I. Physikalisches Institut (IA)
Physik neuer Materialien

RWTH AACHEN UNIVERSITY

Bundesministerium
für Wirtschaft
und Technologie

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

# „On the correlation of grain boundary charge carrier scattering and chemical bonding"

INTRODUCTION…

Thermoelectric materials provide an enticing solution to convert waste heat into electricity. The energy conversion efficiency is balanced by the tradeoff between electron and phonon transport. A good thermoelectric material requires unhindered electron transport but obstructive phonon propagation. To realize this intuitively controversial phenomenon, structural defects are introduced to scatter phonons while remaining electron transmission. Accordingly, nanostructuring to create high-density grain boundaries (GBs) has been widely implemented to improve the thermoelectric properties of materials.

This strategy indeed enhances the performance of some materials, e.g., $Bi_{0.5}Sb_{1.5}Te_3$ and PbTe. However, some materials show degraded performance by introducing GBs, e.g., SnSe and $Mg_3Sb_2$. This indicates GBs can also be detrimental defects because of strong carrier scattering. The controversial effect of GBs raises an important question that **what properties of the GB impact the charge transport**. The charge carrier scattering at GBs results from the dangling bonds that create a space charge layer and potential barrier. The scattering events at the barrier depends on the screening length and mean free path of electrons. In this regard, **the chemical bonding nature in the vicinity of GBs is of crucial importance because it determines the degree of dielectric screening**.

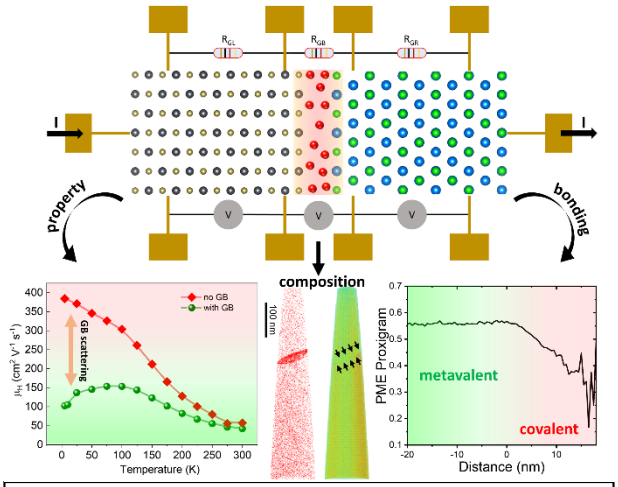


Figure 1: Schematic of the measurement of GB resistivity and corresponding experimental data for Ag-doped PbTe. The GB scattering effect is evidenced at low temperatures. APT determines the GB composition and local probability of multiple events.

THESIS DETAILS…In this Master thesis, we will focus on the local GB resistivity, chemical composition, and chemical bonding for pure PbTe and Ag-doped PbTe compounds. The different GB scattering behaviors will be attributed to the local modification of composition and bonding. All the characterization techniques (focused ion beam, PPMS, atom probe tomography) necessary to obtain a successful Master thesis are available at I. Institut of Physics, RWTH Aachen University.

**References:**

1 Yu et al., Adv. Funct. Mater. **2020**, *30*, 1904862.
2 Yu et al., Mater. Today. **2020**, *32*, 260.

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