DS 59: Thermoelectric Materials, Thin Films, and Nanostructures I (Focused Session – Organisers: Nielsch, Rastelli, Balke)

Time: Friday 11:00–13:00 Location: GER 37

Topical Talk DS 59.1 Fri 11:00 GER 37

Nanocrystalline silicon for thermoelectricity — •Gabi Schierning — Center for NanoIntegration Duisburg-Essen (CeNIDE), University of Duisburg-Essen, 47057 Duisburg, Germany

A main focus in thermoelectricity is on the development and utilization of materials with high availability and sustainability. From this point of view, nanocrystalline silicon is a potential candidate for thermoelectric application, motivating the effort of optimizing its thermoelectric properties. In the first part of the talk, an overview over silicon-based thermoelectrics will be given.

In the second part of the talk, own work will be presented. Our bottom up approach starts with tailored silicon nanoparticles from a gas phase process. Compaction of the nanopowder is done by a dc-current sintering. In a combined experimental and theoretical work it is shown how the developing microstructure during sintering correlates to the percolation paths of the current through the powder. Observed density fluctuations on the micrometer scale are attributed to the specific heat profile of the simulated powder networks.

It is technologically highly demanding to exclude any contamination of the nanopowder with oxygen and moisture. As a result, a Si/SiO_2 core/shell structure is always observed for nanocrystalline silicon powders having been in contact with air. In the sintered body, the initial core shell structure is dissolved. Instead, oxidic precipitates have formed during sintering. The role of these oxidic precipitates with respect to the sintering mechanism and the thermoelectric transport properties will be discussed.

Topical Talk DS 59.2 Fri 11:30 GER 37

Nanoscale Thermoelectrics — •Jan D. König — Fraunhofer IPM, Heidenhofstr. 8, 79110 Freiburg, Germany

The variety of TE materials extends from semiconductors via metalloids to ceramic oxides. Decisive factors for the efficiency of the material, in addition to the highest possible Seebeck coefficient, also known as the thermoelectric power, are a high electrical and at the same time a low thermal conductivity. Here physics has imposed laws; because these properties cannot easily be optimized independently of one another. Modern high ZT materials manage to trick nature to a certain degree: they have a fabricated atomic configuration in which the inner structure of the material restricts the mobility of the phonons, and hence its thermal conductivity, (phonon blocking) while not obstructing or even promoting that of the electrons (electron transmitting). Nanotechnologically produced materials are regarded as especially promising. They are manufactured on the basis of already familiar thermoelectric materials by, for example, embedding nanoparticles in a macroscopic matrix. Recent concepts for nanoscale thermoelectric materials will be discussed.

Topical Talk DS 59.3 Fri 12:00 GER 37

Thermal transport and thermoelectric effect in thin semiconductor membranes — •Matthias Schmidt, Thorben Bartsch, Christian Heyn, and Wolfgang Hansen — Institut für Angewandte Physik, Universität Hamburg, Germany

We study the heat conductance and the thermopower in single-crystalline semiconductor membranes which are fabricated by selective etching of AlGaAs-based heterostructures. The membranes have thicknesses up to a few 100 nm and are grown by molecular beam epitaxy. An airgap of thickness between 5 nm and 500 nm separates the membranes from the substrate and makes possible to establish large thermal gradients both to the substrate as well as within the membrane. In particular, the heat transport between a membrane that is held by few nanometer thin semiconductor columns and the substrate is studied. Furthermore, in thin semiconductor bridges containing a two-dimensional electron system the magneto-thermopower is investigated. The results demonstrate that we are able to establish strong thermal gradients even at very low temperature. With curved membranes in magnetic fields we can establish a system in which the spatial distribution of both the local density of states and the temperature can be controlled simultaneously.

Topical Talk DS 59.4 Fri 12:30 GER 37

Theoretical studies of electrical cross-plane transport in semiconductor multilayer heterostructures — •Peter Kratzer[1] and Vladimir M. Fomin[2] — [1]Faculty of Physics and CeNIDE, University Duisburg-Essen, 47048 Duisburg, Germany — [2]Institute for Integrative Nanosciences, IFW Dresden, 01069 Dresden, Germany

Using epitaxially grown multilayer heterostructures, it has been demonstrated experimentally that low lattice thermal conductivity κ_{ph} can be realized in crystalline samples made from standard semiconductors. In particular, built-in self-assembled quantum dot (QD) stacks offer the possibility to affect both the thermal and the electrical cross-plane transport in a way favorable for thermoelectrics. In this talk, we employ Boltzmann transport theory to explore the role of the electronic structure for further enhancement of the figure of merit Z by increasing its numerator σS^2. For a stack of quantum dots separated by nanometer-thin spacer layers, miniband transport may be used to realize an electronic transport regime with large σS^2 but still low κ_{el}. The geometry-dependent miniband dispersion is obtained from atomistic calculations of the electronic structure of QD arrays. Moreover, due to different quantum states available for scattering, the mean free path of carriers in low-dimensional transport differs strongly from bulk transport. Interesting effects are to be expected if the layer thickness in the structures is reduced below the mean free path. As one example, we predict values of $ZT > 2$ at room temperature for an array of InAs QDs in GaAs for suitably chosen geometry and doping level [Phys. Rev. B **82**, 045318 (2010)].