimated. The stoichiometric concentration charge carriers (holes) was estimated to $n = 1.25 \cdot 10^{21}$ cm^{-3} or $\varepsilon_F = E_F / 2w_1 = 0.36$, where ε_F is the dimensionless Fermi energy [2].

In fig.1. the dependences of the power factor in the direction of molecular conductive chains as a function of absolute temperature is presented for three values of carrier concentration. The dimensionless parameters $D_0 = 0.001$ and $D_1 = 0.8$ describe the scattering on static impurities and on thermally activated defects, respectively. The parameters were estimated by fitting the calculated data for electrical conductivity with experimental results, reported for TTT$_2$I$_3$ crystals, growth from solution [3]. It is observed, that the power factor can be enhanced for a wide range of temperatures by diminution of charge carriers concentration (holes). At 300 K, values of P_{xx} = 3.2, 9.5 and 12.8 mWm^{-1}K^{-1} are predicted for optimized crystals with $n = 1.2$, 0.9 and 0.6 $\cdot 10^{21}$cm^{-3}. Experimentally reported: $P_{exp} \approx 2.4$ mWm^{-1}K^{-1} [3].
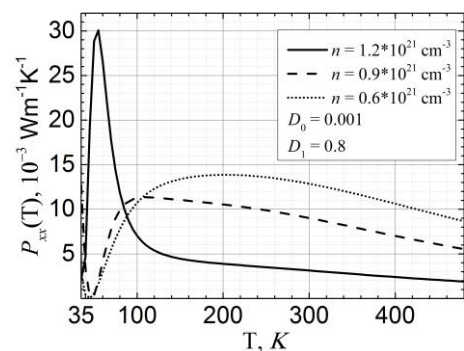

Fig.1. Thermoelectric Power Factor, P_{xx} (T) along TTT chains

[1] L. Isset, *Phys.Rev.B*, (1978), vol. 18, Issue 1, pp. 439-447.
[2] A. Casian, I. Sanduleac, *Materials Today: Proceedings*,(2015), vol. 2, Issue 2, pp. 504-509.
[3] V.F. Kaminskii, M.L. Khidekel', R.B. Lyubovskii and al., *Phys. Status Solidi* A, (1977), vol. 44, pp. 77.