DS 61: Thermoelectric Materials, Thin Films, and Nanostructures III (Focused Session – Organisers: Nielsch, Rastelli, Balke)

Time: Friday 16:00–17:30 Location: GER 37

DS 61.1 Fri 16:00 GER 37

Phonon transport calculations across interfaces using non equilibrium Green's function formalism — •Saeideh Edalati Boostan, Michael Bachmann, Michael Czerner, and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

Modern electronic devices are rapidly approaching nanometer scales, and heat transport in these systems, particularly across embedded interfaces, is critical to their performance. In this work we present a phonon transport model that can calculate heat flow in layered structured systems. We perform ab initio calculations using the abinit package to obtain the interatomic force constants [1]. These force constants are plugged into a non equilibrium Green's function formalism to calculate the transmission function and the temperature dependence of thermal conductivity in the linear ballistic response regime [2, 3].

[1] http://www.abinit.org
[2] S. Datta, Electronic Transport in Mesoscopic Systems, Cambridge Univeristy Press (1995)
[3] P. E. Hopkins, P. M. Noris, M. S. Tsegaye, and A. W. Ghosh, J. Appl. Phys. 106, 063503 (2009)

DS 61.2 Fri 16:15 GER 37

Model calculations of the thermoelectric transport across a back to back Schottky barrier — •Michael Bachmann, Michael Czerner, and Christian Heiliger — Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

We present results of electronic transport calculations across a back to back Schottky barrier [1]. The basic idea of the back to back Schottky barrier is the assumption of additional electronic states in the band gap at grain boundaries. For an n-type semiconductor these states can be filled by electrons from donor levels. This will lead to a negative space charge region directly at the grain boundary and to positive space charge regions on both sides of the grain boundary. We can change the potential profile by varying the total net charge trapped at the grain boundary. For a given total net charge the potential profile is a function of the donor concentrations. The potential profile is obtained by solving the Poisson equation with a finite difference method on a discrete net. From the potential profile we calculate the transmission function using non equilibrium Greens function formalism considering one parabolic band. For the temperature dependency of the chemical potential we consider one Gaussian shaped donor level and impose charge neutrality. The thermoelectric parameters are calculated using the momentum representation of the transmission function weighted with the energy derivative of the Fermi function [2].

[1] C R M Grovenor J.Phys. C: Solid State Phys. 184079 (1985)
[2] H. Fritzsche Solid State Com. Vol. 9 pp. 1813-1815 (1971)

DS 61.3 Fri 16:30 GER 37

Thermoelectric properties of low-dimensional clathrates from first principles — •Deepa Kasinathan and Helge Rosner — Max Planck Institute for Chemical Physics of Solids, Dresden

Type-I inorganic clathrates are host-guest structures with the guest atoms trapped in the framework of the host structure. From a thermoelectric point of view, they are interesting because they are semiconductors with adjustable bandgaps. Investigations in the past decade have shown that type-I clathrates $X_8Ga_{16}Ge_{30}$(X = Ba, Sr, Eu) may have the unusual property of "phonon glass-electron crystal" for good thermoelectric materials. Among the known clathrates, $Ba_8Ga_{16}Ge_{30}$ has the highest figure of merit (ZT 1). To enable a more widespread usage of thermoelectric technology power generation and heating/cooling applications, ZT of at least 2-3 is required. Two different research approaches have been proposed for developing next generation thermoelectric materials: one investigating new families of advanced bulk materials, and the other studying low-dimensional materials. In our work, we concentrate on understanding the thermoelectric properties of the nanostructured Ba-based clathrates. We use semi-classical Boltzmann transport equations to calculate the various thermoelectric properties as a function of reduced dimensions. We observe that there exists a delicate balance between the electrical conductivity and the electronic part of the thermal conductivity in reduced dimensions. Insights from these results can directly be used to control particle size in nanostructuring experiments.

