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Molecular dynamics simulation for emission and propagation of electrons in cathode nano-structures

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14. ABSTRACT
This research resulted in the successful development of simulation code for modeling field, thermionic, and photo electron emission cathodes using a molecular dynamics formalism. This work examined and performed verification testing of many different critical electron emission phenomenology of critical importance to high power microwave (HPM) and radio frequency (RF) amplifiers for electronic warfare, radar, and communication. The software code was provided to AFRL/RDH personnel and now being used to research cathodes and cathodes in HPM devices. The Grant research using the software code investigated mutual space charge effects on field emission from finite emitters embedded in a planar cathode of an infinite diode. It was shown how separation of the emitters can affect the equilibrium current to a significant degree depending on the applied electric field and material parameters of the emitters. Another cathode limiting phenomenon is the classic form of the two-dimensional Child Langmuir law developed by Y.Y. Lau and J.W. Luginsland, which was known not to be valid for emitters of very small diameter or for large ratios of diode spacing to emitter width (large aspect ratio). This FE MD code allowed investigation into how the large aspect ratio emitters of a large cathode exceeded the 2D space-charge limited emission for this regime. In addition, they investigated the effect of non-homogenous work function on the emission current and emittance of a thermionic-field emission cathode. They demonstrated how these parameters are dependant on both the granularity of the cathode structure and its degree of disorganization. A very interesting result was that the emittance improved by almost 30% with large numbers of in-homogenous emitters.

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FINAL PERFORMANCE REPORT

Award no. FA-9550-18-1-7011

Molecular dynamics simulation for emission and propagation of electrons in cathode nano-structures.

PI: Ágúst Valfells

September 2018 – September 2021

Contents

Introduction

This report gives a concise description of the main scientific activity funded by Award no. FA-9550-18-1-7011; participants and collaborators; finances and the output in terms of published work, talks and software improvements.

Overview of scientific activity

In this section, we give an overview of those who worked on the project funded by this grant, the main topics of research and collaborative activities.

Personnel.

The following is a list of faculty, staff and students who worked on this project, either directly or indirectly with a description of their role and how they benefitted from the grant.

Ágúst Valfells, PI. Received support for travel to visit collaborators in Albuquerque.

Andrei Manolescu, Co-PI. Did not use funding from this grant.

Kristinn Torfason, Research Scientist. Primary responsibility for code development and implementation. Involved in all research topics. Part of his salary was from this grant. Received support for travel to visit collaborators in Albuquerque.

Anna Maria Sitek, Research Scientist. Primary researcher on field enhanced thermionic emission. Salary was from this grant. Received support for travel to visit collaborators in Albuquerque.

Currently Associate Professor, Department of Theoretical Physics, Wroclaw University of Science and Technology.

Hákon Valur Haraldsson, MSc student. Worked on mutual space-charge effects between neighbouring emitters. Received financial support from grant. Currently Ph.D. student at Reykjavík University working on modelling of thermal arcs.

Jóhannes Bergur Gunnarsson, BSc student. Worked on deviation from two-dimensional Child-Langmuir law. Received financial support from grant. Currently MSc student in mechatronics engineering at Reykjavík University.

Brynjar Ingi Óðinsson, BSc student. Worked on ion effects. Did not receive financial support, but academic credit.

Hákon Örn Árnason, Ph.D. student. Worked in photoemission model. Received funding from a different grant, but benefitted from code development supported by this grant.

Yuan Zhou, Ph.D. student. Working on developing model for field emission from CNT-fibre. Funded directly by Reykjavík University. Benefitted from code development. Detailed modelling of emission from CNT-fibres is envisioned as follow-up to this project.

Space-charge effects between neighbouring field emitters

This work examined mutual space charge effects on field emission from finite emitters embedded in a planar cathode of an infinite diode. It was shown how separation of the emitters can affect the equilibrium current to a significant degree depending on the applied electric field and material parameters of the emitters. Although the having the model based on planar field emitters rather than protruding emitters is in some ways unrealistic, it has the advantage of isolating space-charge effects on emission from the effects of electrostatic shielding due to surface charge distribution in three-dimensional emitter structures.

