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RWTH AACHEN UNIVERSITY

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

„Understanding the role of nanostructuring in $(GeTe)_x(AgSbTe_2)_{1-x}$ (TAGS) thermoelectric materials based on atom probe tomography studies"

INTRODUCTION…This project aims at achieving fundamental understanding of physical phenomena, specifically of the effects of internal nanostructures, related to thermoelectric (TE) compounds, which may have technological implications for energy conversion and waste heat recovery. TE materials are involved in a variety of devices converting waste heat into electrical energy, as well as for solid-state refrigeration. The energy conversion efficiency is determined by the dimensionless *TE figure of merit, ZT*. Attempts to optimize ZT require reducing the *lattice thermal conductivity*, while maintaining relatively high values of *electrical conductivity*. Today's most common TE materials currently in use exhibit *ZT* values that barely exceed 1[1], which yields device performance of no more than 10% of the Carnot limit[2]. Furthermore, this implies that today's TEGs can be employed for only limited applications in the low power regime (<500 W). To be applicable for greater power levels up to several kW, and to compete with their gas or vapor-based counterparts, increasing *ZT*- values to the range of 2-3 is essential.

THESIS DETAILS…The $(GeTe)_x(AgSbTe_2)_{1-x}$ compounds, also known as TAGS in literature[1], are promising TE materials competing with $AgSbTe_2$ (AST) and $AgPb_xSbTe_{2+x}$ (LAST). Introducing *second-phase precipitates* (see Figure 1(a) observed for AST TE material) as well as lattice point defects to these base alloys is expected to reduce their lattice thermal conductivity, thereby increasing ZT.

The goal of this project is to investigate the formation of the nanostructures (mainly nanoprecipitates) in a solid solution matrix with the atom probe tomography (APT) technique and their effects on the TE properties of the alloy. The matrix composition is also another important aspect of this study mainly when referring to resonance bonding [3]. Related questions such as the thermal stability of single-phase as opposed to two-phase TAGS materials at service temperatures will be considered, as well. In addition, the role of interfaces is addressed. It is important to highlight here that the combination of TE characterization of the Seebeck coefficient, thermal conductivity, and electrical conductivity (done by Matteo Cagnoni at I. Institute of Physics) with advanced materials characterization methods such as APT and correlated APT-EBSD (EBSD-electron backscatter diffraction, see Figure 1(b)) probing on the same tips is unique, and is expected to yield high-impact results. E.g., only few studies of TE materials using APT have been reported so far[4] all imply on the high potential of this combination. On the technological aspect, this will help us adjusting our materials processing to yield better thermal stability, higher ZT-values, and is expected to improve energy conversion efficiency of TE devices.

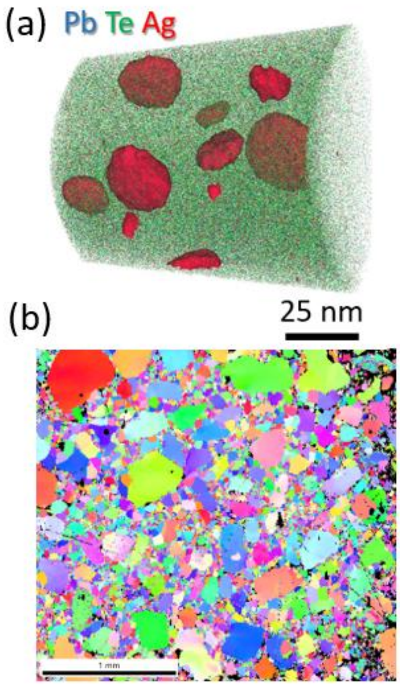

Figure 1. (a) 3D APT map of PbTe thermoelectric material doped with Ag (LEAP 4000X Si). (b) EBSD map of the Ag-doped PbTe showing the its polycrystalline structure.

References

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