

Nanophysics Center, Reykjavik University

Annual Report 2019

Members of the group

During 2018 the Nanophysics Center (Website nano.ru.is) had four full time faculty staff, Andrei Manolescu, Ágúst Valfell, Halldór Svavarsson, Sigurður Ingi Erlingsson, plus Gunnar Þorgilsson who is at ISOR, but still partly affiliated with us. Other members were postdoctoral researchers Anna Sitek and Kristinn Torfason, and also Hifsa Shahid between March and November and Javed Hussain from March to May. Muhammad Taha Sultan, Miguel Urbaneja Torres, and Hákon Örn Árnason were PhD students, who started before 2018, and Kristján Óttar Klausen, Hadi Rezaie, and Hamed Gramizadeh were new PhD students starting in 2019. Hallmann Óskar Gestsson (beginning with March) and Movaffaq Kateb (between with September) worked with us research assistants. Hákon Valur Haraldsson was a Master student. Jóhannes Bergur Gunnarsson, Jónas Már Kristjánsson, and Roberto Aceto were BS students working on a research project with us.

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 Paulo 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.

We hired Hallmann Óskar Gestsson who finished his Master's at Lausanne in 2019, as a research assistant. He joined a project lead by Sigurður I. Erlingsson and Andrei Manolescu on electronic properties of TI nanowires in transverse magnetic field. The combined effect of the transverse magnetic field and the surface character of the TI lead to very interesting transport phenomena that strongly depend on the cross-sectional geometry of the nanowires, e.g. circular, rectangular, or triangular.

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 work is still in the early stages but progressing quickly and the student will graduate in May 2020.

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. A manuscript is in the final stages of writing.

Electronic transport in open nanosystems in the presence of photons.

Andrei Manolescu participated in a project on electronic transport through open systems coupled to cavity photons, in collaboration with Vidar Guðmundsson from University of Iceland, with Valeriu Moldoveanu from National Institute of Materials Physics, Bucharest (Romania) and with Nzar Rauf Abdullah from University of Sulaimani (Iraq). The main published results were about the coupling of two quantum conductors via photons and the role of the electronic states dressed by photons in the charge transport.

Optical properties of core-shell semiconductor nanowires.

Miguel Urbaneja and Andrei Manolescu, with help from other members of the group, finalized the calculation of the radiated electromagnetic field of prismatic core-shell nanowires and submitted a manuscript, to be included in Miguel's PhD thesis. Miguel has also performed calculations on the scattering of light by prismatic nanowires, finalized with a paper published in Optics Express. They also worked together on the charge dynamics in the tubular prismatic geometry, due to a time dependent external field, in continuation of the previous work of Anna Sitek on the electromagnetic absorption due to the transverse modes.

Thermoelectric transport in core-shell semiconductor nanowires.

A new project with this title has been approved for funding by Rannis. Hallmann Óskar Gestsson, who completed his Master's degree in Switzerland in 2018, worked as a research assistant, and calculated states in tubular nanowires with polygonal cross section, using the Dirac Hamiltonian. Transport calculations due to a longitudinal temperature bias are in progress. A new PhD student, Hadi Razaie, started in this project and calculated the current-temperature characteristic of cylindrical nanowires in transverse magnetic field. Also, Movaffaq Kateb obtained phonon spectra and stress maps of triangular and hexagonal prismatic core-shell nanowires.

Majorana states in core-shell prismatic nanowires.

A new PhD student, Kristján Óttar Klausen, started working on this project, being funded by the Reykjavik University within the new system of supporting doctoral studies. The position was obtained in 2018. Kristján has worked on the phase diagram of the topological states in triangular nanowires with hexagonal core. Together with Andrei Manolescu and Sigurdur Erlingsson, he is also working on a Hamiltonian model describing a superconductor-semiconductor heterojunction in the tight binding scheme.

Silicon nanowires.

Preliminary experiments on arrays of silicon-nanowires (SiNWs) performed by Dr. Rodica Plugaru, collaborator from Romania, showed very promising piezoresistance effects of the nanowires embedded in a pressurized gas. A Rannis project proposal submitted in June 2018 to continue this research at RU was rejected in January 2019. A revised version of the application was submitted to Rannis in June 2019. Jonas Mar, an undergraduate student at RU, measured photovoltaic properties of SiNWs arrays with grant from the Students Innovation Fund of Rannis.

