Effect of Lorenz Number Decrease on Thermoelectric Efficiency in Quasi-One-Dimensional Organic Crystals

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In quasi-one-dimensional organic crystals, the relaxation time as a function of carrier energy can exhibit, under certain conditions, a rather high and sharp maximum. It is shown that this maximum and its position on the energy scale influence the electrical conductivity and electronic thermal conductivity in different ways. First, the electrical conductivity is considerably increased. The electronic thermal conductivity is also increased, but to a lesser extent due to the narrower energy interval of carriers that contribute to energy transport. Second, both the electrical conductivity and electronic thermal conductivity achieve maximums, but the latter is displaced to higher carrier concentrations in comparison with the maximum of electrical conductivity. As a consequence, the Lorenz number is decreased for some range of carrier concentration and is increased in other ranges. It is important that there is a large interval of carrier concentrations where the Lorenz number is significantly diminished, and the Fermi level can be moved up to this interval. The Lorenz number may be diminished considerably in comparison with ordinary materials. This is favorable for increase of the thermoelectric figure of merit.

Key words: Thermoelectric, organic crystal, tetrathiotetracene iodide, electronic thermal conductivity, Lorenz number

INTRODUCTION

Recently, significant growth of the thermoelectric figure of merit ZT near room temperature has been obtained in low-dimensional quantum structures—quasi-two-dimensional superlattices, quasi-one-dimensional (Q1D) quantum wires, and structures with quasi-zero-dimensional quantum dots.^{1,2} Several reasons for the increase of ZT in such structures have been established.

The first of these is the growth of the electronic density of states due to quantization of the carrier energy spectrum. The second reason is that, due to additional phonon scattering at structure interfaces³ or to phonon reengineering,⁴ the lattice thermal conductivity is reduced. The main growth of ZT in low-dimensional quantum structures has been obtained just from diminution of the thermal

conductivity, although a contribution from growth of the thermoelectric power factor was also observed.²

Now, the lowest limiting value of thermal conductivity of such structures has practically been achieved. Therefore, only the opportunity to increase the power factor² remains. An increase of the power factor has been measured in *n*- and *p*-type PbTe/PbEuTe quantum-well superlattices.^{5,6} However, theoretical investigations $^{7-10}$ have shown rather limited possibilities to increase the power factor and ZT in such structures. It is known that increase of the electrical conductivity leads to decrease of the thermopower (Seebeck coefficient), so an optimization procedure is needed to obtain the maximum value of the power factor. However, at the same time, increase of the electrical conductivity leads to a proportional increase of the electronic thermal conductivity in accordance with the Wiedemann-Franz law. This reasoning applies when the relaxation time is a smooth function of

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