TT 46: Transport Properties (joint session HL/TT)

Time: Thursday 15:00–17:15 Location: H13

TT 46.1 Thu 15:00 H13

Quasi-Ballistic Transport in Phase-Pure GaAs/InAs Core/Shell Nanowires — •Farah Basarić[1,2], Vladan Brajović[1,2], Gerrit Behner[1,2], Kristof Moors[1], William Schaarman[1], Raghavendra Juluri[3], Ana M. Sanchez[3], Hans Lüth[1,2], Detlev Grützmacher[1,2], Alexander Pawlis[1,2], and Thomas Schäpers[1,2] — [1]Peter Grünberg Institut (PGI9), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology, Jülich-Aachen Research Alliance, Forschungszentrum Jülich and RWTH Aachen University, Germany — [3]Department of Physics, University of Warwick, Coventry CV4 7AL, UK

Core/shell GaAs/InAs nanowires represent tubular conductors due to their insulating core and confined conducting states in the InAs shell. We investigate nanowires with a crystalline phase purity of the InAs shell, where reduced scattering in electronic transport is expected. Low-temperature gate-dependent transport measurements give us insight into different contributions to the oscillatory behavior in the magnetoconductance, as well as the possibility to probe non-local transport phenomena due to large phase coherence length. With temperature-dependent measurements, we resolved the quasi-ballistic transport regime, and estimate the phase coherence length. Both measurements indicate superior transport properties of phase-pure GaAs/InAs nanowires in contrast to previous reports on non-phase pure nanowires. Our findings are an important optimization step for further development of nanowire-based hybrid devices.

TT 46.2 Thu 15:15 H13

Influence of defects and shape of thin InAs nanowires on their thermal conductivity, assessed via machine-learning potentials — •Sandro Wieser[1], YuJie Cen[1], Georg K. H. Madsen[1], and Jesús Carrete[2] — [1]Institute of Materials Chemistry, TU Wien, Wien, Austria — [2]Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-Universidad de Zaragoza, Zaragoza, Spain

Nanowires (NWs) grown from the zincblende (ZB) phase of InAs in the (111) direction commonly contain twin boundary defects consisting of narrow wurtzite (WZ) (001) phase regions between ZB sections. To investigate the impact of these and other defects on heat transport, we employ Green-Kubo equilibrium molecular dynamics simulations utilizing cepstral analysis to efficiently process the noise, and an accurate MACE model trained via active learning strategies to achieve transferability for a wide range of surface conditions.

We show that these twin boundaries reduce the thermal conductivity with respect to that of defect-free WZ-phase (001) NWs by a factor of more than two and that surface conditions lead to lower thermal conductivity values for defect-free ultrathin InAs ZB NWs. Analysis of the shape of twinning NWs reveals that structures mimicking experimentally measured surface configurations can enhance heat transport compared to strictly hexagonal NWs. Additional insights are gained from an analysis of line-group symmetries and vibrational properties for various NW shapes. Furthermore, experimentally motivated symmetric and symmetry-breaking surface defects are studied to reveal more and less influential defect sites.

TT 46.3 Thu 15:30 H13

Ab-initio heat transport in defect-laden quasi-1D systems from a symmetry-adapted perspective — •Yujie Cen[1], Sandro Wieser[1], Georg Kent Hellerup Madsen[1], and Jesús Carrete Montaña[2] — [1]Institute of Materials Chemistry, TU Wien, A-1060 Wien, Austria — [2]Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-Universidad de Zaragoza, Zaragoza, Spain

Due to their aspect ratio and wide range of thermal conductivities, nanotubes hold significant promise as heat-management nanocomponents. However, one major limitation preventing their widespread use is the typically high thermal resistance that arises from defects or contact with other materials. An intriguing question is the role that structural symmetry plays in thermal transport through those defect-laden sections. However, the ab-initio study of lattice thermal transport is hindered by factors such as the large number of atoms involved and the artifacts introduced by formalism designed for 3D systems.

We employ an Allegro-based machine learning potential to calculate the force constants and phonons of single and multi-layer MoS_2-WS_2 nanotube with near-DFT accuracy and efficient scaling. Subsequently, we combine representation theory with the mode-resolved Green's function method to calculate detailed phonon transmission profiles across defects, and connect the transmission probability of each mode to structural symmetry. while more drastic symmetry breakdowns might be expected to increase scattering and thermal resistance, our results show they actually reduce it by the suppression of selection rules and opening more phonon transmission channels.

TT 46.4 Thu 15:45 H13

Analysis of the electrical transport properties of MBE grown cubic Galliumnitride (c-GaN) sample structures — •Hannes Hergert[1,2], Mario F. Zscherp[1,2], Silas A. Jentsch[1,2], Jörg Schörmann[1,2], Sangam Chatterjee[1,2], Peter J. Klar[1,2], and Matthias T. Elm[1,2,3] — [1]Center for Materials Research, Heinrich-Buff-Ring 16, 35392 Giessen — [2]Institute of Experimental Physics I, Heinrich-Buff-Ring 16, 35392 Giessen — [3]Institute of Physical Chemistry, Heinrich-Buff-Ring 17, 35392 Giessen

