DS 14: Thermoelectric Thin Films and Nanostructures II

Time: Tuesday 14:00–15:30 Location: H8

Topical Talk DS 14.1 Tue 14:00 H8

Thermal Conductivity of Thermoelectric Materials Embedded with Nanoparticles — •Yee Kan Koh and David Cahill — Dept. of Materials Sc. and Eng., University of Illinois, Urbana, USA

Over the past decade, nanostructures are prevalently explored to reduce the thermal conductivity of existing thermoelectric materials and hence enhance the thermoelectric efficiency. In this regard, nanoparticles or nanodots embedded in a matrix could be effective in scattering phonons and thus reducing the thermal conductivity. We report here our thermal conductivity measurements of two important classes of thermoelectric materials, i.e., InAlGaAs embedded with ErAs nanoparticles and PbTe/PbSe nanodot superlattices (NDSLs). The samples are grown by our collaborators at UC Santa Barbara and MIT Lincoln Laboratory. We measured the thermal conductivity by time-domain thermoreflectance. From our measurements, we found that reduction of the thermal conductivity by ErAs nanoparticles is less significant in InAlGaAs than in InGaAs. By measuring TDTR in frequency domain, we showed that 3% of ErAs nanoparticles is sufficient to scatter phonons with mean-free-paths of 300-1000 nm. In contrast to InAlGaAs, we found that PbSe nanodots do not reduce the thermal conductivity of NDSLs below the alloy limits. All of our measurements approach the thermal conductivity of bulk homogenous alloys with the same average composition. We attribute this observation to short mean-free-paths of phonons in PbTe and small acoustic impedance mismatch between PbTe/PbSe. Our work provides guidelines for future work on thermoelectric materials embedded with nanoparticles.

DS 14.2 Tue 14:30 H8

Thermoelectric efficiency in stacks of n-type InAs/GaAs quantum dots — Vladimir M. Fomin[1] and •Peter Kratzer[2] — [1]Institut für Integrative Nanowissenschaften (IIN), Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, D-01069, Dresden — [2]Fakultät für Physik und Center for Nanointegration (CeNiDE), Universität Duisburg-Essen, D-47048, Duisburg

We investigate the effect of the electron miniband energy spectrum of periodic 1D stacks of self-assembled InAs/GaAs quantum dots (QDs) with different geometrical parameters on their electronic transport employing the Boltzmann transport equation. The electron minibands are calculated within tight-binding and Kronig-Penney models. The transport relaxation time reveals a significant dispersion as a function of the wave vector in the stacking direction. The chemical potential is related to the concentration of electrons of the conduction band taking into account the minibands and a continuum. From the numerical analysis of the electric and thermal conductivities, the Seebeck coefficient and the figure-of-merit, we conclude that a 1D stack of QDs achieves a geometry-controlled enhanced efficiency as a thermoelectric converter in certain windows of the donor concentration. Reducing the QD height for a fixed stacking period is favourable for an increase of the figure-of-merit.

A fruitful collaboration with O. G. Schmidt and A. Rastelli and a financial support under the DFG SPP 1386 and the ESF Exchange Grant 2157 within the activity ‘Arrays of Quantum Dots and Josephson Junctions’ are gratefully acknowledged.

DS 14.3 Tue 14:45 H8

Thermal Conductivity Of Single Crystalline SiGe/Si Multilayers Below The Amorphous Limit — •Armando Rastelli, Fabio Pezzoli, Peixuan Chen, Mathieu Stoffel, and Oliver G. Schmidt — Institut für Integrative Nanowissenschaften, IFW Dresden, Helmholtzstr. 20, 01069 Dresden

We report on the fabrication, structural properties and cross-plane thermal conductivity measurements of multilayers of epitaxial SiGe self-assembled nanodots in Si matrix. Thermal conductivity measurements are performed with the differential 3-omega method using metal strips on top thin (30 nm thick) dielectric layers deposited by atomic layer deposition. With this approach we are able to reliably determine the cross-plane thermal conductivity of semiconductor layers as thin as 30 nm. Moreover we present a new method for error evaluation, which, based on Monte Carlo simulation, takes into account the uncertainties of all parameters entering in the model equations used to determine the thermal conductivity. The study reveals a rather linear dependence of the thermal conductivity on the SiGe interlayer spacing. For the thinnest Si-spacer thickness available (3 nm), our single-crystalline SiGe structure shows thermal conductivity values well below those of amorphous Si. Finally we discuss the results and possible routes to further reduce the thermal conductivity.

DS 14.4 Tue 15:00 H8

Half Heusler thin film superlattices for thermoelectrics — •Tino Jaeger[1], Christian Mix[1], Xenija Kozian[2], Benjamin Balke[2], Sascha Populoh[3], Anke Weidenkaff[3], Claudia Felser[2], and Gerhard Jakob[1] — [1]Institut für Physik, Universität Mainz, Staudinger ,Weg 7, 55099 Mainz, Germany — [2]Institut für Anorganische Chemie und Analytische Chemie, Universität Mainz, Staudinger Weg 7, 55099 Mainz, Germany — [3]EMPA - Eidgenössische Materialprüfung und -forschungs Anstalt Festkörperchemie und Katalyse, Ueberlandstrasse 129, 8600 Duebendorf, Switzerland

Due to rising energy costs and carbon dioxide concentration in the atmosphere interest on thermoelectric materials has strongly increased. The energy efficiency of thermoelectric devices has to be increased to expand the commercial usage. Here, efficiency is given by the figure of merit that is increased by a large Seebeck coefficient, large electrical conductivity and small thermal conductivity. Due to their electronic band structure half-Heusler alloys are appropriate candidates for such materials. Using thin film technology we prepare superlattices in order to increase the figure of merit. A superlattice based on NiTiSn and $NiZr_{0.5}Hf_{0.5}Sn$ is supposed to decrease the thermal conductivity due to phonon scattering at the interfaces. The epitaxial multilayer structures are synthesized by sputter technique in argon atmosphere. A four-circle X-ray diffractometer allows the analysis of the crystal structures and the orientation of several layers with respect to each other. Resistivity, thermal conductivity and Seebeck coefficients are measured for different multilayers.

DS 14.5 Tue 15:15 H8

Engineering the thermopower in semiconductor-molecule junctions: towards high thermoelectric efficiency at the nanoscale — Daijiro Nozaki, Haldun Sevincli, Wu Li, •Rafael Gutierrez, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, D-01062 Dresden, Germany

We propose a possible route to achieve high thermoelectric efficiency in molecular junctions by combining a local chemical tuning of the molecular electronic states with the use of semiconducting electrodes. The former allows to control the position of the HOMO transmission resonance with respect to the Fermi energy while the latter fulfills a twofold purpose: the suppression of electronlike contributions to the thermopower and the cut-off of the HOMO transmission tails into the semiconductor band gap. As a result a large thermopower can be obtained. Our results strongly suggest that large figures of merit in such molecular junctions can be achieved [1].

[1] Engineering the thermopower in semiconductor-molecule junctions: towards high thermoelectric efficiency at the nanoscale, D. Nozaki, H. Sevincli, W. Li, R. Gutierrez, and G. Cuniberti, arxiv preprint: cond-mat 0908.0438 (2009).