DS 33: Thermoelectric materials II: Reduced dimensionality (Focused session – Organizers: Meyer, Heiliger)

Time: Thursday 11:15–12:45 Location: H 2032

Topical Talk DS 33.1 Thu 11:15 H 2032

Calculation of thermoelectric properties of nanostructured semiconductors — •Peter Kratzer and Gregor Fiedler — Fakultät für Physik and Center for Nanointegration (CeNIDE), Universität Duisburg-Essen, Duisburg, Germany

Epitaxial nanostructuring, e.g. in the form of superlattices, enables high figure of merit ZT even with perfectly crystalline samples of standard semiconductors. One decisive factor is the reduction of thermal conductivity, as demonstrated e.g. for an array of self-assembled SiGe quantum dots (QDs) in Si [Nature Materials **9**, 491 (2010)]. Complementing these efforts, our work uses electronic structure + Boltzmann transport theory to explore the chances for increasing σS^2 in ZT.

We employ the tight-binding method to calculate the conduction-band states in an array of Ge QDs in Si. It is found that the strained Si between the QDs supports low-lying dispersive states, while the strongly compressed region between two vertically stacked QDs leads to a resonance in the conduction band. The consequences of the modified electronic structure for thermoelectric properties will be discussed.

In a more general framework, the role of transitions between bound and free states in a superlattice for the cross-plane transport relaxation time is investigated. If the mean free path of the phonons mediating these transitions exceeds the superlattice period, combined non-equilibrium effects of the electron and phonon system need to be considered. We predict an additional contribution to the thermopower that is similar to the phonon drag, but scales linearly with the number of superlattice periods and extends to higher temperatures.

DS 33.2 Thu 11:45 H 2032

Giant thermoelectric efficiency in single electron transistors with superconducting island — •Christopher Eltschka[1] and Jens Siewert[2,3] — [1]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany — [2]Departamento de Química Física, Universidad del País Vasco, 48080 Bilbao, Spain — [3]Ikerbasque, Basque Foundation for Science, 48011 Bilbao, Spain

It is well known that dimensional reduction of the electron dynamics may enhance the thermodynamic efficiency [1,2]. A special case of such reduced dimensionality is the single-electron transistor (SET) where at low temperatures electron transport is governed by Coulomb blockade effects. We specifically consider an SET with superconducting island (NSN SET) in the parity regime. We find a dramatically enhanced value for the figure of merit ZT. By extending the statistical interpretation of the thermopower by Matveev [3] to the figure of merit, we are able to explain this high value purely from the statistical distribution of transport. This statistical interpretation of ZT indicates a general strategy to increase ZT which might be useful also in the analysis of other systems.

[1] L. D. Hicks, M. S. Dresselhaus, Phys. Rev. B 47, 12727 (1993)

[2] G. D. Mahan, J. O. Sofo, Proc. Natl. Acad. Sci. 93, 7436 (1996)

[3] K. A. Matveev, Statistical and Dynamical Aspects of Mesoscopic Systems. Proceedings of the XVI Sitges Conference on Statistical Mechanics (2000)

DS 33.3 Thu 12:00 H 2032

Nano-sized semiconductor pillars for thermoelectric applications — •Thorben Bartsch, Matthias Schmidt, Christian Heyn, and Wolfgang Hansen — Institut für Angewandte Physik, Jungiusstr. 11, D-20355 Hamburg,Germany

Nanostructures are an attempt to enlarge the efficiency of thermoelectric devices by drastic reduction of the thermal conductivity and enhancement of the electrical properties [1]. We fabricate novel, epitaxially grown air-gap heterostructures that contain a nanometer sized air gap stabilized by epitaxial semiconductor pillars with length of only few nanometers. Caused by the small dimension and the low density of the pillars, the thermal conductance is several orders of magnitude smaller than in comparable bulk structures. The measured conductance can be described with a simple model of ballistic phonon transport through the pillars [2]. Here, first experimental results will be discussed that probe the thermoelectric properties of the semiconductor nanopillars in the air-gap heterostructures.

[1] K. Nielsch et al. Adv. Energy Mater. 1, 713 (2011)

[2] Th. Bartsch et al. submitted , published on arXive:http://arxiv.org/abs/1111.1164

DS 33.4 Thu 12:15 H 2032

Suppression of phonon heat conduction in undulated nanowires — Denis L. Nika[1], Alexandr I. Cocemasov[1], Calina I. Isacova[1], Dmitrii V. Crismari[1], Alexander A. Balandin[2], •Vladimir M. Fomin[3], and Oliver G. Schmidt[3,4] — [1]Lab. PIN "E. Pokatilov", Dep. Theor. Physics, Moldova State U., MD-2009 Chisinau, Republic of Moldova — [2]Nano-Device Lab., Dep. Electrical Engineering, U. California-Riverside, CA 92521 Riverside, U.S.A. — [3]Institute for Integrative Nanosciences, IFW-Dresden, D-01069 Dresden, Germany — [4]Material Systems for Nanoelectronics, Chemnitz University of Technology, D-09107 Chemnitz, Germany

We have theoretically demonstrated that the phonon heat flux can be significantly suppressed in Si, Si/SiO_2 and Si/Ge nanowires with periodical modulation of their cross-section [undulated nanowires (UNWs)] in comparison with generic Si nanowires in a temperature range from 50 K to 400 K. The phonon energy spectra in UNWs are calculated in the framework of five-parameter Born – von Karman-type and six-parameter Valence Force Field models of lattice dynamics. A 4- to 10-fold reduction of the heat flux in UNWs is explained by the exclusion of phonon modes trapped in UNWs segments from the heat flow. Discussions with A. Rastelli and X. Zianni are gratefully acknowledged. The work was supported by the IB BMBF under Project MDA 09/007, the DFG SPP 1386 under Project RA1634/5-1 and Moldova State Project 11.817.05.10F. The work at UCR was supported by FENA.

DS 33.5 Thu 12:30 H 2032

Thermoelectric power factor of a 70 nm Ni-nanowire in a magnetic field — •Rüdiger Mitdank[1], Martin Handwerg[1], Corinna Steinweg[2], William Töllner[3], Mihaela Daub[4], Kornelius Nielsch[3], and Saskia F. Fischer[1] — [1]Novel Materials, Institut für Physik, Humboldt Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany — [2]Werkstoffe und Nanoelektronik, Ruhr-Universität Bochum, 44780 Bochum, Germany — [3]Institute of Applied Physics, Universität Hamburg, Jungiusstr. 11, 20355 Hamburg, Germany — [4]Max Planck Institute of Microstructure Physics, Weinberg 2, 06120, Germany.

Thermoelectric (TE) properties of a single nanowire (NW) are investigated in a microlab which allows the determination of the Seebeck coefficient S and the conductivity σ [1]. A significiant influence of the magnetization of a 70 nm ferromagnetic Ni-NW on its power factor S*σ is observed. Mainly, an evident relationship between magnetoresistance and magneto-thermopower was found, confirming Mott's relation. We detected a strong magneto-thermopower effect of about 10% and an anisotropic magneto resistance as a function of an external magnetic field B in the order of 1%. At B = 0 T we determined the absolute value of S = - (19 +- 2) μV/K. At zero field the figure of merit ZT = 0.02 was calculated using the Wiedemann-Franz- law for the thermal conductivity. The TE efficiency increases in a transversal magnetic field (B =0.5 T) due to an enhanced power factor by nearly 20%.

[1] http://arxiv.org/abs/1111.1873