TiO₂ thin films with embedded GeSi nanoparticles.

This project started in 2016 and it was funded by Rannis with an M-ERA.NET collaboration with National Institute of Materials Physics from Romania. The PhD student Muhammad Taha Sultan, supervised by Halldór Svavarsson, finalized his thesis with a new series of four published papers on using High Power

Impulse Magnetron Sputtering to produce GeSi nanoparticles or nanocrystals. Taha wrote one more paper on a method without annealing, still in under review.

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. Emission, current and brightness of the electron beam are calculated and examined how they are affected. A random pattern also being studied on a square grid similar to the checkerboard model. Some preliminary results were shown at the ICOPS conference and a paper is now being prepared for publications. Other geometries such as circular patches with different work functions and Voronoi diagrams are in the starting phase. Ion's and collisions have been added to the MD code and simulations are being done by Amanda Loveless at Purdue University. Recombination effects for the ion's will be added later.

Anna Sitek included in the code the effect of the temperature on the field emission, based on the formula derived by Kevin Jensen. The preliminary results show strong enhancement of emission in the presence of both processes, i.e., for the thermo-field emission. Moreover, the strong impact of space-charge effects was observed for higher fields and temperatures. Further, she created a model of polygonal cathode which is now being tested.

A paper based on the work of Hákon Valur Haraldsson, on mutual space-charge effects between neighboring field emitters, was submitted for publication in Physics of Plasmas. Jóhannes Bergur Gunnarsson performed a new series of simulations in order to obtain corrections to the two-dimensional Child-Langmuir law at small dimensions. This work is being prepared for submission to the IEEE Transactions on Electron Devices. On the experimental side Taha Sultan and Hákon Örn Árnason obtained a reproducible photoemission signal using annealed GaAs cathode emitters.

Grants and other financial resources

High photoconductive oxide films functionalized with GeSi nanoparticles for environmental applications (PhotoNanoP) M-ERA.NET project 2016-2019, in collaboration with National Institute of Materials Physics from Romania. RU team leader Halldór Svavarsson, RU budget 108000 Euro.

Core-shell nanoantennas, The Icelandic Research Fund, PI Andrei Manolescu, 41.3 mil. ISK (2016-2019).

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

DC vacuum-microdiode arrays as tunable THz sources, The Icelandic Research Fund, PI Ágúst Valfell, 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 Valfell, 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, Kristján Óttar Klausen and Hamed Gramizadeh, were provided by the research funds of Reykjavik University, the two positions being obtained in 2018.

Fund for one summer student, Jonas Mar, from Student's Innovation Fund of Rannis. 0.900 mil. ISK (20019).

Events related to the activity of the center (short visits, presentations, theses, etc.)

20-21 February, visit of Dr. Jason Foley AFOSR, US, Materials and Physics Division, to discuss possible new projects on condensed matter.

15 March, Andrei Manolescu gives talk entitled "Localization of electrons in semiconductor tubular nanowires" and the Physics Department of Oslo University.

22 May, talk by Andrei Manolescu, at Icelandic Physical Society Conference, on excitons in core-shell nanowires with polygonal cross section.

29 May, talk by Andrei Manolescu, on excitons in core-shell nanowires, at the International Workshop of Materials Physics, organized by National Institute of Materials Physics, Bucharest, Romania,

9-18 May, Dr. Nicolina Pop from University of Timisoara, Romania, visited our group and gave a presentation on the ionization and recombination rates of gas atoms relevant for the field enhancement effect in vacuum diodes with gas residuals.

10-22 June, Kristján Óttar Klausen participates at Physics Summer School on Quantum Frontiers, organized by Nordita in Stockholm.

24-26 June, Halldór G. Svavarsson gave a talk on Effect of H₂/Ar plasma exposure: influence of short and protracted intervals, in *3rd international workshop on thin films for electronics, electro-optics, energy and sensors* (TFE3S), Reykjavik, Iceland,

24-26 June. Muhammad Taha gave a talk on Growth of SiGe nanocrystals in SiO₂ matrix by applying HiPIMS: On the way to crystallization bypassing the need of annealing in *3rd international workshop on thin films for electronics, electro-optics, energy and sensors* (TFE3S), Reykjavik, Iceland.