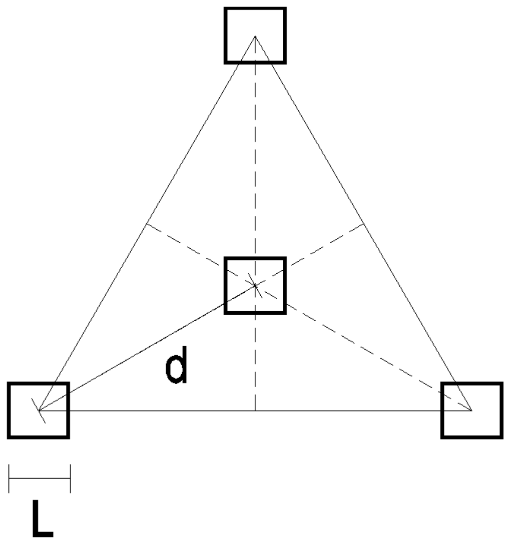

Figure 1. Top view of configuration of planar field emitting squares in an equilateral triangle array. These patches are on the cathode of a planar diode.

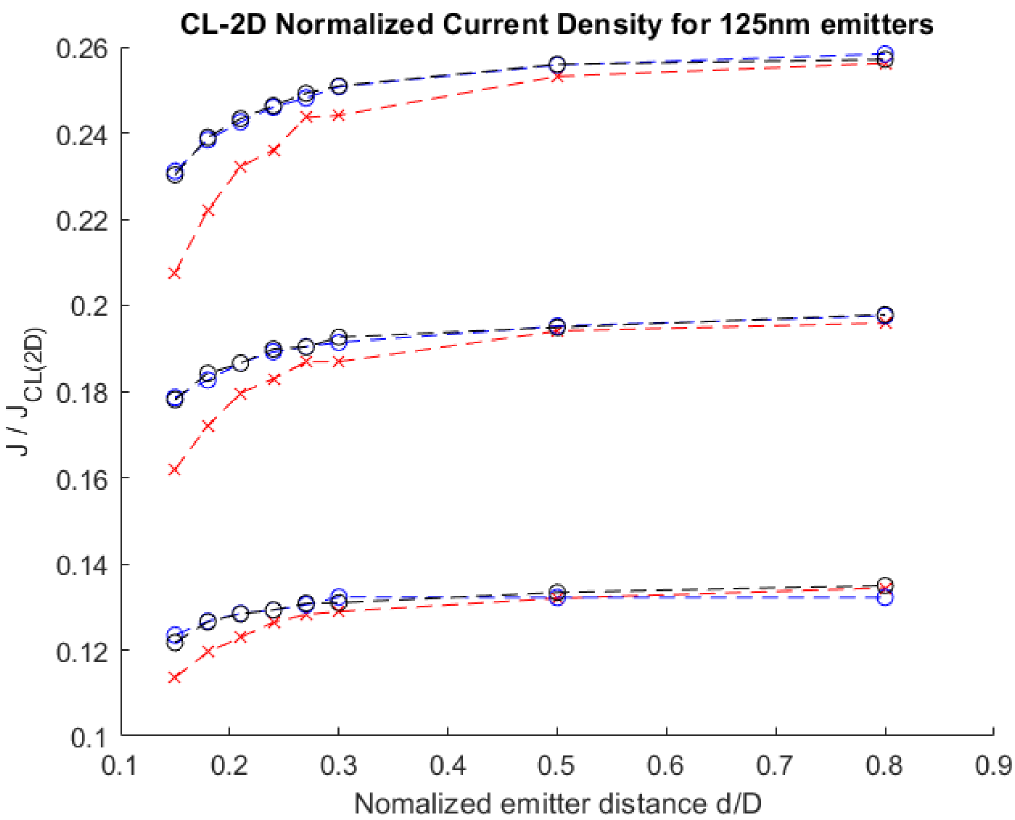

Figure 2. Effect of emitter proximity in a four-emitter system for 125nm edge length and three different gap voltages. The average current density is normalized by the current density as predicted by the 2D Child-Langmuir law. Here the gap spacing is, D = 1000nm, work function 2.2eV, the emitter spacing, d, is varied. The gap voltage for the topmost, middle and bottom set of curves is 2750V, 2500V and 2250V respectively. The red curves (x) show the normalized current density from the central emitter, and the green black and blue curves (o) show the normalized current density from the outer emitters.

