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Thermoelectric properties of nanostructured tetrathiotetracene iodide crystals: 3D modeling

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Abstract

A more complete three-dimensional (3D) physical model for nanostructured crystals of tetrathiotetracene iodide, TTT_2I_3, is presented. The restrictions on the thermoelectric figure of merit *ZT* that this model involves are determined. At the same time, the criteria of application of simplified 1D model are defined more precisely. In TTT_2I_3 crystals the carriers are holes. As earlier, two interaction mechanisms of holes with acoustic phonons are considered, generalized for 3D case. One interaction is similar to that of polaron and other to that of deformation potential. Interaction of carriers with impurities and defects is also taken into account. Along chains (*x* direction) the transport mechanism is of the band type, but in the transversal directions it is of hopping type. The electrical conductivity σ_{xx}, the thermopower (Seebeck coefficient) S_{xx}, the electronic thermal conductivity κ^e_{xx} and $(ZT)_{xx}$ along the conductive chains have been modelled for the first time in the 3D model. Optimal parameters which predict a considerable increase of $(ZT)_{xx}$ are determined.

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Keywords: Tetrathiotetracene iodide; nanostructured crystals; electrical conductivity; thermopower; thermoelectric figure of merit.

1. Introduction

Organic materials attract more and more attention for thermoelectric applications because they have much more diverse properties in comparison with the inorganic ones and their electronic structure is well tunable through molecular chemistry and doping procedures. Besides, organic materials usually have lower thermal conductivity, can be easier produced, are cost effective and are environmentally friendly. In the past two decades big efforts were

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undertaken to investigate the thermoelectric applications of organic materials, especially of conducting polymers (see the review [1]).

Poly(3,4-ethylenedioxythiophene) (PEDOT) doped by poly(styrenesulphonate) (PSS) is promising as an organic-based thermoelectric material due to its stability in air and potential for very high electrical conductivity (measured over 300,000 Sm^{-1}) [2]. By optimizing the carrier concentration a value of the thermoelectric figure of merit $ZT = 0.42$ has been measured in *p*-type [2, 3] and 0.20 in *n*-type [4] materials. Thermoelectric modules containing *n-p* single couples were fabricated by printing [5]. In (PEDOT:PSS) thin films *ZT* value of 0.31 was achieved at room temperature [6], very good result.

It was demonstrated that the nanocomposites of organic and inorganic components may have better thermoelectric performance than either component [7-9]. And really, the highest value of $ZT = 0.57$ at room temperature was measured in phenyl acetylene-capped silicon nano particles [10]. Different theoretical models have been also developed [11-14] in order to describe the thermoelectric transport in organic materials.

In molecular nanowires of conducting polymers values of $ZT \sim 15$ and of thermoelectric power factor $\sim 5\square 10^4$ $W/m\cdot K^2$ at room temperature were predicted [15] in spite of hopping conducting mechanism that usually gives smaller carrier mobility than the band model.

The quasi-one-dimensional (Q1D) organic crystals attract a special attention. Values of $ZT \sim 20$ have been predicted in highly conducting charge transfer organic crystals, if the crystal purity is sufficiently high [16] assuring huge mobilities. These results were obtained in strongly one-dimensional approximation, when the crystal is formed from 1D conductive molecular chains packed into a three-dimensional (3D) structure. In not very pure crystals of tetrathiotetracene-iodide, TTT_2I_3, grown from