HL 65: Transport Properties II (Theory)

Time: Wednesday 17:00–18:15 Location: ER 164

HL 65.1 Wed 17:00 ER 164

Boltzmann equation approach to rectification at a potential step — •Stephan Rojek, Daniel Urban, Fred Hucht, and Jürgen König — Theoretische Physik, Universität Duisburg-Essen and CeNIDE, 47048 Duisburg, Germany

We study theoretically a two-dimensional electron gas with two regions separated by a potential step. A bias voltage parallel to the potential step leads to a transverse voltage proportional to the square of the applied bias voltage. This effect can be exploited for rectification, since the transverse voltage does not depend on the bias polarity. Our analysis is motivated by recent experiments [1, 2].

We model the system by means of the Boltzmann equation in the relaxation time approximation. We consider different relaxation times for scattering processes with energy transfer larger and lower than k_BT based on inelastic and elastic scattering processes, respectively. In order to study the rectification effects, the distribution function has to be calculated to second order in the applied electric field. The contributions from the bulk to the transverse voltage promise to be relevant for the measured data. Direct effects of the potential step depend on the energy dependence of the relaxation times. The potential step leads to a finite charge accumulation on the length scale of the energy diffusion length. The transverse electric field of this non-uniform charge distribution can be the leading contribution to the transverse voltage. We discuss the relevance of our results for the measurements in Ref. [1, 2].

[1] A. Ganczarczyk *et al.*, arXiv:0804.0689v3 (2009).
[2] A. Ganczarczyk *et al.*, AIP Conf. Proc. **1199**, 143 (2009).

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Multiscale modeling of silicon nanowire FETs for sensor applications — Daijiro Nozaki, •Jens Kunstmann, Felix Zörgiebel, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, Germany

We present a theoretical framework for the calculation of charge transport through nanowire-based Schottky-barrier field-effect transistors (FETs) that is conceptually simple but still captures the relevant mechanisms of the transport process [1]. Our approach combines two approaches on different length scales: (1) the finite element method is used to model realistic device geometries and to calculate the electrostatic potential across the Schottky barrier by solving the Poisson equation, and (2) the Landauer-Büttiker approach combined with the method of non-equilibrium Green's functions is employed to calculate the charge transport through the device. Our model correctly reproduces typical I-V characteristics of FETs, and the dependence of the saturated drain current on the gate field and the device geometry are in good agreement with experiments. Our approach is suitable for 1D Schottky-barrier FETs of arbitrary device geometry and it is intended to be a simulation platform for the development of nanowire-based sensors.

[1] D. Nozaki, J. Kunstmann, F. Zörgiebel, and G. Cuniberti, Nanotechnology 22, 325703 (2010).

HL 65.3 Wed 17:30 ER 164

Effect of pH value and ionic strength on transport characterics of nanowire FETs — •Daijiro Nozaki, Jens Kunstmann, Felix Zörgiebel, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany

For the development of ultra sensitive electrical bio/chemical sensors based on nanowires, the influence of the liquid environment such as the pH value, ionic strength of the solution, and the surface charge on the electron transport has to be understood. For this purpose, we implemented a modified Poisson-Boltzmann theory into a previously-developed multiscale model [1], which combines two models on different scales: (1) the finite element method for the calculation of electrostatic potential and (2) a Landauer transport approach based on non-equilibrium Green's functions formalism to calculate the charge transport through the device. We investigated the changes of the electric potential and transport characteristics due to the ionic concentration, the pH value, and surface charge densities, systematically. Using this model, we could reproduce the reduction of sensitivity of the sensors due to the screening effect from the electrolyte. [1] D. Nozaki, J. Kunstmann, F. Zörgiebel, and G. Cuniberti Nanotechnology 22, 325703 (2010).

HL 65.4 Wed 17:45 ER 164

Towards a Unifying Framework of AC Quantum Transport for Nanodevices including Scattering — •Diego Kienle — Theoretische Physik I, Universit\"at Bayreuth, 95440 Bayreuth

At present there is a significant need to model and understand dynamic quantum transport in realistic nanoscale devices including non-idealities e.g. due to scattering to ultimately guide the development of novel quantum devices operating at terahertz (THz) frequencies, even exploiting plasmon waves for THz sensing and emission. To step towards this goal, we discuss in this talk a general approach for linear AC quantum transport formulated by means of Non-Equilibrium Green Functions (NEGF) that is able to simultaneously handle the open nature of transport incorporated through self-energies, the complex dielectric environment typical for realistic devices, and most importantly the self-consistent dynamic coupling of the space-dependent AC charge and potential, the latter being essential to capture the plasmonic response of the system. Employing this approach, it is then discussed how scattering due to charged impurity atoms placed along the channel impacts the high-frequency response of nanodevices, specifically their plasmonic THz spectrum by example of a p-type carbon nanotube transistor. It is shown that particularly positively charged impurities cause a severe degradation of the THz plasmon modes, which vanish when the impurity concentration is sufficiently high. In this case, the AC response is solely determined by the single-particle excitation spectrum. [1] D. Kienle and F. Leonard, PRL 103, 026601 (2009). [2] D. Kienle, M. Vaidyanathan, and F. Leonard, PRB 81, 115455 (2010).

HL 65.5 Wed 18:00 ER 164

The effect of edge reconstruction in the electronic transport through transition metal dichalcogenide nanoribbons — •Mahdi Ghorbani Asl[1,2], Agnieszka Kuc[1], Gerd Schön[2], and Thomas Heine[1] — [1]Research Center for Functional Materials and Nanomolecular Science, Jacobs University Bremen, Bremen, Germany — [2]Institut für Theoretische Festkörperphysik, Karlsruher Institut für Technologie (KIT), Karlsruhe, Germany

Transition metal dichalcogenides, TX2 (T = Mo and W; X = S, Se, and Te), have become a focus of the substantial recent research, especially in their 2D crystalline forms in the wake of comprehensive research on graphene. Recent experiments have demonstrated that TX2 exhibit promising potentials for the next generation electronics [1]. However, a nanoflake or a nanoribbon can show different physical properties because of quantum confinement effects. In particular, edge atoms may influence the electronic transport properties of such low-dimensional materials. Using density functional based tight-binding (DFTB) method [2] combined with the Green's function technique [3], we have developed a code for coherent quantum transport calculations. We investigate the electron transport properties with a focus on the nature of the edge states in different type of nanoribbons.

[1] B. Radisavljevic, A. Radenovic, J. Brivio, V. Giacometti1 and A. Kis, Nature Nanotech 6, 147 (2011). [2] G. Seifert, D. Porezag, and T. Frauenheim, Int. J. Quantum Chemistry 58, 185 (1996) [3] S. Datta, Quantum transport: Atom to transistor, Cambridge University Press (2005).