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MS20-O5 The influence of mobile monovalent ions on structures and properties of multinary thermoelectric tellurides

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Crystal structures and thermoelectric properties in the system $(GeTe)_nSb_2Te_3$ (GST materials) are dominated by high concentrations of vacancies associated with diffusion-controlled phase transitions.[1] Partially replacing Ge by twice the amount of monovalent cations M^+ reduces the number of vacancies and yields stable compounds without reconstructive phase transitions. In the case of Li, the lattice thermal conductivity is as low as that of compounds with high vacancy concentrations, indicating that Li acts as a "pseudo vacancy".[2] Such materials reach thermoelectric figures of merit ZT up to ca. 1. Varying the ratio of M^+, Ge^{2+} and Sb^{3+} enables the adjustment of the vacancy concentration and consequently the Li mobility. Thus, $LiGe_{3.5}Sb_2Te_7$ or $LiGe_{11.5}Sb_2Te_{15}$ exhibit lower thermal conductivities (0.4 and 1.6 $Wm^{-1}K^{-1}$, respectively) than the vacancy-free variants $Li_2Ge_3Sb_2Te_7$ and $Li_2Ge_{11}Sb_2Te_{15}$ (1.3 and 2.5 $Wm^{-1}K^{-1}$). [2] As corroborated by superionic Li-ion conductivity in Li_2Te, the mobility of Li may lead to PLEC (phonon liquid/electron crystal) behavior at elevated temperature. [7]Li solid-state NMR spectra clearly indicate Li mobility. Motional narrowing of the NMR signal sets in at temperatures slightly above room temperature. Compounds with vacancies exhibit higher Li mobilities, correlation times are in the order of magnitude of 10^{-3} s at ca. 300 K and less at higher temperatures.

Using Na instead of Li is also possible whereas samples with Cu contain precipitates of copper tellurides. The interplay of doping GST and nanoscale heterostructures leads to ZT values of 1.5 and higher.

Since SnSe emerged as a promising and cheap thermoelectric material,[3] related substitution strategies in the system Sn/Sb/Se seem intriguing. $SnSb_2Se_4$ with a chain-like "sulfosalt" structure [4] is an n-type semiconductor with a high Seebeck coefficient; however, the ZT value is limited by the low electrical conductivity, similar to that of comparable sulfosalts. Formally adding Na_2Se leads to p-type $Na_2SnSb_2Se_5$ which crystallizes in a NaCl-type structure and is surprisingly stable against air and moisture.

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MS21 Structural disorder and materials' properties at ambient and non-ambient conditions

Chairs: Dmitry Chernyshov, Vaughan Gavin

MS21-O1 Lattice dynamics and elastic properties from thermal diffuse scattering

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Diffuse scattering from thermally populated phonons contains important details on the lattice dynamics. The intensity distribution of thermal diffuse scattering across reciprocal space allows for the identification and localization of phonon anomalies and naturally encodes the phonon eigenvectors [1]. In this presentation, the audience will be introduced to the theoretical background, recent developments on model calculations and the use of pertinent software for computing the intensity distribution in 3D reciprocal space [2]. Important aspects of the experimental implementation and data treatment are discussed and the methodology is illustrated by a representative set of recent examples [3-5]. I will show how distinct features in the lattice dynamics leave their footprint in the intensity distribution, such as soft and low energy phonon modes (see Figure 1), similarities in the electronic potential and symmetry relations upon phase transitions. Finally, the possibility for extracting the full elasticity tensor from thermal diffuse scattering is discussed and an outlook to application at high pressures is presented.

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