Results from this work were published in IEEE Transactions on Plasma Science and in the Master's thesis of Hákon Valur Haraldsson.

Deviation from 2D Child-Langmuir law

The classic form of the two-dimensional Child Langmuir law developed by Y.Y. Lau and J.W. Luginsland was known not to be valid for emitters of very small diameter or for large ratios of diode spacing to emitter width (large aspect ratio). How it broke down was not understood, nor was there a clear picture of the physics of space-charge limited emission for this regime. In our work we extended the two-dimensional Child-Langmuir law to large aspect ratios and emitter widths on the microscale and smaller. The model was based on a circular emitting patch embedded in the cathode of an infinite planar diode. Molecular dynamics based simulations were used to calculate *I-V* curves for the diode for a large range of applied field strength, diode gap size, and emitter radius. The curves showed significant deviation from the conventional 2D Child-Langmuir law when the emitter size was decreased to the microscale and/or the aspect ratio was made very large. An analytic model based on discrete emission of electrons from a point source could be used to quantitatively explain the current characteristics of the diode for very small emitting areas. We also described how the applied field strength affects the radius at which transition to the point emitter regime takes place, and showed how the predicted current ceases to depend on the the ratio between the diode spacing and charactristic width (aspect ratio) as the aspect ratio becomes large.

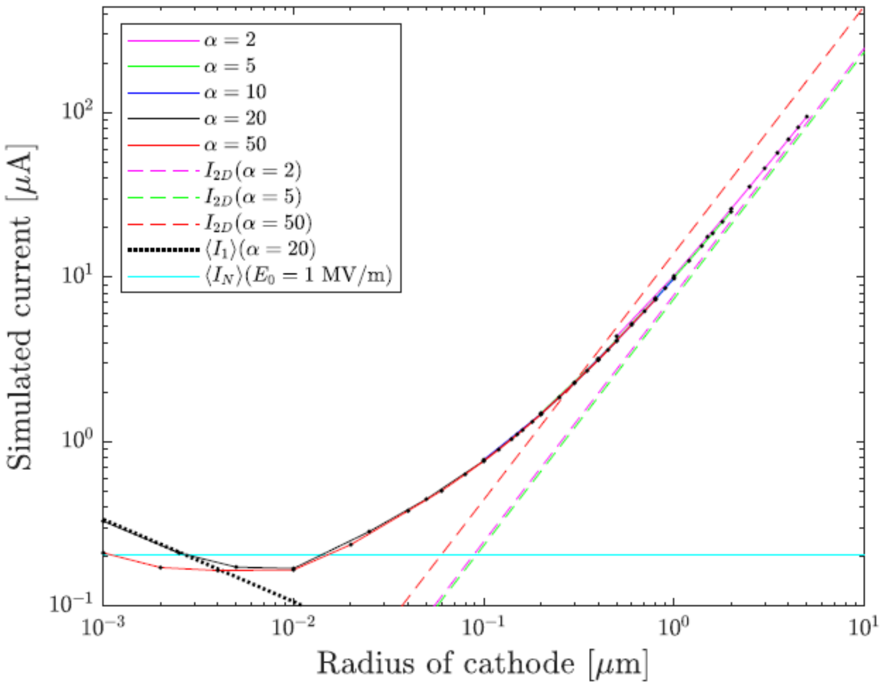

Figure 3. Current from an emitting area of finite radius for an applied field of 1 MV/m and different aspect ratios (α). Solid curves are obtained from simulation. Dashed lines labelled as I_{2d} are calculated from the conventional two-dimensional Child-Langmuir law. The dotted line is obtained from a point emitter Coulomb blockade model. The horizontal solid line stems from a multiple electron point emitter model.

This work was published in the IEEE Transactions on Electron Devices and at ICOPS 2020.

Non-homogeneous work function effects on field emission

In this work we examined an infinite planar diode with a finite emitter area embedded in the cathode. The emitting area was divided into an N×N array of square checks that were assigned a work function of either 2.5eV or 2.0eV. Simulations were done for both a regular checkerboard-like pattern of checks with alternating values of work function, and for checks with randomly assigned work function. A very large number of MD based simulations for different operating parameters and configurations were used to generate data on beam current, emittance and brightness as well as on the charge distribution from the cathode. We could demonstrate how these parameters are dependant on both the granularity of the cathode structure and on it degree of disorganization. Furthermore, we could qualitatively explain these results in terms of our previous work on field emission from finite areas with uniform work function, and in terms of our understanding of mutual space-charge effects between neighboring field emitters as described previously in this summary.

