HL 19: Thermoelectricity

Time: Tuesday 11:30–12:45 Location: H33

HL 19.1 Tue 11:30 H33

Simulating time dependent thermoelectric transport with t-Kwant — •Phillipp Reck, Adel Kara Slimane, and Geneviève Fleury — SPEC, CEA, CNRS, Université Paris-Saclay, CEA Saclay, 91191 Gif sur Yvette Cedex, France

Recent theoretical works suggest that the thermoelectric efficiency of a nanodevice could be greatly enhanced if it is suddenly pushed out of equilibrium with the use of an external time-dependent parameter [1-3]. In those studies, quantum dot models were considered and the thermoelectric properties were calculated analytically with a non equilibrium Green's function (NEGF) approach. Instead, we are developing an extension to the t-Kwant library [4] which will enable us to study numerically time-dependent thermoelectric transport in arbitrary (non-interacting) tight-binding models. It is based on a wave function approach, equivalent to the NEGF approach but drastically more efficient from a numerical point of view.

In this talk I will briefly introduce t-Kwant and discuss how to generalize it to thermoelectric transport. I will show that we reproduce previous results in the literature within derived the NEGF formalism for the resonant level model [1,5] and discuss first results for the dynamic thermoelectric transport in more complicated nanodevices.

[1] A. Crépieux et al., Phys. Rev. B 83, 153417 (2014)
[2] H. Zhou et al., Scientific Reports 5, 14870 (2015)
[3] A.-M. Daré and P. Lombardo, Phys. Rev. B 93, 035303 (2016)
[4] B. Gaury et al., Physics Reports 534, 1 (2014)
[5] F. Covito et al., J. Chem. Theory Comput. 14, 2495 (2018)

HL 19.2 Tue 11:45 H33

Synthesis of organic-inorganic hybrids based on mesoporous silicon and PEDOT:PSS — •Haider Haseeb, Klaus Habicht, and Tommy Hofmann — Helmholtz-Zentrum Berlin für Materialien und Energie (HZB), Berlin, Germany

This contribution thoroughly discusses synthesis routes to combine mesoporous silicon and the conductive polymer blend, polyethylendioxythiophene:polystyrenesulfonate (PEDOT:PSS) in novel organic-inorganic hybrid materials. The synthesis of self-supporting, mesoporous silicon membranes by means of electrochemical etching is described in detail. Post treatment in hydrogen peroxide and hydrofluoric acid subsequently proves to be a versatile approach to widen the average pore size from 8 nm in as-etched samples to 25 nm in post-treated samples. The increased pore size and fine-tuned wetting properties of diluted PEDOT:PSS solutions are crucial for liquid imbibition into the pore space and thus for the synthesis of the hybrids. Microscopic SEM studies and gas adsorption isotherms are invaluable tools to reveal morphological properties of the synthesized samples. They readily show changes in pore size distributions, specific surfaces and porosities upon chemical treatment. They also provide stringent proof for successful incorporation of PEDOT:PSS into mesoporous silicon. Our contribution discusses in an outlook - the synthesized samples in the context of novel organic-inorganic thermoelectric hybrids.

HL 19.3 Tue 12:00 H33

Phonons in mesoporous silicon: the influence of nanostructuring on the dispersion in the Debye regime — •Tommy Hofmann and Klaus Habicht — Helmholtz Zentrum Berlin für Materialien und Energie, Berlin, Deutschland

This contribution presents a comprehensive scattering study of nanostructured silicon [1]. Neutron and x-ray scattering experiments elucidate structural and dynamical properties of electrochemically etched, porous silicon membranes with pores roughly 8 nm across. In particular, inelastic cold neutron scattering techniques reveal the phonon dispersion of the nanostructured, single crystalline samples in the linear Debye regime for energy transfers up to 4 meV whereas inelastic thermal neutron scattering experiments provide access to the dispersion closer to the zone boundary. A modified dispersion relation characterized by systematically reduced sound velocities manifests itself in altered elastic properties of porous silicon when compared to bulk silicon. Its relevance for nanostructured silicon as thermoelectric material of interest is discussed. In this context, we give an outlook on phonon lifetime measurements to ascertain directly phonon scattering rates in nanostructured silicon by means of neutron spin-echo studies.

