Nanophysics Center, Reykjavik University
Annual Report 2020

Members of the group

In 2020 The Nanophysics Center (Website nano.ru.is) four full time faculty staff, Andrei Manolescu, Ágúst Valfells, Halldór Svavarsson, Sigurður Ingi Erlingsson, plus Gunnar Þorgilsson who is at ISOR, but still partly affiliated with us. Four other members were postdoctoral researchers Anna Sitek, Kristinn Torfason, Muhammad Taha Sultan and Movaffaq Kateb. The group included several PhD students who started their program earlier, Kristján Óttar Klausen, Hadi Rezaie, Hamed Gramizadeh, Hákon Örn Árnason, and Miguel Urbaneja Torres who graduated in February. A new PhD student joined the group in the beginning of the year, Elham Aghabalaei Fakhri and a new Master student in June, Rachel Elizabeth Brophy. Hallmann Óskar Gestsson and Hákon Valur Haraldsson, former Master students, worked with us for several months each, and also Jóhannes Bergur Gunnarsson, BS student.

Main research projects: participants, results, work in progress

Magnetoresistance oscillations in systems with spin-orbit coupling.
This is a collaboration between Sigurður I. Erlingsson and Prof. J. Carlos Egues at the University of Sao Paulo, Sao Carlos. The main result is an equation that describes beatings in the Shubnikov-de Haas oscillations in a 2D electron gas with both Rashba and Dresselhaus interaction. The central feature of the project is a new approximation scheme that works well for strong spin-orbit coupling and high Landau-level index. A new PhD student, Hamed Gramizadeh, was recruited and funded by the Reykjavik University within the new system of supporting doctoral studies. There are also students at the University of Sao Paolo who are working on Shubnikov-de Haas oscillations in topological insulator system, who Sigurður I. Erlingsson is co-supervising. We have extended the theory work to include an experimental group at the University of Basel, Switzerland, who are doing magnetotransport measurements.

Topological insulator (TI) nanowires.
Hallmann Óskar Gestsson continued his calculations on electronic spectra and transport in topological insulator nanowires with prismatic geometry, closely supervised by Sigurður Erlingsson. He obtained a 3-months grant from the Rannis Student Innovation Fund during the summer of 2020. He is now finalizing a manuscript which will present results that relate how different cross-sectional shapes affect the transport properties in the presence of a perpendicular magnetic field.

Magnetization dynamics and gap formation in 2D topological edge-states
Sigurður I. Erlingsson is working on a project along with Prof. Martin Leijnse at Lund University, Sweden, and Simon Wozny, Msc student at Lund. The project is a continuation of the work Simon did in magnetic impurities in helical edge states. Now the focus is on having time-dependent magnetic impurities, i.e. rotating magnetic moments, and how the gap behaves as the frequency of rotation is changes. The student defended his MSc in summer 2020 and is now working on adding transport calculations. The student is currently finalizing a manuscript that will present the transport in the presence time-dependent magnetic impurities.

Emergence of edge electronic states in 1D molecular chains
Sigurður I. Erlingsson joined project lead by Pavel Jelinek and Karel Vyborny at the Institute of Physics in Prague, the Czech Republic, on edge states in complicated molecular chains SIE and Karel Vyborny lead the theoretical part which involved extending the standard Su-Schrieffer-Heeger model that had two atoms per unit cell to more complicated molecules involving 10 atoms per unit cell. The manuscript has already appeared on arXiv.

Thermoelectric transport in core-shell semiconductor nanowires.
This is a Rannis funded project where Hadi and Movaffaq made significant progress in calculating the heat transported by nanowires using the software LAMMPS. Their results suggest that the geometry of the nanowires, circular or prismatic, is important for heat transport. In particular it appears that the triangular cross section is more favorable to heat transport along the nanowire than other geometries, for nanowires with 5-20 nm diameters and several hundreds of nm length. They also calculated the thermoelectric current carried by the electrons in a core-shell nanowire in the presence of a temperature bias beyond the linear response described by the Seebeck coefficient.

Majorana states in core-shell prismatic nanowires.
The PhD student Kristján Óttar Klausen, obtained his own doctoral grant from Rannis, for two years, in June 2020. He made progress in computing the energy states of a superconductor shell surrounding a semiconductor shell and their oscillations in the presence of a magnetic field reminding of the Little-Parks oscillations. He also made important steps in the direction of transport calculations in this systems by combining two computer codes, one for the energy states and one for the transmission function derived with the Green's function method. Kristján published a book in Springer, entitled "A treatise on the magnetic vector potential", which is based on his Master thesis plus a number of extensions related to his present project on Majorana states.