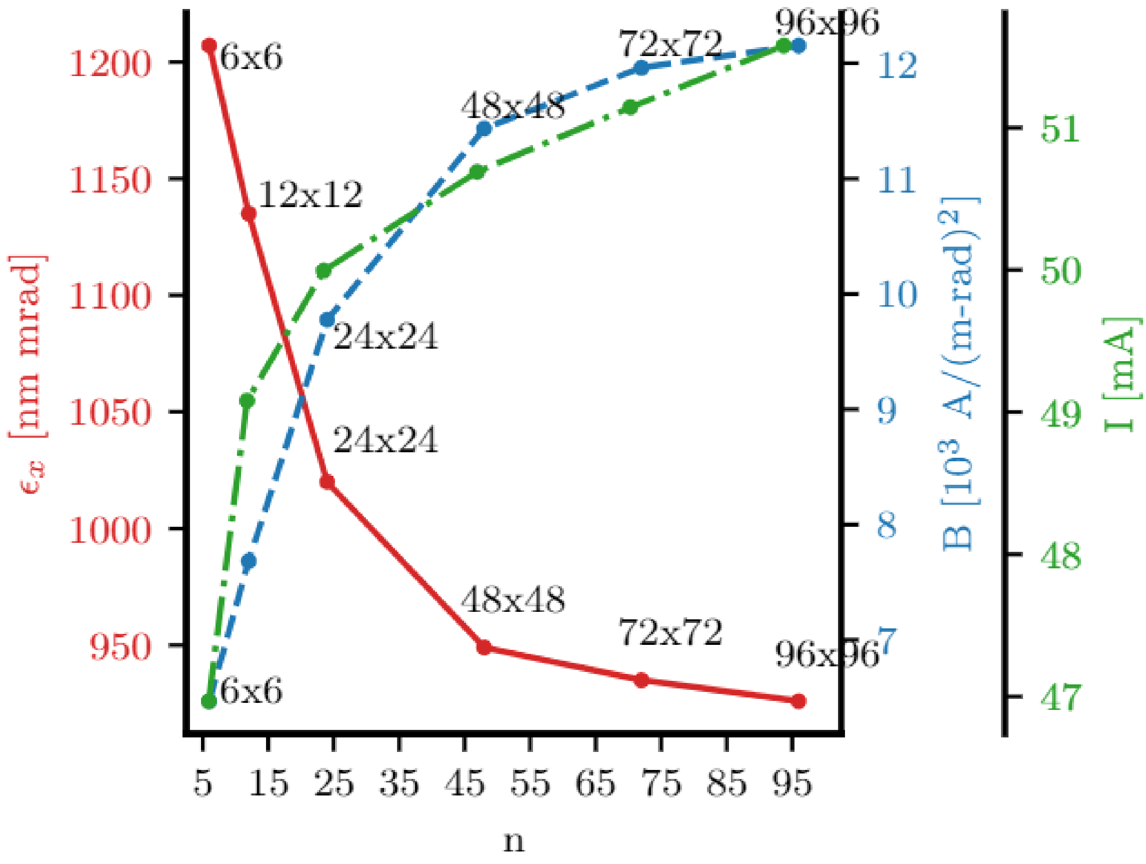

Figure 4. Emittance and brightness as a function of *N* of the checkerboard size *N*×*N*. The red line shows the emittance, the blue line shows the brightness, and the green line the current.

An interesting result was that a low work function cathode with a small number of widely distributed patches with high work function provided a higher quality beam in terms of current and brightness, than a similar cathode with uniformly low work function.

This work was published in the IEEE Transactions on Electron Devices and presented at ICOPS 2019 and ICOPS 2020.

Thermal-field emission

The primary motivation for this work was a visit to Patrick Soukiassians lab at CEA-SACLAY in November 2018 where Ágúst Valfells and Kristinn Torfason met with Dr. Soukiassian, John Boeckl, Tyson Back, and Ludovic Doulliard. There we learned about their capabilities with LEEM/PEEM experiments and the possibility of understanding emission from thermionic cathodes with a heterogeneous work function. The work was also motivated by discussions in 2017 with Y.Y. Lau and his collaborators regarding how the Miram curve describing current-temperature characteristics from a thermionic cathode might be affected by cathode heterogeneity.

