I. Physikalisches Institut (IA)
Phasenwechselmaterialien
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Topic for a Master Thesis

„Convergence of band valleys in IV-VI compounds for enhanced thermoelectric performance “

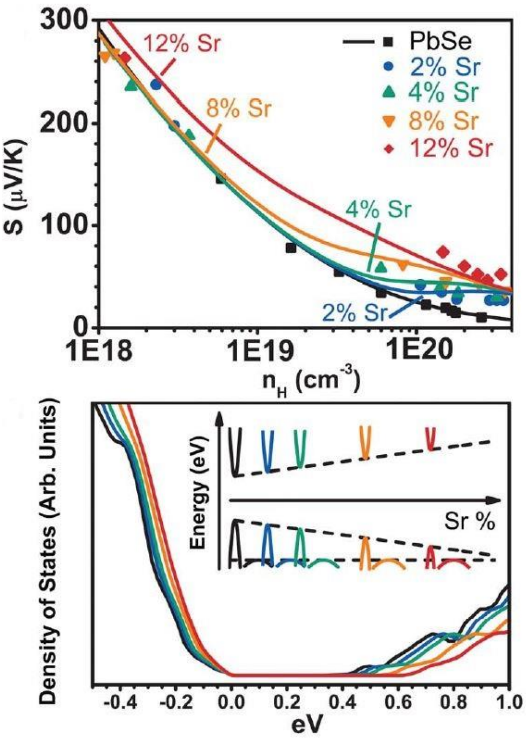

Fig 1: Effect of the convergence of band valleys on the thermoelectric performance. Increasing the valley degeneracy leads to a larger density-of-states and an enhanced Seebeck coefficient. Taken from Wang et al, 2014.

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, which makes the phase space of the problem very large. 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 convergence of band valleys[3]. As a matter of fact, 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 $S^2\sigma$.

Convergence of band valleys have been already employed in IV-VI compounds such as PbTe[5] and PbSe[6] to enhance the thermoelectric performance. In principle, the energy difference between the valence-band valleys can be engineered by alloying in order to strongly increase the density-of-states around E_F, resulting in very large values of m^*_{DOS} and enhanced $S^2\sigma$.

Goal of this thesis is to systematically understand convergence of band valleys in IV-VI compounds. To this end, Fourier-transform infrared spectroscopy, ellipsometry and Seebeck coefficient measurements will be performed on samples with different stoichiometry in order 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.

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