Atomistic calculations of 2D materials.
Andrei Manolescu participated in a project on structural properties of two dimensional materials derived by atomistic calculations, led by Nzar Rauf Abdullah from University of Sulaimani (Iraq). The studied materials were graphene codoped with B and N, graphene-like BC_6N and BSi_6N layers. The focus is on the mechanical and thermoelectric properties of these materials.

Molecular dynamics pf perovskite materials
The mater student Rachel Brophy started her project on computer simulations of the lattice dynamics of perovskite materials like $CH_3NH_3PbI_3$ with the goal of describing the migration of the Iodine ions which are known to contribute to the degradation of the material during the photovoltaic process. She is supervised by Movaffaq Kateb, Andrei Manolescu, and Halldór Svavarsson. The numerical simulations are performed using the LAMMPS software. This project is a continuation of the EEA funded international project on perovskite photovoltaics, closed in 2017, where our group was a partner. A second proposal for EEA funding on this subject was submitted in 2018, and approved in the end of 2020, for three years.

Piezoresistance of Silicon nanowires.
A new doctoral student, Elham Aghabalaei Fakhri, was hired in this project, funded by Reykjavik University, supervised by Halldór Svavarsson and Snorri Ingvarsson at UI. With a new fabrication method they could obtain a disordered arrays of Silicon nanowires with 20-50 nm diameter. They began measurements of their resistance variation in the presence of stress induced by a blown gas. The results were very promising, but the control of the gas blow, and the quality of the electrical contacts between metallic electrodes and the nanowires need to be improved.

Electronic properties of vacuum diodes.
Kristinn Torfason is studying surface inhomogeneities using the molecular dynamics code. A checkerboard model is being used to study the effects of areas with different work functions. Emittance, current and brightness of the electron beam have been calculated and examined how they are affected. A random pattern is also being studied, on a square grid, similar to the checkerboard model. Some results were shown at the ICOPS conference and a paper has been sent for publication in November. A checkerboard model for the prolate spheroidal tip geometry is being considered. Other geometries such as circular patches with different work functions and Voronoi diagrams are still in the initial phase. Ions and collisions have been added to the MD code. Recombination effects for the ions are in progress. An algorithm to generate a cathode surface with a background work function and with random islands of a different work function has been coded separately, and is being implemented in the simulations. One first goal is to compare the simulated current characteristics under photoemission with the recent experimental results obtained by our group, described in the second next paragraph.

Anna Sitek included in the code the effect of the temperature on the emission from nonuniform cathodes , based on the formula derived by Kevin Jensen, and studied the emission from cathodes with two values of work function forming a checkerboard pattern on the cathode surface. The results show that the current obtained from a checkerboard cathode is always larger than the averaged value of the currents from uniform cathodes with the same work functions as those on the checkerboard cathode. For the intermediate temperatures corresponding to the transition between source- and space-charge-limited regimes, the current from lower work function areas considerably exceeds the space-charge-limited value for the whole systems. Moreover, beams of the best quality, i.e. characterized by the largest brightness were also obtained for the transition range. These results were accepted for publication in Phys. Rev. Applied.

Jóhannes Bergur Gunnarsson finished a series of simulations in order to obtain corrections to the two-dimensional Child-Langmuir law at small dimensions. His work was published in the IEEE Transactions on Electron Devices. Taha Sultan and Hákon Örn Árnason obtained a experimentally a reproducible photoemission signal using inhomogeneous cathodes based on GaAs annealed in the presence of Ge. The fabrication, the structure of the cathodes, and the current characteristics were included in a manuscript submitted for publication.

Grants and other financial resources

Thermoelectric transport in core-shell nanowires, The Icelandic Research Fund, Andrei Manolescu and Sigurdur Ingi Erlingsson, 51.1 mil. ISK (2019-2022)

A possible basis for quantum computation: Majorana zero modes in tubular nanowires, The Icelandic Research Fund, doctoral grant, Kristján Óttar Klausen, 13 mil. ISK (2020-2021).

DC vacuum-microdiode arrays as tunable THz sources, The Icelandic Research Fund, PI Ágúst Valfells, 44.9 mil. ISK (2017-2020)

Vacuum electronics, The Icelandic Research Fund, postdoctoral fellowship Kristinn Torfason, 24.5 mil ISK (2017-2020)

Molecular dynamics simulations for emission and propagation of electrons in cathode nanostructures, US Air Force Office of Scientific Research (AFSOR), PI Ágúst Valfells, 180000 USD (2018-2021).