Work on modifying the MD code to enable efficient simulation of thermionic emission up to the space-charge limit began in February 2019. It was primarily done by Dr. Anna Sitek and Kristinn Torfason. Dr. Sitek subsequently carried out validation of the code and conducted the simulations of thermal-field emission from a microscopic emitter with heterogeneous work function, similar to that used for simulations of field emission from an inhomogeneous cathode.

The results of our simulations were in line with the results of Dr. David Chernin et al. which were published earlier in 2020. Namely, we observed how, as temperature was increased, the current came initially almost solely from those areas with low work function. As the temperature was increased further more current was emitted from areas of higher work function. In turn space-charge forces caused the current from the low work function regions to peak and subsequently decrease as current density became uniform throughout the interior of the emitting area. The physics of this process can be explained in terms of mutual space-charge interaction and the results of our work on the two-dimensional Child-Langmuir law described above.

Additionally, we observed that there is an optimum temperature for brightness of the beam being emitted; that rounding of the Miram curve is not only due to inhomogeneity of the work function on the cathode, but can also come due to edge effects if the emitter is of finite size; and we showed how the beam quality improved (in terms of current density and brightness) as the cathode became more fine-grained.

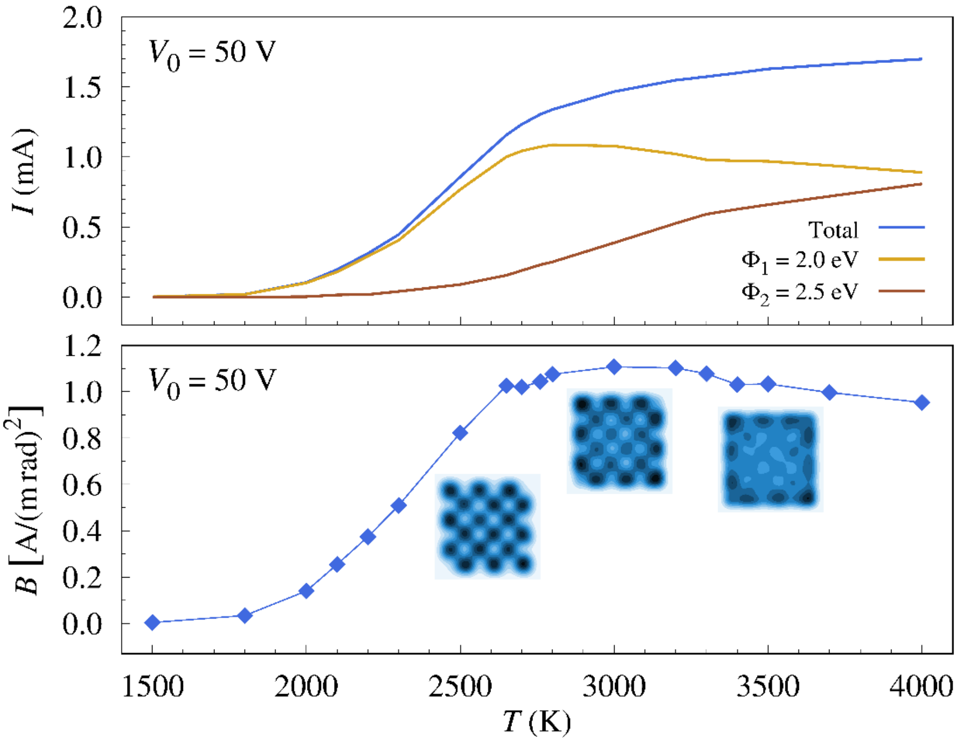

Figure 5. Current (top) and brightness (bottom) as a function of temperature. In the top figure the total current is displayed separately from the current from low and high work function areas. In the bottom figure the electron density at the cathode can be seen for three different temperatures.

