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CALPHAD-assisted synthesis of Hf-free Half Heusler thermoelectrics with high ZT~1.2

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Besides the well-known skutterudites and Zintl phases, Half Heusler (HH) alloys currently are the most promising candidates for thermoelectric (TE) devices at elevated temperatures: they can be used in a wide temperature range and their starting materials are abundant and cheap. Particularly via nano structuring of TiNiSn-based thermoelectric materials by top-down (ball milling) and bottom-up (spinodal decomposition/precipitation) mechanisms. We have accomplished multicomponent HH alloys with attractive ZTs for n-type TE materials based on (Ti, Zr)-Ni-Sn. These values were achieved on the basis of a profound knowledge not only of isothermal phase relations, temperature dependent solubilities but also of the solidification/annealing behavior.

The detailed experimental investigation of the constitution of both relevant systems Ti-Ni-Sn, Zr-Ni-Sn as well as (Ti, Zr) NiSn - (Ti,Zr)Ni2Sn including liquidus projections and Scheil solidification diagrams, as well as CALPHAD modelling, provided the necessary basis for an elaborate synthesis (annealing/hot-pressing) route in order to reproducibly get a suitable microstructure. Exploiting furthermore the system inherent but coherent binodal/spinodal demixing and precipitation at sub solidus temperatures within the sections TiNiSn-ZrNiSn and ($Ti_{0.5}Zr_{0.5}$) Ni1+xSn we were able to achieve for the n-type half Heusler alloy a ZTmax = 1.2 at 825 K. The demixing is a balanced effect of (i) destabilization of the solid solution by a positive enthalpy of mixing compensated by elastic strain energy (coherent binodal) but also (ii) by the stabilizing effect of the entropy of mixing. The experimental data are backed by SEM/TEM analyses as well as by DFT results.

Speaker Biography

Peter Franz Rogl has completed his PhD at the age of 25 years from University of Vienna, Austria. He is full professor of physical chemistry of materials at University of Vienna, Austria. He has over 700 publications. His publication H-index is 49 and he has been serving as an editorial board member of reputed Journals.

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