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

I. Physikalisches Institut (IA)
Nanocharacterization for advanced functional materials
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Topic for a Master's Thesis

Research on the Optimization of Low-Temperature Thermoelectric Properties of $Bi_{1-x}Sb_x$-based Alloys via Compositional Tuning

Thermoelectric (TE) materials can directly convert heat into electricity and vice versa without any byproducts, providing a sustainable and clean energy solution. Recently, in some high performance thermoelectric systems have revealed that their exceptional properties from a unique distinct metavalent bonding mechanism. This unconventional bonding lead to high carrier mobility and intrinsically low lattice thermal conductivity.

The $Bi_{1-x}Sb_x$ alloy, a low temperature n-type thermoelectric material with great application potential in the 20-200 K range, particularly for single-crystal Bi-Sb alloys, has attracted extensive attention in the field of cooling. Bi and Sb exhibit complete solid solubility across the entire compositional range, which means a homogeneous solid solution structure can be formed regardless of the atomic ratio between the two elements. And when the Sb content (x) ranges from 7% to 22%, the material exhibits narrow-gap semiconducting behavior, Furthermore, variations in Sb content not only tune the bandgap but also induce lattice distortions, which are expected to drive the evolution of metavalent bonding (MVB) characteristics. What is the relationship between the changes in thermoelectric performance under different compositions and the $Bi_{1-x}Sb_x$ structure? how does the degree of Peierls distortion in the Bi1-xSbx structure influence the electron delocalization of MVB?

Goal of the study:

Pure Bi and pure Sb are regarded as semimetals, the band structure show the slight overlap between conduction and valence band, exhibits incipient MVB features. Bi–Sb alloys exhibit MVB characteristics, therefore, it is essential to investigate the relationships among composition-bonding–structure–property. The Bi1-xSbx single crystals (x = 0.09, 0.12, 0.15) were synthesized in vertical Bridgman oven. The thermoelectric properties were measured using the Thermal Transport Option in a physical property measurement system (PPMS). Microstructures and chemical bonding mechanisms of these samples were characterized by atom probe tomography (APT).

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