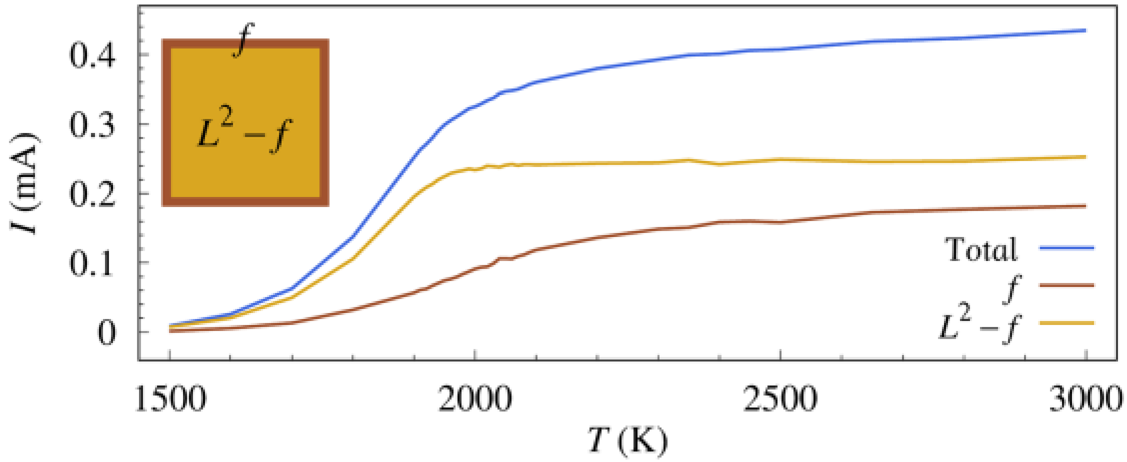

Figure 6. The total current (blue) from a square emitting area with a uniform work function and side length L = 3µm of uniform work functiion, shown with partial currents stemming from the frame region of width t = 0.167µm (brown) and interior region (yellow).

This work was published in two articles in Physical Review Applied (one of which was selected as an Editor's Suggestion) and at ICOPS 2020.

Ion effects

From initial simulations, we observe that presence of a background gas in the microdiode (gap spacing 1µm, side length of emitter area is 1µm) has an effect on the current. Even in the absence of ionization, collisions with a background gas increase the field emitted current in a diode. This is presumably due to scattering of the electrons that leads to more transverse spreading of the electrons and subsequently less space charge directly above the emitting area. Ionization causes further increase in the diode current. Ionization further increases the current due to a positive charge layer forming in front of the cathode. A two time-step propagation model has been introduced to efficiently model ion motion in a consistent manner with electron emission and propagation, and a recombination model is being developed. With these two models in place, we will proceed with examining ion effects on the diode dynamics for a longer time scale than has been done heretofore with our basic ionization and scattering model.

Some of this work was presented at ICOPS 2019.

Photoemission, CNT-fibres, and other related work

Hákon Örn Árnason has, as a part of his doctoral studies, been simulating photoemission from a microscopic emitter. His first efforts are on the effects of laser pulse-length and amplitude on electron emission and propagation from a planar emitter of about one micron in length-scale. Initial results indicate that for a given laser amplitude and a variable pulse duration, that is short compared to the time it takes for electrons to transit the anode-cathode gap, there is exists a pulse length that gives maximum brightness for the electron beam bunch that is emitted. Hákon will also look at the effects of heterogeneous cathode surfaces on beam quality for photoemission in a similar vein as was done previously for thermionic and field emission.

Yuan Zhou has recently joined the Reykjavík University Nanophysics Group as a doctoral student. She is currently modelling charge induced on a CNT fibre (represented simply as a conducting cylinder) due to a free external charge. Using these results, she will examine the suitability of extending the image charge approach that we successfully used in our MD code to more general emitter geometries.

Kristinn Torfason is currently conducting simulations on electron emission from LaB_6 using work function data from John Boeckl and Tyson Back. We will present preliminary results at ICOPS 2022.

Collaboration

Research activity on this project began with a visit by Ágúst Valfells and Dr Kristinn Torfason to CEA-Saclay from November 14th – 16th 2018 supported by an Erasmus grant. The purpose of this trip was to meet Dr John Boeckl and Dr Tyson Back, who were conducting LEEM/PEEM experiments in the laboratory of Dr Patrick Soukiassian. Currently, Kristinn Torfason is modelling emission from LaB_6 based on work function data provided by Dr Boeckl and Dr Back.

