I. Physikalisches Institut (IA) Physik neuer Materialien
RWTH AACHEN UNIVERSITY

I. Institute of Physics (IA)
Nanocharacterization for advanced functional materials
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Topic for a Master's Thesis

Thermoelectric crystals of doped Tin selenide with metavalent bonding

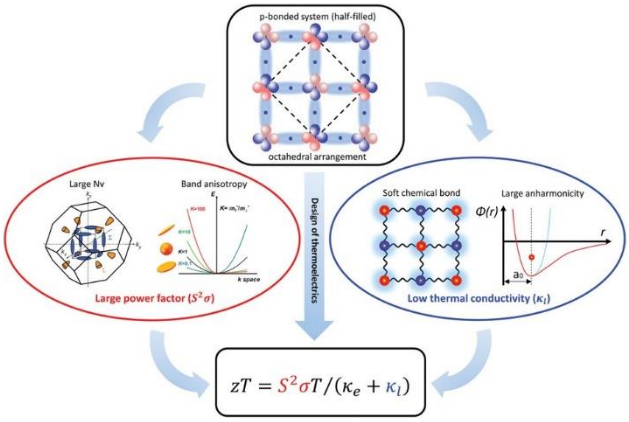

Fig. 1: Chalcogenide thermoelectrics empowered by an unconventional bonding mechanism.

INTRODUCTION Thermoelectric solid energy conversion technology provides a reliable way to use waste heat for power generation. Tin selenide (SnSe) as a new promising thermoelectric material exhibits one of the lowest lattice thermal conductivities (κ_l, refer to the formula in Fig. 1) known for crystalline materials, and **cubic SnSe with high symmetry has larger degeneracy number than orthorhombic SnSe, which favors a high Seebeck coefficient *S*. The phase transition alloy from orthorhombic to cubic structure was realized in $AgSbSe_2$ doped SnSe.** Heterogeneous element alloying or doping can be used to reduce κ_l by introducing defects to enhance phonon scattering, adjusting the nature of the chemical bonds, and thus optimizing the thermoelectric properties. Chalcogenides utilizing metavalent bonding (MVB) are characterized by high Grüneisen parameters and therefore have low κ_l.

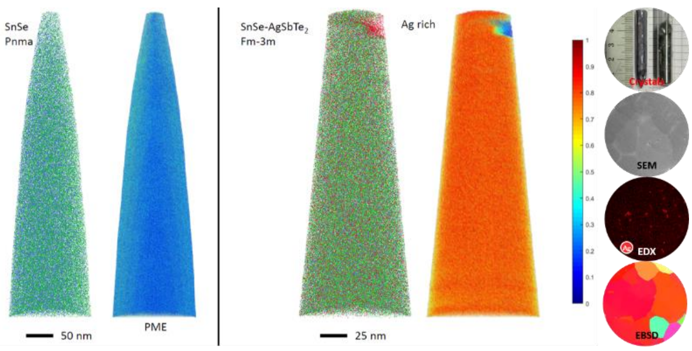

Fig. 2: Experimental data for pure and $AgSbTe_2$-doped SnSe. APT reconstructed the 3D distribution of atoms and the PME comparison.

Alloys such as $AgSbTe_2$ have been successfully used to modulate carrier concentration n_H and reduce lattice thermal conductivity *k* in many cubic IV-VI thermoelectrics. We confirmed the cubic structure of the SnSe-$AgSbTe_2$ alloy by EBSD, while EDX showed some Ag-rich precipitates, which are related to the formation of defects such as cation vacancies in the MVB phase (Fig. 2). The doped SnSe showed a higher "probability of multiple events" (PME) than that of pure SnSe using laser-assisted atom probe tomography (APT), which is related to its unconventional bond-breaking mechanism, while many other Ag-containing IV-VI compounds doped with SnSe can be investigated based on the property characteristics of chalcogenide with MVB.

THESIS DETAILS We will prepare Ag-V-VI_2 alloyed SnSe crystals through the Bridgman oven (Fig. 3) which can accurately control the temperature and automatically grow crystals through the set program, and then characterize the microstructures by XRD and EDX, measure the optical properties by Ellipsometry and FTIR-Spectrometer, and investigate the bonding mechanism by APT. All the techniques necessary to obtain a successful Master's thesis are available at I. Institute of Physics, RWTH Aachen University.

Fig. 3: Bridgman oven.

References:

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[2] H.X. Wang et al. "Band flattening and phonon-defect scattering in cubic SnSe–AgSbTe2 alloy for thermoelectric enhancement." Materials Today Physics (2021). https://www.sciencedirect.com/science/article/pii/S254252932030122X?casa

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