Funds from individual research accounts provided by the School of Science and Engineering were used for travel to conferences, for guest scientists, and for software license.

Funds for two PhD students, Elham Aghabalaei Fakhri and Hamed Gramizadeh, were provided by the research funds of Reykjavik University, the two positions being obtained in 2020 and 2018, respectively.

Funds for one summer student, Rachel Elizabeth Brophy, from Student's Innovation Fund of Rannis. 0.900 mil. ISK (20019).

Funds from Landsvirkjun obtained by Andrei Manolescu within the Sustainability Institute and Forum (SIF) at Reykjavik University, for research on photovoltaics, 0.650 mil. ISK.

Events related to the activity of the center (short visits, presentations, theses, etc.) were severely limited due to the Covid related crisis

25 February, PhD student Miguel Urbaneja Torres defends his doctoral thesis. His supervisor was Andrei Manolescu, and the external examiner was Professor Guido Goldoni from Modena University, Italy.

27 February, talk by Pof. Guido Goldoni entitled Spin physics in one-dimensional semiconductor nanomaterials

6 December, online presentation by Kristinn Torfason at ICOPS2020 conference, entitled Effects of surface inhomogeneities in field and thermal-field emission

Journal papers (e-prints, accepted, or published)

Aleš Cahlík, Jack Hellerstedt, Jesús I. Mendieta-Moreno, Martin Švec, Vijai M. Santhini, Simon Pascal, Diego Soler-Polo, Sigurdur I. Erlingsson, Karel Výborný, Pingo Mutombo, Ondrej Marsalek, Olivier Siri, Pavel Jelínek, Significance of nuclear quantum effects in hydrogen bonded molecular chains, submitted for publication arXiv:2007.14657 (2020).

P. Zhang, Y.S. Ang, A.L. Garner, Á. Valfells, J.W. Luginsland, L.K. Ang, Space-charge limited current in nanodiodes: Ballistic, collisional, and dynamical effects, submitted for publication (invited perspective paper) in Journal of Applied Physics (2021).

K. Torfason, A. Sitek, A. Manolescu, Á. Valfells, Dynamics of a Field Emitted Beam from a Microscopic Inhomogeneous Cathode, submitted for publication, arXiv:2011.13731 (2020).

A. Sitek, K. Torfason, A. Manolescu, and A. Valfells, Space-charge effects in the field-assisted thermionic emission from nonuniform cathodes, accepted for publication in Physical Review Applied, (2021) selected as an Editors' Suggestion, arXiv:2009.13616 .

J. B. Gunnarsson, K. Torfason, A. Manolescu, A. Valfells, Space-Charge Limited Current from a Finite Emitter in Nano- and Microdiodes, IEEE Transactions on Electron Devices **68**, 342 (2021), arXiv:2010.01334 .

H. V. Haraldsson, K. Torfason, A. Manolescu, and A. Valfells, Molecular Dynamics Simulations of Mutual Space-Charge Effect between Planar Field Emitters, IEEE Transactions on Plasma Science **48**, 1967 (2020) DOI: 10.1109/TPS.2020.2991582.

M. T. Sultan, A. Manolescu, H. G. Svavarsson, A. Valfells, Solid-state dewetting of silver-thin films: self-assembled nano-geometries, IOPSciNotes https://iopscience.iop.org/article/10.1088/2633-1357/abcea2 (2020).

M. T. Sultan, J. T. Gudmundsson, A. Manolescu, H. G. Svavarsson, Structural and photoluminescence study of TiO2 layers with self-assembled Si1-xGex nanoislands, J. Appl. Phys. **128**, 085304 (2020).

I. Stavarache, C. Logofatu, M. T. Sultan, A. Manolescu, H. G. Svavarsson, V. S. Teodorescu, M. L. Ciurea, SiGe nanocrystals in SiO2 with high photosensitivity from visible to short-wave infrared, Scientific Reports **10**, 3252 (2020).

M.T. Sultan, J. T. Gudmundsson, A. Manolescu, V. S. Teodorescu, M. L. Ciurea, H. G. Svavarsson, Obtaining SiGe nanocrystallites between crystalline TiO2 layers by HiPIMS without annealing, Applied Surface Science **511**, 145552 (2020).