Ágúst Valfells, Kristinn Torfason, and Anna Sitek attended a workshop on cathodes organized by Dr. John Harris at AFRL Albuquerque in December 2019. Several ideas for experiments were discussed, with the most promising ones aimed at investigating mutual space charge effects between emitters in close proximity. This trip was financed by the AFOSR grant.

We have collaborated with Professor Allen Garner of Purdue University on various scientific issues, including his ongoing experiments on the effects of ions present in the vacuum gap of a microscale diode, on electron emission. Amanda Loveless, a Ph.D. student of Professor Garner, worked on simulations of ion effects.

Dr Nicolina Pop from the University of Timisoara, Romania, visited Reykjavík University, supported by Erasmus funding. She shared her expertise on ionization and recombination in low temperature plasmas, which helped us to introduce appropriate models for those processes into our code.

There have been several meetings (teleconferences and physical meetings at conferences) discussing collaboration. One particular field of interest has been modelling of field emission from CNT-fibres. The plan has been to use DFT simulations by Dr. Renee van Ginhoven at Sandia Labs as a basis for surface potential models in the emission code. Unfortunately, this has not been completed but we hop that it can be done in a follow up project.

The Covid pandemic has disrupted collaboration in 2020 and 2021. Administrative and organizational load at Reykjavík University and partner institutions has drastically increased and travel restrictions have limited opportunities for visits and attendance at scientific connferences and workshops.

Financial report

The following table shows monthly cash flow for the project. All amounts are in Icelandic *króna* (except when otherwise indicated). The exchange rate with the dollar has varied over the grant period as can be seen from the table. Please note the abbreviations used in the *remarks* column: **AS**, **KT**, **JBG**, **HVH**, refer to salary and payroll costs for Anna Maria Sitek, Kristinn Torfason, Jóhannes Bergur Gunnarsson, and Hákon Valur Haraldsson respectively. All costs are related to salaries except for ISK 651.118 paid in December 2019 for travel and accommodation in connection with the cathode workshop at Kirtland Air Force Base attended by Ágúst Valfells, Kristinn Torfason and Anna Sitek. It took somewhat over 4 months to hire a research scientist after receiving the grant. Thus, Anna Sitek commenced work on the project in mid-February 2019. Note that there was a 6-month period when no salaries were drawn from this grant as Anna Sitek and Kristinn Torfason had other duties, and as a result, the work was extended for 6 months beyond the original period. The 116.441

ISK that have not yet been allocated will be used to pay part of one month's salary for Yuan Zhou, who is working on the CNT fibre modelling and is partially funded by Reykjavík University.

Period	**Payments received**	**Payments made**	**Remarks**
October 2018	7,078,800.00	0	$60,000 from funding agency
November 2018	0	0	
December 2018		0	
January 2019		0	
February 2019		273,606	AS (1/2 month)
March 2019		547,211	AS
April 2019	7,326,000.00	547,211	$60,000 from funding agency, AS
May 2019		547,211	AS
June 2019		931,069	JBG + AS
July 2019		547,211	AS
August 2019		547,211	AS
September 2019		547,211	AS
October 2019		931,069	HVH + AS
November 2019		931,069	HVH + AS
December 2019		1,198,329	AS, Albuquerque trip
January 2020		547,211	AS
February 2020		547,211	AS
March 2020		547,211	AS
April 2020		547,211	AS
May 2020	2,199,150	547,211	$15,000 from funding agency, AS
June 2020		547,211	AS
July 2020		547,211	AS
August 2020		547,211	AS
September 2020		547,211	AS
October 2020		1,094,422	AS + KT
November 2020		1,094,422	AS + KT
December 2020		1,094,422	AS + KT

January 2021			
February 2021			
March 2021	5,721,300		$15,000 from funding agency
April 2021			
May 2021			
June 2021			
July 2021		555,096	KT
August 2021		555,096	KT
September 2021		555,096	KT
October 2020		555,096	KT
November 2020		555,096	KT
December 2020		555,096	KT
January 2021		780,415	KT
February 2021		780,415	KT
March 2021		780,415	KT
April 2021		780,415	KT
All	22,325,250	22,208,809	

Output

In this chapter, we describe some of the main conclusions of each of the research subjects. A more thorough treatment will be given in the planned journal papers.

