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

I. Institute Of Physics (IA)
Phase Change Materials
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Topic for a Master's Thesis (English)

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„Investigation of the Chemical Bonding Mechanisms in Ag-V-VI_2 compounds"

Ag-V-VI_2 compounds are very promising and attractive due to their unique properties and potential applications in many fields such as thermoelectrice (TE), where an exceptionally high thermoelectric figure of merit has been reported. To understand the good thermoelectric performance and explore the application of Ag-V-VI_2 compounds in other fields, it is of vital importance to reveal the underlying mechanism, i.e. the chemical bonding.[1] As has been demonstrated, the unique property portfolio of materials with metavalent bonding is highly relevant to the excellent thermoelectric performance. Therefore, understanding of the chemical bonding mechanism in Ag-V-VI_2 compounds can be beneficial for the further improvement of TE performance.

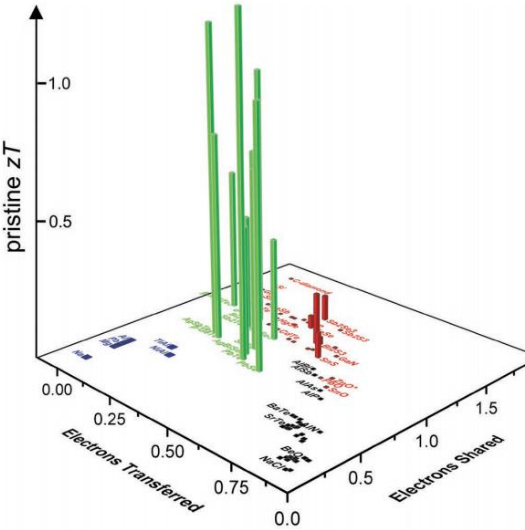

Fig.1 the zT value of different intrinsic materials.

Atom Probe Tomography (APT) has the unique ability of performing 3D analysis and provides an opportunity to obtain 3D structural images on the near-nm scale and also 3D compositional images on almost ppm scale. More importantly, the applied high electric field during APT measurements can regularly break chemical bonds via field evaporation.[2] This bond breaking process is related to the bonding mechanism inside the sample and is responsible for many unique properties in both phase change memory (large dielectric constant) and thermoelectric materials (anharmonicity). Hence this unique technique provides an effective way to distinguish different bonding mechanisms.

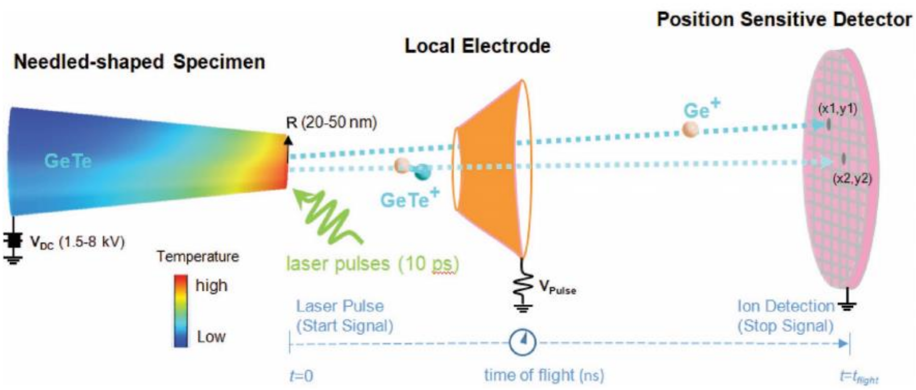

Fig.2 Schematic of atom probe tomography.

The scope of this thesis will be the investigation of the laser-assisted evaporation behavior and the bond breaking process in APT. To achieve this purposes, four Ag-V-VI_2 compounds and some alloys will be studied, and many advanced analytical techniques, such as XRD, FTIR, SEM/FIB and APT will be employed in this thesis. We are looking for a master student who is interested in advanced characterization techniques.

[1] Yu, Yuan, et al. "Chalcogenide Thermoelectrics Empowered by an Unconventional Bonding Mechanism." *Advanced Functional Materials* (2019): 1904862.

[2] Zhu, Min, et al. "Unique Bond Breaking in Crystalline Phase Change Materials and the Quest for Metavalent Bonding." Advanced Materials 30.18 (2018): 1706735.

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