I. Physikalisches Institut (IA)
Physik neuer Materialien

I. Physikalisches Institut (IA)
Phasenwechselmaterialien
Prof. Dr. rer. nat. Matthias Wuttig

Topic for a Bachelor Thesis

“Engineering the band structure of IV-VI compounds for enhanced thermoelectric performance”

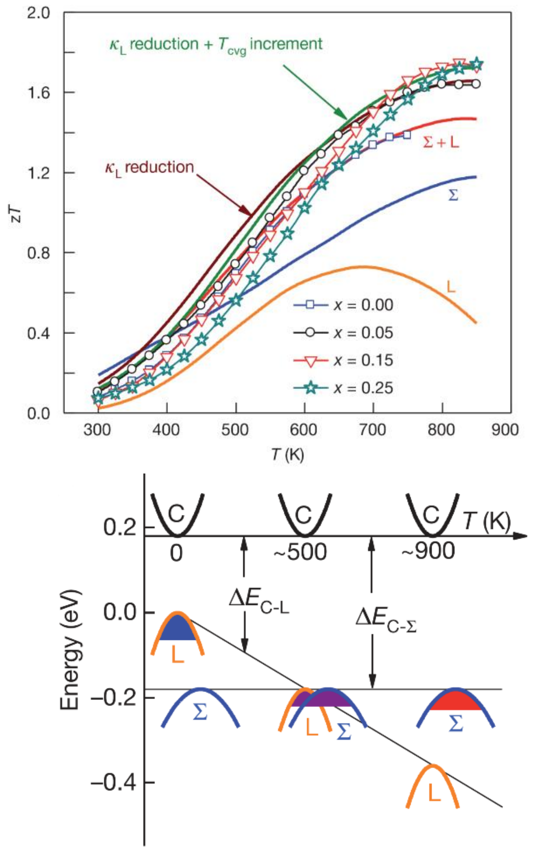

Fig 1: Effect of the convergence of band valleys on the thermoelectric performance. Increasing the valley degeneracy leads to a larger density-of-states and an enhanced Seebeck coefficient. Taken from Pei et al, 2011.

Thermoelectric materials could play an important role in a global sustainable energy solution by enabling the conversion of waste heat into electricity. The thermoelectric figure of merit is defined as:

$$zT = \frac{S^2\sigma}{k}T,$$

where S is the Seebeck coefficient, σ is the electrical conductivity, k is the thermal conductivity and T is temperature[1].

Maximization of zT requires the optimization of a variety of conflicting properties, resulting in a very complex problem. As consequence, several approaches have been attempted and several material classes have been studied for thermoelectric applications[2].

A possible root is to enhance the power factor $S^2\sigma$ by multivalley electron transport[3]. S is proportional to $m_{DOS}^* = N^{2/3}m^*$[4], where N and m^* are the valley degeneracy and the effective mass at the Fermi level E_F. Increasing the number of valleys with energy around E_F results in a larger N and in a subsequent increase of $S^2\sigma$.

A possible approach to obtain multivalley transport is to engineer the band structure of the material class under study by alloying miscible compounds. The goal is to increase the valley degeneracy at the Fermi level and obtain very large values of m_{DOS}^*, hence enhanced $S^2\sigma$.

Goal of this thesis is to systematically understand convergence of band valleys in IV-VI compounds, already successfully employed in PbTe:PbSe alloys[5]. To this end, Fourier-transform infrared spectroscopy, ellipsometry and Seebeck coefficient measurements will be performed on samples with different stoichiometry to detect changes in the positions of the valence-band valleys and to link them to changes in the density-of-states. Systematic trends with stoichiometry might enable the definition of atomistic design rules for band valleys convergence in IV-VI compounds and related alloys to maximize the thermoelectric performance.

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Matteo Cagnoni
✉ cagnoni@physik.rwth-aachen.de
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