4-5 July, visit of Dr. Nicklas Anttu, from Alto University, Finland, and talk entitled "Absorption modeling with FMM, FEM and FDTD".

10 July, Miguel Urbaneja Torres, invited talk "Transverse polarization light scattering in tubular semiconductor nanowires", at ICTON 2019 conference, Angers, France.

14 August-9 September, Joao Vito Ignacio Costa. Visiting PhD student from Sao Carlos, Brazil. Working on the Shubnikov-de Haas project.

23-27 September, Anna Sitek, poster "*Localization-dependent properties of prismatic nanowires*", Nanowire Week 2019, Pisa, Italy.

8-22 November, visit of Dr. Valeriu Moldoveanu from National Institute of Materials Physics, Romania, collaborator on the project on thermoelectric transport at nanoscale.

10-17 November, Kristján Óttar Klausen visits the research group led by Thomas Schaeper in Juelich, Germany.

26 November, PhD student Muhammad Taha Sultan defends his doctoral thesis. His supervisor was Halldór Svavarsson, and the eternal examiner was Marin Alexe, professor at University of Warwick, UK.

13 December, Dr. Victor Kuncser, head of Department of Magnetism at National Institute of Materials Physics, Romania, gives the presentation “Anisotropy related magneto-functionalities in low dimensional systems”.

17 – 18 December, Ágúst Valfells, Anna Sitek, and Kristinn Torfason attend workshop on cathodes at Air Force Research Laboratory, Kirtland Air Force Base, Albuquerque, NM, USA. Ágúst gives a talk entitled “Molecular dynamics based simulations of emission and propagation at the microscale: Space-charge effects, mutual interaction between emitters, and inhomogeneous cathodes”.

19 December, Anna Sitek receives the habilitation from Wroclaw University of Science and Technology.

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

M. Urbaneja Torres, K. O. Klausen, A. Sitek, S. I. Erlingsson, V. Gudmundsson, A. Manolescu, Anisotropic electromagnetic field emitted by core-shell semiconductor nanowires driven by an alternating current, submitted for publication, [arXiv:1912.10284](https://arxiv.org/abs/1912.10284) (2019).

V. Moldoveanu, I. V. Dinu, A. Manolescu, V. Gudmundsson, Backaction effects in cavity-coupled quantum conductors, *Phys. Rev B* **100**, 125416 (2019), [arXiv:1909.03630](https://arxiv.org/abs/1909.03630).

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, submitted for publication, [arXiv:1908.05712](https://arxiv.org/abs/1908.05712) (2019).

M. Urbaneja Torres, A. Sitek, A. Manolescu, Anisotropic light scattering by prismatic semiconductor nanowires, *Optics Express* **27**, 25502 (2019).

V. Moldoveanu, A. Manolescu, V. Gudmundsson, Generalized Master Equation approach to time-dependent many-body transport, *Entropy* **21**, 731 (2019), [arXiv:1908.00354](https://arxiv.org/abs/1908.00354).

A. Sitek, M. Urbaneja-Torres, A. Manolescu, Corner and side localization of electrons in irregular hexagonal semiconductor shells, *Nanotechnology* **30**, 454001 (2019) [arXiv:1907.06764](https://arxiv.org/abs/1907.06764).

V. Gudmundsson, N. R. Abdullah, C.-S. Tang, A. Manolescu, V. Moldoveanu, Cavity-photon induced high order transitions between ground states of quantum dots, *Annalen der Physik*, **531**, 1900306 (2019), [arXiv:1905.10883](https://arxiv.org/abs/1905.10883).

N. R. Abdullah, C.-S. Tang, A. Manolescu, V. Gudmundsson, Manifestation of the Purcell effect in current transport through a dot-cavity-QED system, *Nanomaterials* **9**, 1023 (2019) [arXiv:1905.07492](https://arxiv.org/abs/1905.07492).

D. V. Anghel, G. A. Nemnes, I. Pintilie, A. Manolescu, Modelling J-V hysteresis in perovskite solar cells induced by voltage poling, *Physica Scripta* **94**, 125809 (2019).