DS 61.4 Fri 16:45 GER 37

Thermoelectric power of nanostructured thin Au films — •Sebastian Schnurr, Ulf Wiedwald, and Paul Ziemann — Institut für Festkörperphysik, Universität Ulm, Albert-Einstein-Allee 11, 89069 Ulm, Germany

The effect of ordered arrays of nanostructures like nanopillars (periodicities 50 - 100 nm) on the Seebeck coefficient S of thin polycrystalline Au films (thickness t = 10-100 nm) is investigated as function of temperature in the range 6-300 K. Nanostructures are prepared by combining a micellar approach [1] with reactive ion etching. Reference measurements of S were performed on thin continuous films. At low temperature a phonon drag peak is found, which is significantly reduced as compared to bulk Au for thicker films while it completely vanishes for film thicknesses below 20 nm. At ambient temperature, S follows a $[1 - \exp(-a \cdot t)]$-dependence similar to a recent report on thin Pt films [2].

For nanostructured Au films the ratio of the average grain size to the periodicity of nanostructures becomes important. For small grains (10-15 nm) electron scattering at grain boundaries dominates leading to a complete suppression of the influence of nanostructures. In the limit of large grains, however, scattering at nanostructures takes over decreasing S significantly below the reference level while its temperature dependence between 100 K and 300 K practically vanishes.

[1] U. Wiedwald et al., Beilstein J. Nanotechnol. 1, 24 (2010).
[2] M. C. Salvadori et al, Appl. Phys. Lett. 88, 133106 (2006).

DS 61.5 Fri 17:00 GER 37

Complex Chalcogenides for Thermoelectrics: Microstructure Analysis of $AgPb_{18}SbTe_{20}$ — •Susanne Perlt[1], Thomas Höche[1], Jayaram Dadda[2], and Eckhard Müller[2] — [1]Leibniz Institute of Surface Modification, Leipzig — [2]German Aerospace Center, Institute of Materials Research, Köln

The thermoelectric (TE) bulk material $AgPb_{18}SbTe_{20}$ (LAST-18) is a highly promising candidate for application in the mid-temperature range. The manufacturing process needs to be controlled in such a way, that the figure of merit, ZT [1], gets maximized. In this respect, a high electronic conductivity σ, a high thermopower S, and a low thermal conductivity κ are crucial. The high TE performance of LAST is assumed to be caused by the nanoscale precipitates formed by nucleation and growth and/or spinodal decomposition [2].
The presented LAST samples are fabricated via different melting routes and annealing treatments in order to find favourable conditions, i.e. to get a homogeneous material on the microscale but introduce precipitates on the nm scale.
Based on properties monitored by a Seebeck scanning microprobe, structure-property relationships are studied by SEM and TEM analysis. Site-specific lift-out of TEM lamellae are made by focused ion beam (FIB) machining. High-resolution STEM is giving insight into the atomistic structure of the nanostructures.

[1] D. Bilc et al., Phys. Rev. Lett. **93**, 146403 (2004)
[2] J. Androulakis et al., J. Am. Chem. Soc. **129**, 9780 (2007)

DS 61.6 Fri 17:15 GER 37

First principle calculations of nanostructured LAST materials — Jadranka Dokic and •Beate Paulus — Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin

First principle calculations based on different density functionals are performed in order to explain the effects which occur in a solid environment on a microscopical level upon nanostructuring. We are especially interested in, so called LAST-m ($AgPb_mSbTe_{m+2}$) crystals which contain a small percentage of silver and antimony atoms incorporated in a lead telluride matrix. The enhancement of thermoelectric efficiency in doped-PbTe is stated to be a consequence of the local increase in the density of states (DOS) over a narrow energy range. Therefore we will analyze the influence of single atom impurities and AgSb pair impurities in various nanostructures within the parent material PbTe.

The influence of different doping ratios, relative distances between the impurities, structural relaxations due to doping onto the DOS is determined and discussed. In addition formation energies of the nanostructured solids will be studied and relative stabilities evaluated.