

Topic for a Master Thesis

„Venturing the Vulcano: Investigating the Bond Breaking of Chalcogenides using Atom Probe Tomography“

Chalcogenide-based phase change materials play a crucial role in numerous applications, including non-volatile rewritable storage devices, topological insulators, and photonic phase modulators. These materials exhibit distinct properties. By linking chemical bonding and physical properties, the concept of metavalent bonding arises [1]. In metavalent materials, bonding involves competition between localization and delocalization of the electrons.

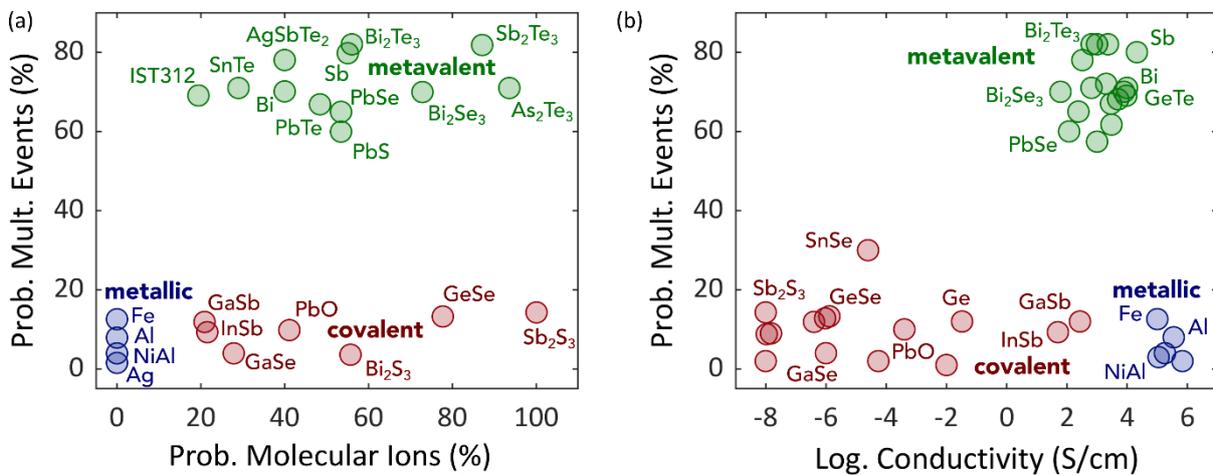


Figure 1: The Probability of Multiple Events allows the differentiation of different bond types. Metavalent Materials show a distinct region of electric conductivity.

By utilizing atom probe tomography, one of the indicators for metavalent bonding can be determined, which serves as a parameter for unique evaporation behavior known as the Probability of Multiple Events. Metallic systems can be distinguished from covalent and metavalent systems by their absence of molecular ions [2]. Additionally, this sophisticated method combines mass spectrometry with the spatially resolved evaporation of single atoms, enabling three-dimensional characterization of features within a 100nm sized prepared tip [3].

This master's thesis project aims to enhance our understanding of the correlation between Multiple Events and metavalent bonding by expanding our knowledge on the edges of our so-called volcano plots, focusing on a variety of transition metal chalcogenides and other exotic alloys.

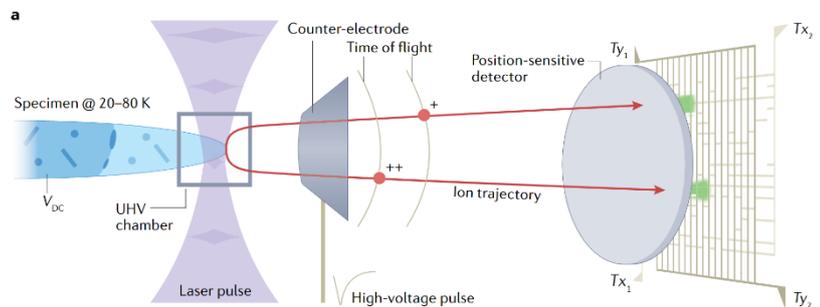


Figure 2: The schematic setup of a Local Electrode Atom Probe. Using the effect of field evaporation, single atoms are evaporated and measured for its time of flight. Taken from [3].

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

[2] Cojocaru-Miredin et al. "Atom Probe Tomography: a Local Probe for Chemical Bonds in Solids", Advanced Materials, (2024).

[3] Gault et al. "Atom Probe Tomography", Nature Review Methods Primers, (2021).