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Thermoelectric Properties of Nanostructured Tetrathiotetracene Iodide Crystals in a Two-Dimensional Model

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Previously, it has been predicted that nanostructured crystals of tetrathiotetracene iodide are very promising candidates for thermoelectric applications. However, these predictions are based on a strictly one-dimensional (1D) model. In order to verify these conclusions, a two-dimensional (2D) model is elaborated which explicitly takes into account the weak interaction of carriers with the nearest conductive chains. It is shown that for crystals with a rather low degree of purity this interaction does not affect significantly the results obtained by the 1D approximation, but for ultra-pure crystals this interaction can no longer be neglected.

Keywords: Tetrathiotetracene Iodide, Interchain Interaction, Two-Dimensional Crystal Model, Thermoelectric Figure of Merit.

RESEARCH ARTICLE

1. INTRODUCTION

The necessity to recover into electricity even a part of the enormous quantity of waste low grade thermal energy requires an increasing effort in the search and investigation of new, more efficient thermoelectric (TE) materials with higher possible thermoelectric figure of merit ZT and of reasonable productions costs. During the last decade two major directions in the search of suited materials have been emerged. One direction is connected with bulk multi component systems, such as clathaters[1] and filled scutterudite systems,[2] containing many atoms in the elementary cell and thus having complex electronic and phonon spectra. For these material classes ZT values of up to 2.2 at 800 K were obtained[3] in chalcogenides $AgPb_mSbTe_{2+m}$. The other direction is connected with low-dimensional quantum structures of 2D, 1D, 0D. In this case, $ZT = 2.4$ was measured in Bi_2Te_3–Sb_2Te_3 superlattices[4] and impressively high ZT values of 3 and even 3.5 were reported by Harman in PbTeSe quantum dot superlattices.[5]

The main source of ZT enhancement in such materials and structures is caused by the reduction of thermal conductivity, although contributions by an increasing power factor P were also observed. For n-type PbTe/PbEuTe quantum wells Harman et al. have measured[6] a value of P of the order $6.2–6.6 \cdot 10^{-3}$ W/m K^2. In p-type structures $P \sim 1.6 \cdot 10^{-2}$ W/mK^{-2} was observed.[7] Also, it was predicted theoretically[8,9] for such (100) and (111) oriented n-quantum wells $P_{100} = 1.75 \cdot 10^{-2}$ W/mK^2 and $P_{111} = 1.08 \cdot 10^{-2}$ W/mK^2, and a maximum value of $\sim 2.5 \cdot 10^{-2}$ W/mK^2 for p–type quantum wells.[10]

A much higher (100-fold) reduction in the lattice thermal conductivity was realized in silicon nanowires, and a value of $ZT \sim 0.6$ was obtained at room temperature[11] and $ZT \sim 1$ at 200 K (Ref. [12]), although it is known that bulk Si is a poor thermoelectric.

However, the fabrication technology of such quantum-well structures is rather complicated and expensive. Besides, this approach solely cannot produce big quantities of such materials. Therefore, the search and investigation of new materials with high potential for thermoelectric applications proceeds to be an important and urgent problem of materials science.

In the last time organic materials attracted increasing attention by investigators as materials with more diverse properties and being less expensive than the well-known inorganic ones. There are already promising results, e.g., in poly (3,4-ethylenedioxy-thiophene) (PEDOT) a value of $ZT = 0.25$ has been measured,[13] and $ZT = 0.42$ at room temperature was obtained[14] in PEDOT: PSS. It is predicted that in this class of materials $ZT = 1$ can be achieved.[15] To our knowledge, a highest value of $ZT = 0.57$ at room

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