D. J. Carney, H. G. Svavarsson, H. Hemmati, Alexander Fannin, Jae W. Yoon, R. Magnusson; Refractometric sensing with periodic nano-indented arrays: Effect of structural dimensions. *Sensors* **19** (2019)

M. T. Sultan, J. T. Gudmundsson, A. Manolescu, V. S. Teodorescu, M. L. Ciurea, H. G. Svavarsson, Efficacy of annealing and fabrication parameters on photo-response of SiGe in TiO₂ matrix, *Nanotechnology* **30**, 365604 (2019).

M. T. Sultan, V. S. Teodorescu, J. T. Guðmundsson, A. Manolescu, M. L. Ciurea, H. G. Svavarsson, Fabrication and characterization of Si_{1-x}Ge_x nanocrystals in as-grown and annealed structures: A comparative study, *Beilstein Journal of Nanotechnology* **10**, 1873 (2019).

M. M. Sonner, A. Sitek, L. Janker, D. Rudolph, D. Ruhstorfer, M. Döblinger, A. Manolescu, G. Abstreiter, J. J. Finley, A. Wixforth, G. Koblmüller, H. J. Krenner, Break-down of corner states and carrier localization by monolayer fluctuations in radial nanowire quantum wells, *Nano Letters* **19**, 3336 (2019).

N. R. Abdullah, C.-S. Tang, A. Manolescu, V. Gudmundsson, The photocurrent generated by photon replica states of an off-resonantly coupled dot-cavity system, *Scientific Reports* **9**, 14703 (2019).

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M. T. Sultan, A. Manolescu, J. T. Gudmundsson, K. Torfason, G. A. Nemnes, I. Stavarache, C. Logofatu, V. S. Teodorescu, M. L. Ciurea, H. G. Svavarsson, Enhanced photoconductivity of SiGe nanocrystals in SiO₂ driven by mild annealing, *Applied Surface Science* **469**, 870 (2019)

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

Contributions to conferences

M. Urbaneja Torres, A. Sitek, A. Manolescu, Transverse polarization light scattering in tubular semiconductor nanowires, ICTON 2019 Angers, IEEE Xplore Digital Library <https://ieeexplore.ieee.org/document/8840569> (2019), [arXiv:1905.02268](https://arxiv.org/abs/1905.02268).

Kristinn Torfason, Ágúst Valfells, Andrei Manolescu, Simulations of Surface Inhomogeneities in Field Emission, ICOPS PPPS 2019, Orlando, Florida, 23-28 June 2019, IEEE Nuclear and Plasma Sciences Society.

Amanda Loveless, Kristinn Torfason, Ágúst Valfells, Allen Garner, Investigation of Electron Emission Using Molecular Dynamics Simulations, ICOPS PPPS 2019, Orlando, Florida, 23-28 June 2019, IEEE Nuclear and Plasma Sciences Society.

M.T. Sultan, J. T. Gudmundsson, A. Manolescu, M. L. Ciurea, H. G. Svavarsson: Growth of SiGe nanocrystals in SiO₂ matrix by applying HiPIMS: On the way to crystallization by-passing the need of annealing, in proceedings of *3rd International workshop on thin films for electronics, electro-optics, energy and sensors* (TFE3S), Reykjavik, Iceland, 24-26 June, 2019.

M.T. Sultan, J. T. Gudmundsson, A. Manolescu, M. L. Ciurea, H. G. Svavarsson: Effect of H₂/Ar plasma exposure: influence of short and protracted intervals, in proceedings of *3rd International workshop on thin films for electronics, electro-optics, energy and sensors* (TFE3S), Reykjavik, Iceland, 24-26 June, 2019.

Research plans for 2020

Thermoelectric and heat conduction of nanowires.

Lateral optical absorption of arrays of Silicon nanowires.

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

Charge dynamics in core-shell nanowires.

Shubnikov – de Haas oscillations and spin-orbit coupling.

Thermoelectric transport in topological nanowires.

Vacuum electronics: Thermal-field emission for inhomogeneous work function, arrays of hyperbolic tips, core-shell like emitters, space-charge effects in the I-V characteristics of photoemission from annealed GaAs emitters.