I. Physikalisches Institut (IA)
Physik neuer Materialien

RWTH AACHEN UNIVERSITY

I. Physikalisches Institut (IA)
Phase-Change Materials
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Topic for a Bachelor Thesis

„Characterization of the pseudo-binary line In_3SbTe_2-SnTe: Determination of structural and optical properties“

Materials can be categorized by examining their properties, including band gap, effective coordination number, electrical and optical conductivity, Born effective charge, and more. Based on such properties and quantum chemical identifiers a classification into metallic, covalent, ionic, and metavalent bonding appears appropriate. For any material, where the crystal structure is known, quantum chemical calculations yield the chemical bond identifiers ES and ET, which refer to the number of electrons shared (ES) and electrons transferred (ET) between adjacent atoms. Plotting these in a map for various materials reveals the proper separation of the different bond types along with their different properties, cf. Fig. 1 (or https://materials-map.rwth-aachen.de/ for the representation including properties). Metavalent bonding is defined by a competition between electron localization and electron delocalization resulting in a unique property portfolio. SnTe and In_3SbTe_2 are identified to be metavalent and metallic, respectively. However, both occur in a rocksalt-like crystal structure with similar lattice constants allowing for isostructural alloying. Investigating the property portfolio along the pseudo-binary line yields insights about the pronounced changes in properties by crossing the tipping point towards complete electron delocalization and closing the band gap.

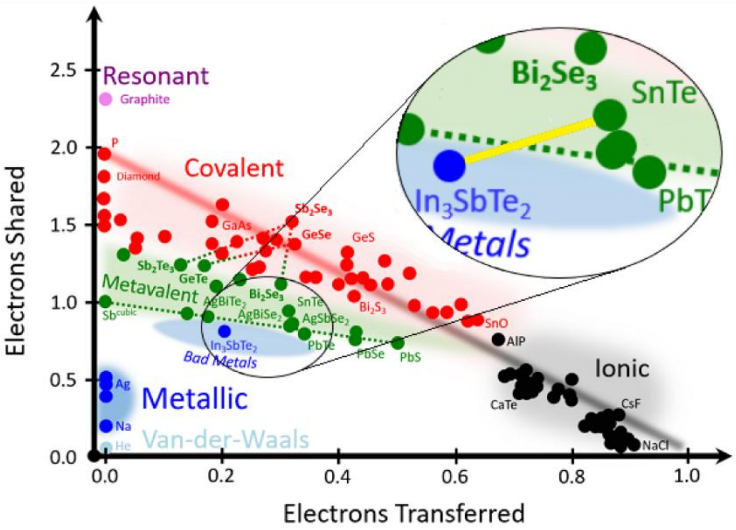

Fig 1: Bonding map of materials. *Along the pseudo-binary line between SnTe and In_3SbTe_2 the border between metavalent and metallic bonding is crossed. Taken from [1] and modified.*

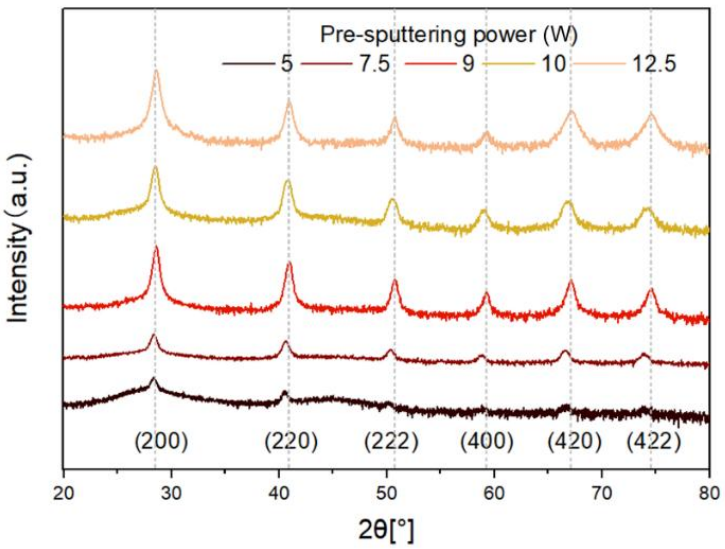

Fig 2: XRD patterns *of IST-SnTe with ratio of approx. 45:55 at different substrate temperatures (defined by different powers).*

Goal of the study:

In this study several alloys on the pseudo-binary line between In_3SbTe_2 (IST) and SnTe are produced by heated plasma assisted co-sputter deposition. Properties like crystallization temperature T_x, crystal structure with X-ray diffraction (XRD) and optical properties, i.e. the dielectric function, over a broad spectral range shall be investigated. For the latter, a combination of ellipsometry, fiber grating and Fourier-transform infrared (FTIR) spectroscopy will be used. Consequently, a software will be utilized to model the measured data.

In a previous study, the substrate temperature and pre-annealing conditions had a strong impact on the crystallization behavior of different IST-SnTe stoichiometries. Now, this recipe should be used to produce comparable thin films to investigate the stoichiometric influences on the optical properties. Additionally, Hall-Bar geometry samples should be produced for future electrical transport investigations.

[1] Guarneri *et al.*, Metavalent Bonding in Crystalline Solids: How Does It Collapse? Advanced Materials 33, 2102356 (2021)

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