SSNN 13P **THERMOELECTRIC POWER FACTOR OF TETRATHIOTETRACENE-IODIDE ORGANIC CRYSTALS IN THE 3D MODEL**

I. I. Sanduleac*, A. I. Casian
Technical University of Moldova, Chisinau, Moldova
*E-mail: sanduleac_ionel@yahoo.com

Nanostructured organic crystals of TTT_2I_3 are very prospect materials for thermoelectric applications. The crystals are needle-shaped and consist of segregate stacks of TTT molecules and iodine ions. Due to the pronounced quasi-one-dimensionality and to the property that allows the formation of non-stoichiometric compounds, the thermoelectric figure of merit of these crystals, *ZT*, may be increased by optimizing the concentration of conducting holes, as it was predicted theoretically [1]. Earlier [2] it was demonstrated on the basis of a bi-dimensional (2D) model that the interchain interaction has a small influence on the transport and thermoelectric properties in the direction of molecular chains (*x* direction) when the purity level is not very high. By the other side, for ultra-pure crystals, the interaction mentioned above becomes significant. For these reasons it is necessary to analyze the 3D complete model. Theoretical model was developed taking into account the narrow conduction band in the *x* direction (~ 25 k_0T_0, T_0 is the room temperature) and the hopping transport in transversal (*y* and *z*) directions. The Hamiltonian of the system is applied in the tight-binding electrons and nearest neighbor's approximations, and contains two electron-phonon interactions: of deformation potential and of polaron type. The scattering on point-like, electric neutral and randomly distributed impurities is also taken into account.
Transport coefficients are calculated using the Kubo formula for electrical conductivity and the linearized Boltzmann equation. The ratio of transfer energy between nearest molecules in the transversal direction w_2 and w_3 on the longitudinal w_1 one is denoted by $d = w_2/w_1 \approx w_3/w_1 = 0.013$.
Electrical conductivity and power factor as function of dimensionless Fermi energy $\varepsilon_F = E_F/2w_1$ are presented in Figs.1, 2. The impurity scattering is described by the parameter $D_0 = 0.1, 0.04, 0.02$.

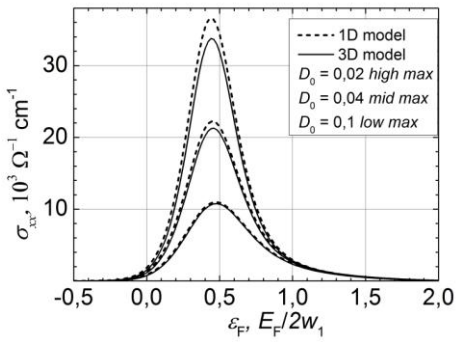

Fig.1. Electrical conductivity in the *x* direction as function of ε_F.

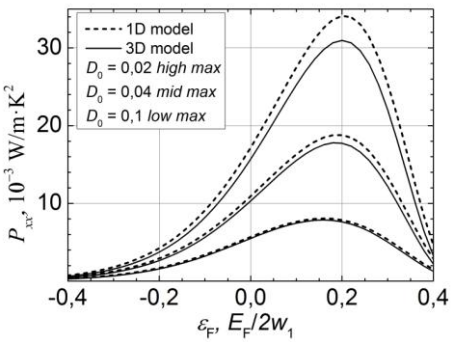

Fig.2. Power factor *P*, as function of ε_F.

The results of numerical calculations in the 3D crystal model show an increasing influence of interchain interaction when the crystal purity is increased. The same behavior was predicted theoretically in previous papers for 2D model approximation [3]. In such a way, for stoichiometric compounds ($\varepsilon_F = 0.33$), the relative deviations of simplified 1D model approximation from the more realistic 3D one are: 3.6 %, 6.1 % and 9.5 % for electrical conductivity and 9.8 %, 15 %, 21 % for thermoelectric power factor when $D_0 = 0.1, 0.04, 0.02$. Consequently, for TTT_2I_3 organic crystals with $\sigma \sim 10^4\ \Omega^{-1}\ cm^{-1}$ and lower at room temperature it is applicable the simpler 1D model approximation. For purer crystals the complete 3D model must be considered.

[1] A. I. Casian, *Thermoelectric Handbook, Macro to Nano, Ed. By D. M. Rowe*, *CRC Press*, 2006, Chap.36.
[2] A. I. Casian, I. I. Sanduleac. *J. of Nanoelectronics and Optoelectronics*, **7**, 2012, 706 – 711.
[3] I. I. Sanduleac, A. I. Casian, J. Pflaum., *J. of Nanoelectronics and Optoelectronics*, **9**, 2014, 247 – 252.