DS 11: Thermoelectric and Phase Change Materials

Time: Thursday 15:00–16:00 Location: H3

DS 11.1 Thu 15:00 H3

Bond strength and force constants in RESbS — •Franziska Zahn[1], Christopher Benndorf[2], Hans H. Falk[1], Konrad Ritter[1], Sergiu Levcenko[1], Edmund Welter[3], Oliver Oeckler[2], and Claudia S. Schnohr[1] — [1]Felix Bloch Institute for Solid State Physics, Leipzig University, Germany — [2]Institute of Inorganic Chemistry and Crystallography, Leipzig University, Germany — [3]Deutsches Elektron Synchrotron DESY, Hamburg, Germany

Our recent study on bond strength in different materials has shown that elemental Sb exhibits characterics of regular covalent and multicenter bonding based on the behavior of force constants with increasing interatomic distance. *RE*SbS are Sb-containing rare-earth (*RE*) pnictide chalcigenides that show special electronic and magnetic properties. They consist of different layeres, including Sb monolayers that alternate with *RE*-S double layers. To study the structural and vibrational properties of *RE*SbS with *RE* = La, Ce, Pr, and Nd in more detail, extended X-ray absorption fine structure spectroscopy (EXAFS) was performed at the Sb K-edge at ten different temperatures ranging from 20 to 295 K. The temperature dependence of the bond length variation σ^2 (mean square relative displacement) was evaluated using a correlated Einstein model, providing static disorder and force constants. The behavior of the force constants with incrasing interatomic distance is compared to other materials and to elemental Sb in particular. This contributes to the fundamental understanding of physical properties of *RE*SbS and their potential origin.

DS 11.2 Thu 15:15 H3

Enhancing mechanical flexibility and thermoelectric efficiency of amorphous TiNiSn — •Denis Music — Department of Materials Science and Applied Mathematics, Malmö University, SE-205 06 Malmö, Sweden

Thermoelectrics can convert heat to electricity without greenhouse gas emissions and hold significant potential as energy sources for wearable devices. Current research focuses on designing compounds that combine high conversion efficiency with mechanical flexibility. Half-Heusler phases, such as TiNiSn, demonstrate promising chemical stability and thermoelectric efficiency, but their inherent brittleness limits their application in flexible devices. To address this shortcoming, amorphous TiNiSn thin films were synthesized by sputtering on various substrates, such as Kapton, silk, and paper, to evaluate their bending response. These thin films show good adhesion to the substrates, as predicted by density functional theory, and do not delaminate under mechanical loading. Bending tests up to 154 degrees reveal minimal crack formation, indicating a high degree of flexibility. Consequently, amorphous TiNiSn is a promising candidate for flexible thermoelectric devices. To further enhance the thermoelectric efficiency of these devices, density functional theory and Boltzmann transport theory were employed to tune the electronic structure and identify suitable doping elements among 3d and 4d transition metals. Experiments were carried out to validate these predictions, yielding an order of magnitude increase in performance at room temperature.

DS 11.3 Thu 15:30 H3

Atomic arrangement in MBE grown chalcogenide thin films: structural investigation based on LEED-IV — •Maximilian Buchta[1], Christoph Ringkamp[1], Lucas Bothe[1], and Matthias Wuttig[2] — [1]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany — [2]I. Institute of Physics (IA), RWTH Aachen University, Germany

If chalcogenides such as GeTe or Sb2Te3 are confined to reduced dimensions, for instance by reducing the film thickness, distortions in the atomic arrangement of the crystal emerge, which have been investigated by techniques such as X-ray diffraction (XRD). However, for the chalcogenides SnTe and SnSe, density functional theory (DFT) predicts pronounced distortions not only for thin films but also at the vicinity of the surface, which cannot be resolved by XRD. Further, as the distortions occur in both out-of-plane and in-plane directions, advanced structural characterization techniques are necessary to determine the atomic arrangement. In this work, Low Energy Electron Diffraction (LEED) Intensity vs. Electron Energy (LEED-IV) curves will be utilized to determine the surface atomic arrangement of tin-based chalcogenide thin films (SnTe and SnSe), grown by Molecular Beam Epitaxy (MBE), providing direct experimental evidence for structural predictions based on DFT.

DS 11.4 Thu 15:45 H3

Characterization of Nucleation and Growth Processes in the Phase Change Material GeTe upon Laser-Induced Switching — •Ramon Pfeiffer, Pascal Schröder, Elias Hildebrand, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, Germany

We have investigated how germanium telluride (GeTe) phase change material behaves during laser-induced switching at a wavelength of 658 nm. Starting with an amorphous GeTe matrix, which we have crystallized using laser pulses, GeTe has been reverted back to an amorphous state before recrystallizing it again. To analyze concomitant changes, we have examined individual crystal grains using electron backscatter diffraction (EBSD) and topographic changes by atomic force microscopy (AFM). Additionally, we have explored larger spot sizes during the second crystallization phase to assess the influence of a crystalline matrix on nucleation and growth dynamics within the material. These experiments revealed distinct nucleation and growth mechanisms that depend on the parameters used for crystallization.