TECHNISCHE UNIVERSITÄT WIEN
Vienna University of Technology

INSTITUT FÜR FESTKÖRPERPHYSIK
Institute of Solid State Physics

Wiedner Hauptstraße 8-10//138, 1040 Wien, AUSTRIA – T: +43 1 58801 13801 / F: +43 1 58801 13899 – E: sekretariat@ifp.tuwien.ac.at

EINLADUNG zum IFP-SEMINAR

Thema: **New Strategies for finding new High-ZT Thermoelectric materials**

Vortragender: **Wilfried Wunderlich**
Tokai University, Mat.Sci. Dept. , 259-1292 Hiratsuka, Japan

Host: Silke Bühler-Paschen

Termin: **Mittwoch, 12. September 2012, 14:00 Uhr**

Ort: TU Wien, Institut für Festkörperphysik
Freihaus Seminarraum 138B, Turm C, 7. OG (rote Leitfarbe)
Wiedner Hauptstraße 8-10, 1040 Wien

Abstract:

Devices based on thermoelectric materials (TE) are considered as one of the clean energy sources helping to solve the severe global warming problem by CO_2-emission. Both, thermoelectric power generation (TEG) based on the Seebeck-effect as well as Peltier-coolers require materials with large figure of merit $ZT=S2\sigma T/\kappa$. While $ZT>3$ is desired to widespread the field of applications, present bulk materials reach $ZT=1.5$, and nano-structured materials are reported to reach around $ZT=3$.

This lectures first summarizes the engineering possibility of thin-film structures on known thermoelectrics, such as BiTe, Nb-$SrTiO_3$ [1] and (TiZr)NiSn [2]. Epitaxial layers might be strained according to the orientation relationship to the substrate. This structural effect can reduce the bandgap, but there is also a more-or-less large space-charge region due to the contact potential, also referred to in literature as confinement of a two-dimensional electron gas (2DEG). Utilizing these effects for new TE-devices is discussed.

The second part of the lecture focuses on the search to new bulk TE-materials. The main key parameter for thermoelectric is the proper charge carrier concentration, but since the development of new thermoelectric devices in the 1960-ies, more key parameters have been found, such as small band-gap, a large density of states near the band gap, degenerated bands with large effective electron mass, phonon-glass electron-gas (PGEC) behavior, strong electron-phonon coupling (EPC), and a proper shape of the Fermi surface. The later contribution has recently become popular due to direct visualization of the band-structures in angle-resolved photoemission spectroscopy (ARPES) [3]. Results on FeSi [4] confirm, that Kramers-Kroning analysis of the THz- spectra together with Raman spectroscopy can visualize the inharmonic interatomic potential required for good thermoelectrics.

The complexity of the search to high ZT materials is a multi-parameter problem and requires the use and application of new concepts as regression analysis in knowledge discovery.

[1] W. Wunderlich et al. Physica B 404 (2009) 2202-2212
[2] W.Wunderlich et al J. Electr. Mat. 40 (2011) 583
[3] Y. L. Chen et al., Science 325, 178 (2009); Y.Pei, G.J.Snyder et al. Nature 473(2011)66
[4] S. Paschen PRB(1997)12916, D. Menzel et al., Phys. Rev. B 79 (2009) 165111

FWF
Der Wissenschaftsfonds.