H. Rezaie Heris, M. Kateb, S. I. Erlingsson, and A. Manolescu, Thermoelectric properties of tubular nanowires in the presence of a transverse magnetic field, Nanotechnology **31**, 424006 (2020), arXiv:2006.13328.

K. O. Klausen, A. Sitek, S. I. Erlingsson, A. Manolescu, Majorana Zero Modes in Nanowires with Combined Triangular and Hexagonal Geometry, Nanotechnology **31**, 354001 (2020), arXiv:2004.14991.

Kristján Óttar Klausen, A Treatise on the Magnetic Vector Potential, Springer 2020, https://www.springer.com/gp/book/9783030522216, DOI: 10.1007/978-3-030-52222-3.

V. Gudmundsson, N. R. Abdullah, C.-S. Tang, A. Manolescu, V. Moldoveanu, Self-induction and magnetic effects in electron transport through a photon cavity, Physica E 127 (2021) 114544 (2021), arXiv:2005.10914.

N. R. Abdullah, H. O. Rashid, A. Manolescu, V. Gudmundsson, Interlayer interaction controlling the properties of AB- and AA-stacked bilayer graphene-like BCN and SiC, Surfaces and Interfaces **21**, 100740 (2020), arXiv:2008.10888.

N. R. Abdullah, H. O. Rashid, C.-S. Tang, A. Manolescu, V. Gudmundsson, Properties of BSi_6N monolayers derived by first-principle computation, Physica E **127**, 114556 (2021), arXiv:2008.03782.

N. R. Abdullah, H. O. Rashid, C-S Tang, A. Manolescu, V. Gudmundsson, Modelling electronic, mechanical, optical and thermal properties of graphene-like BC_6N materials: Role of prominent BN-bonds, Phys. Lett. A **384**, 126807 (2020), arXiv:2003.08467.

N. R. Abdullah, H. O. Rashid, M. T. Kareem, C.-S. Tang, A. Manolescu, V. Gudmundsson, Effects of bonded and non-bonded B/N codoping of graphene on its stability, interaction energy, electronic structure, and power factor, Phys. Lett. A **384**, 126350 (2020), arXiv:2002.11377.

N. R. Abdullah, C.-S. Tang, A. Manolescu, V. Gudmundsson, Oscillations in electron transport caused by multiple resonances in a quantum dot-QED system in the steady-state regime, Physica E **123**, 114221 (2020), arXiv:1903.03655.

N. R. Abdullah, C.-S. Tang, A. Manolescu, V. Gudmundsson, The interplay of electron-photon and cavity-environment coupling on the electron transport through a quantum dot system, Physica E **119**, 113996 (2020), arXiv:1908.05712.

See also http://nano.ru.is/publications

Contributions to conferences

K. Torfason, A. Sitek, Á. Valfells, A. Manolescu, Effects of surface inhomogeneities in field and thermal-field emission, ICOPS2020

J. B. Gunnarsson, K. Torfason, A. Manolescu, Á. Valfells, Deviations from the Child-Langmuir law at the microscale, ICOPS2020

R. Magnusson, K. J. Lee, H. Hemmati, P. Bootpakdeetam, J. Vasilyev, F. A. Simlan, N. Razmjooei, Y. H. Ko, S. Zhang, Sun-Goo Lee, H.G. Svavarsson. Properties of resonant photonic lattices:Bloch mode dynamics, band flips, and applications: SPIE-Photonics West conference, 1-6 February, San Francisco, USA, 2020

H.G. Svavarsson, M.T. Sultan, K.J. Lee, S. Das and R. Magnusson. Hydrogenated silicon films for low-loss resonant reflectors operating in the visible region in 3rd IEEE Research and applications of photonics defense, RAPID, 10-12 August 2020

Research plans for 2021

Thermoelectric and heat conduction of nanowires.

Piezoresistance and other stress effects in disordered arrays of Silicon nanowires.

Molecular dynamics of perovskite materials for photovoltaics applications

Majorana states in tubular nanowires: core shell geometry including the superconductor.

Shubnikov – de Haas oscillations and spin-orbit coupling.

Thermoelectric transport in topological nanowires.

Vacuum electronics: Thermal-field emission for inhomogeneous work function, Miram curves, arrays of hyperbolic tips, core-shell like emitters, space-charge effects in the I-V characteristics of photoemission from inhomogeneous cathodes. Space charge limited emission from a hyperbolic tip.