Code improvements

The capabilities of the MD code improved significantly in work done under this grant. A combined thermionic-field emission model based on the work by Jensen [1] was implemented in the code. A model for scattering and ionization of nitrogen gas was introduced based on empirical data [2,3]. A two time-scale propagation model has been introduced to account for the different mobility of electrons and ions in the system. A model for recombination and electron attachment is underway. Post-processing capabilities have been extended to improve diagnostics of the electron beam. This includes tracking of individual electrons in phase space to better understand the dynamics of emittance growth, brightness and I-V characteristics due to heterogeneity. Adaption to GPU use has begun, though it is only incipient. Image charge models for generalized cathode geometries

Dissemination

Journal publications

1. A. Sitek, K. Torfason, A. Manolescu, Á. Valfells, "Edge Effect on the Current-Temperature Characteristics of Finite-Area Thermionic Cathodes ", *Phys. Rev. Applied*, doi: 10.1103/PhysRevApplied.16.034043 (2021).
2. K. Torfason, A. Sitek, A. Manolescu, Á. Valfells, "Dynamics of a Field Emitted Beam From a Microscopic Inhomogeneous Cathode", *IEEE Transactions on Electron Dev.*, doi: 10.1109/TED.2021.3063210 (2021).
3. 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 Dynamic Effects", *J. Appl. Phys.*, doi:10.1063/5.0042355 (2021). (**INVITED, FEATURED**)
4. A. Sitek, K. Torfason, A. Manolescu, and Á. Valfells, "Space-Charge Effects in the Field-Assisted Thermionic Emission from Nonuniform Cathodes", *Phys. Rev. Applied.*, **15**, 014040 (2021). (**EDITOR'S SUGGESTION**)
5. J.B. Gunnarsson, K. Torfason, A. Manolescu, and Á. Valfells, "Space-Charge Limited Current from a Finite Emitter in Nano- and Microdiodes", *IEEE Transactions on Electron Dev.*, **68**, 342 (2021).
6. H.V. Haraldsson, K.Torfason, A. Manolescu, and Á. Valfells, "Molecular Dynamics Simulations of Mutual Space-Charge Effect Between Planar Field Emitters", *IEEE Trans. Plasma Sci.*, **48**, 1967 (2020).

Conference Presentations

1. J.B. Gunnarsson, K. Torfason, A. Manolescu, and Á. Valfells, "Deviation from the 2-D Child-Langmuir Law at the Microscale", ICOPS 2020, Singapore December 6 – 10 2020.
2. K. Torfason, A. Sitek, Á. Valfells, and A. Manolescu, "Effects of Surface Inhomogeneities in Field and Thermal-Field Emission", ICOPS 2020, Singapore December 6 – 10 2020.
3. K. Torfason, Á. Valfells, A. Manolescu, "Simulations of Surface Inhomogeneities in Field Emission", ICOPS, 2019, Orlando, FL, USA, June 23-28 2019.
4. A. Loveless, K. Torfason, Á. Valfells, A. Garner, "Investigation of Electron Emission using Molecular Dynamics Simulations", ICOPS, 2019, Orlando, FL, USA, June 23-28 2019.

Other

1. Á. Valfells, A. Manolescu, A. Sitek, H.V. Haraldsson, J.B. Gunnarsson, and K. Torfason, "Molecular dynamics based simulations of emission and propagation at the microscale", talk given at cathode workshop, Albuquerque, December 2019.
2. Á. Valfells, "Molecular dynamics simulations of vacuum diodes", talk given during visit to CEA, Saclay, France, November 2019.

The molecular dynamics code has been shared with Dr Allen Garner at Purdue University and Dr Travis Garrett at AFRL. A user handbook is being updated.

References

[1] K.L. Jensen, *Introduction to the Physics of Electron Emission*, (John Wiley and Sons, Hoboken New Jersey, 2018).

[2] Y. Itikawa, Cross Sections for Electron Collisions with Nitrogen Molecules, *Journal of Physical and Chemical Reference Data*, **35**, 31 (2006).

[3] J.C. Nogueira, M.A. Eschiapati Ferreira, Doubly Differential Cross Section for Electrons Scattered by Nitrogen, *Brazilian Journal of Physics*, **25**, 14 (1995).