Contribution ID: **56** Type: **Invited Speaker**

Thermoelectric Half Heusler phases to harvest waste heat

Thursday 25 May 2017 09:50 (25 minutes)

Thermoelectric materials have the ability to convert a heat flow into an electrical charge carrier flow (energy flow). TiNiSn-based thermoelectric half-Heusler phases (noncentrosymmetric, cubic MgAgAs-type) have proven to be excellent thermoelectrics. The large-scale production and particularly nanostructuring of materials by preferably system-inherent phases need a profound knowledge not only of isothermal phase relations, temperature dependent solubilities but also of the solidification behavior.
The present paper covers a detailed experimental investigation of the constitution of the [Ti,Zr]-Ni-Sn systems including a liquidus projection and a Scheil diagram, as well as a CALPHAD calculation of the entire constitution diagrams. For the binary systems TiNiSn-ZrNiSn and TiNiSn-HfNiSn, thermodynamic spinodal/binodal curves have been determined from solubility data and DFT calculations. With the relevant elastic moduli also the corresponding critical points of coherent spinodal demixing were calculated.
From a series of compounds $Ti_{1-x-y}Zr_xHf_yNiSn$ and respective Sn/Sb substituted alloys the thermoelectric behavior was characterized in the temperature range from 4.2 to 875 K. Due to a particularly low thermal conductivity at a high Seebeck coefficient, Hf-containing n-type alloy reached a figure of merit ZT = 1.5 at 850 K whereas for Hf-free, n-type $Ti_{0.5}Zr_{0.5}NiSn_{0.98}Sb_{0.02}$ a ZT ˜ 1.2 at 850 K was found yielding an thermoelectric leg-efficiency of η ˜ 11

Author: Prof. ROGL, Peter (1Christian Doppler Laboratory for Thermoelectricity at the Institute of Materials Chemistry and Research, University of Vienna)

Co-authors: Dr GRYTSIV, Andriy (Christian Doppler Laboratory for Thermoelectricity); Mr SAUERSCHNIG, Philipp (Institut für Physikalische Chemie,Univ. Vienna); Prof. VRESTAL, Jan (Department of Chemistry, Masaryk University, Brno, Czechia); Prof. YUBUTA, Kunio (Institute for Materials Research, Tohoku University, Sendai, Japan); Dr ROGL, Gerda (Christian Doppler Laboratory for Thermoelectricity); Prof. BAUER, Ernst (Christian Doppler Laboratory for Thermoelectricity, Institute of Solid State Physics, Vienna University of Technology); Dr ROMAKA, Vitaliy (Department of Materials Science and Engineering,Lviv, Ukraine)

Presenter: Prof. ROGL, Peter (1Christian Doppler Laboratory for Thermoelectricity at the Institute of Materials Chemistry and Research, University of Vienna)

Session Classification: A6: Condensed Matter and Accelerators

Track Classification: Condensed Matter Physics