[1] T. Hofmann, D. Wallacher, R. Toft-Petersen, B. Ryll, M. Reehuis, and K. Habicht. Phonons in mesoporous silicon: the influence of nanostructuring on the dispersion in the Debye regime. Microporous and Mesoporous Materials, 243:263*270, 5 2017.

HL 19.4 Tue 12:15 H33

Structure and Thermoelectric Characterization of Li-substituted Bismuth Palladium Oxide — •Hong Hai Nguyen, Jan-Ekkehard Hoffmann, Klaus Habicht, and Katharina Fritsch — Helmholtz-Zentrum Berlin für Materialien und Energie , Hahn-Meitner-Platz 1, 14109 Berlin

Bismuth palladium oxide (Bi_2PdO_4) has recently been theoretically proposed as a promising thermoelectric oxide. The material is predicted to display an intrinsically low thermal conductivity κ related to Bi anharmonicity and good electrical properties due to the presence of PdO_4 square planar motifs, and a high power factor PF=σS^2 upon hole doping. In this talk, we present experimental work on the synthesis of polycrystalline and bulk samples of Bi_2PdO_4 and Li-substituted $Bi_2Pd_{1-x}Li_xO_4$ and report on their structural characterization by means of powder diffraction measurements. We confirm the incorporation of Li at the Pd site from Rietveld refinements of our neutron diffraction data. Measurements of the TE properties reveal a very low κ close to the amorphous limit for all studied samples, in excellent agreement with theory. Moreover, we find that Bi_2PdO_4 is electrically insulating, leading to a rather low PF over the whole temperature range studied, while the Seebeck coefficient is high - in disagreement with theory. Surprisingly, incorporation of tiny amounts of Li (x=0.02) leads to an increase in electrical conductivity by two orders of magnitude. Overall, the measured PF is found to be considerably smaller than theoretically predicted which we attribute to the theoretical assumption of a much larger intrinsic charge carrier density and mobility.

HL 19.5 Tue 12:30 H33

Silicon Nitride Interface Engineering for the Realization of Dopant-free MOSFETs — •Benjamin Richstein[1,2], Thomas Grap[1,2], Lena Hellmich[1], and Joachim Knoch[1] — [1]Institute of Semiconductor Electronics, RWTH Aachen, Germany — [2]Peter Grünberg Institute 11, FZ Jülich, Germany

Dopants are necessary in standard CMOS-technology as they enable conductivity in silicon and provide low contact resistances. Moreover, degenerate doping avoids carrier freeze out in low temperature applications. However, in deep nanoscale MOSFETs even at very high dopant concentrations only a few dopants reside in typical device volumes resulting in strong variability. Furthermore, the nanoscale size leads to deactivation of dopants increasing parasitic source/drain resistances. Thus, new concepts are required to avoid the problems with dopants in small MOSFETs. Therefore we show a study on silicon nitride interface engineering. Very thin silicon nitride layers in the sub-nm regime are fabricated to suppress the penetration of the metal wave function of S/D-contacts into the bandgap of silicon. This leads to a Fermi-Level-Depinning and a decrease of the Schottky-barrier in Schottky-MOSFETs. As a result, the contact resistivity decreases and the ambipolar behavior can be suppressed. The metal work functions of S/D-contact metals are utilized to obtain N-, or PMOS-like behavior. Dopant-free ohmic contacts were fabricated and characterized at room and very low temperatures. Additionally, Schottky-MOSFETs with S/D-contacts consisting of a thin silicon nitride layer and different contact metals are fabricated to demonstrate unipolar behavior.