Due to its lack of internal polarization fields cubic gallium nitride (c-GaN) is a promising semiconductor system for 'more-than-Moore' applications such as high-power electronics or optoelectronic devices. The analysis of its electrical transport properties is challenging since the molecular beam epitaxy (MBE) growth of high-quality c-GaN thin films requires a complex substrate architecture in order to accommodate the lattice mismatch between c-GaN and the 3C-SiC template. However, a reliable characterization of the electrical transport properties of c-GaN is crucial for the design of advanced functional devices. Here we analyze the electrical transport properties of the whole sample structure (MBE grown c-GaN/c-AlN thin films onto a 3C-SiC/Si template) with different c-GaN thicknessses using electrochemical impedance spectroscopy (EIS) as well as angle- and temperature-dependent magnetoresistance (MR) measurements. MR measurements reveal the existence of a highly conductive channel while EIS measurements allow the determination of the position of the channel between the c-AlN thin film and the 3C-SiC layer.

15 min. break

TT 46.5 Thu 16:15 H13

Fabrication and Characterisation of Short-channel Junctionless Nanowire Transistors — •Alessandro Puddu — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

The downscaling limitations of conventional planar transistors require the investigation of alternative device configurations. Because of their excellent electrostatic control and intrinsic scalability, junctionless nanowire transistors (JNTs) present a feasible solution and are highly desirable for next-generation electronics. The key factor that characterizes the JNTs is the absence of pn-junctions. This provides several benefits, such as an easier fabrication process since the devices do not require abrupt doping profiles within the nanowire channel, which is now uniformly doped.

This work focuses on the fabrication and characterisation of short-channel Si JNTs. A top-down approach based on e-beam lithography (EBL) and inductively coupled plasma reactive ion etching (ICP-RIE) was used to fabricate the Si nanowires. The device characterisation showed improved performances due to the channel length shrinking.

TT 46.6 Thu 16:30 H13

***Ab initio* investigation of drag effect in germanium** — •Dwaipayan Paul and Nakib Protik — Humboldt-Universität zu Berlin, Zum Großen Windkanal 2, 12489 Berlin, Germany

In a system of interacting electrons and phonons, the transport of one induces transport in the other. This phenomenon is known as the electron-phonon drag effect [1]. Now, an important milestone in the history of drag physics is the first recorded measurement of this phenomenon in germanium [2]. Here we present the results of our *ab initio* computations of the thermoelectric transport coefficients of germanium for various temperatures and charge carrier concentrations using the `elphbolt` code [3]. We investigate how the various scattering channels in the system enable this material to exhibit strong drag phenomena.

[1] Gurevich, Yu G., and O. L. Mashkevich. "The electron-phonon

drag and transport phenomena in semiconductors." Physics Reports 181.6 (1989): 327-394.

[2] Frederikse, H. P. R. "Thermoelectric power of germanium below room temperature." Physical Review 92.2 (1953): 248.

[3] Protik, Nakib H., et al. "The elphbolt ab initio solver for the coupled electron-phonon Boltzmann transport equations." npj Computational Materials 8.1 (2022): 28.

TT 46.7 Thu 16:45 H13

Anomalous Knudsen effect signaling long-lived modes in 2D electron gases — •Grigorii Starkov and Björn Trauzettel — Institute for Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany

Careful analysis of electron collisions in two spatial dimensions leads to the conclusion, that the odd harmonics of the electron distribution function decay much slower in comparison to the even ones at finite temperatures. Focusing on a channel geometry with boundary scattering, we show, that such behaviour of the odd decay rates leads to a characteristic behaviour of the resistance that we dub anomalous Knudsen effect: increasing temperature leads to decreasing resistance, that quickly slows down and turns into growth. The further increase of temperature exhibits the usual Gurzhi peak in the resistance related to the crossover from ballistic to hydrodynamic transport. The simultaneous observation of the Gurzhi peak preceded by an anomalous Knudsen dip can serve as a concrete signature of the long-lived modes in the 2D electron transport at low temperatures.

TT 46.8 Thu 17:00 H13

Quantum confinement and stoichiometry fluctuations in nm-thin SiGe layers — •Daniel Dick[1,2,3,4], Florian Fuchs[1,2,3], Sibylle Gemming[2,4], and Jörg Schuster[1,2,3] — [1]Center for Micro- and Nanotechnology, TU Chemnitz, Germany — [2]Center for Materials, Architecture and Integration of Nanomembranes, TU Chemnitz, Germany — [3]Fraunhofer Institute for Electronic Nanosystems (ENAS), Chemnitz, Germany — [4]Institute of Physics, TU Chemnitz, Germany

We simulate biaxially strained SiGe layers of varying thickness in the range of a few nanometers, as found in the base layer of heterojunction bipolar transistors (HBTs). At this length scale, local fluctuations in atomic concentrations can strongly influence the electronic properties of the device, especially the distribution of dopants like e.g. boron. Even at high doping concentrations, only a single atom is present at a 1 nm^2 cross section of the layer on average.

Employing a new parameterization of silicon and germanium in the framework of extended Hückel theory (EHT), we calculate the local band gap for different permutations of the atomic structure. Various distributions of boron atoms are simulated. We study the impact of locally increased and decreased concentrations on the band gap. By varying layer thickness, we evaluate the effects of quantum confinement and how it impacts transport properties of the thin layer in contrast to bulk material.