Miniworkshop on Surface Science and Field Electron Emission

This mini-workshop aims at introducing a new research line of the Surface Science group at the Physics Institute of Universidade Federal Fluminense: Field Electron Emission Science. The workshop brings together scientists from around the world who work in this area and in related problems, facilitating discussion and interaction on various topics, including fundamental physics, computational simulation, instrumentation, and experimental work. The list of speakers includes Prof. Thiago de Assis, who will be soon hired at that Physics Institute, and Dr. Richard Forbes, who is a visiting researcher of a PrInt/CAPES project from 12 September to 5 October 2024. The organizers of the mini-workshop thank all the speakers for accepting the invitation to present their works and wish that the event be successful for advancing international cooperation in the area and advancing the research in our Institute.

Fábio David Alves Aarão Reis

General Chair - Miniworkshop on Surface Science and Field Electron Emission

This workshop is financially supported by CAPES and FAPERJ.

Date: Thursday (09/19/2024)

Time: 9 a.m. – 5 p.m. (Physics Institute – Universidade Federal Fluminense – Niterói – Rio de Janeiro - Brazil)

Program

(9:00 a.m.) **Nonequilibrium Statistical Physics at Surfaces and Interfaces**, Fábio David Alves Aarão Reis (IF-UFF) [Pg. 3]

(9:30 a.m.) **Field Electron Emission Theory and Its Future**, Richard Gordon Forbes (University of Surrey - U.K.) [Pg. 4]

Coffee Break (10:15 a.m. – 10:35 a.m.)

(10:35 a.m.) **Field emission microscopy as a tool for characterizing scanning probe microscopy,** Alexandr Knápek (Institute of Scientific Instruments of the Czech Academy of Sciences - Czech Republic) [Pg. 5]

(11:05 a.m.) **Multi-scale simulations for electron emission and diffusion from metal surfaces under high electric field**, Andreas Kyritsakis (University of Tartu, Faculty of Science and Technology, Institute of Technology – Estonia/ Helsinki Institute of Physics and Department of Physics, University of Helsinki -) [Pg. 6]

(11:35 a.m.) **Improved Method of Calculating Apex Fields for an Array of Identical Carbon-Nanotube-Like Posts in Close Proximity to a Counterelectrode**, Thiago Albuquerque de Assis (IF-UFBA/IF-UFF - Brazil) [Pg. 7]

12:05 p.m – 2:00 p.m. Lunch

(2:00 p.m.) **Field electron emission: Modern tasks and open challenges**, Sergey Filippov (Ioffe Institute – St. Petersburg - Russia) [Pg. 8]

(2:30 p.m.) **Towards a new class of AlGaN/GaN vacuum field effect transistors**, Marc Cahay/Nathaniel Hernandez (Spintronics and Vacuum Nanoelectronics Laboratory, University of Cincinnati; Wright-Patterson Air Force Base, OH - USA) [Pg. 9]

(3:00 p.m.) **Characteristics from Bendable Single Tip Field Emitters**, Fernando Fuzinatto Dall'Agnol (UFSC Blumenau - Brazil) [Pg. 10]

(3:30 p.m.) **Nanowire-, nanoring-, and crack-template-based transparent conductive films: Mean-field approach and computer simulations of effective electrical conductivity of random metallic nanowire networks**, Yuri Yu. Tarasevich (Astrakhan State University, Astrakhan - Russia/IF-UFF - Brazil) [Pg. 11]

Coffee Break (4:00 p.m. – 4:20 p.m.)

Discussion Session (4:20 p.m. – 5p.m.)

- **(4:20 p.m.) Field Emission Properties of Cold Rolled Graphene Sheets Prepared by Chemical Vapor Deposition,** Nathaniel Hernandez (Spintronics and Vacuum Nanoelectronics Laboratory, University of Cincinnati; Wright-Patterson Air Force Base, OH - USA)
- **(4:35 p.m. – 5:00 p.m.) Future projects and prospects.**

Nonequilibrium Statistical Physics at Surfaces and Interfaces

Fábio David Alves Aarão Reis

Physics Institute, Fluminense Federal University, Avenida Litorânea, 24210-340,
Niterói, RJ, Brazil

This talk summarizes the recent work of my multi-institutional research group, which uses computational and analytical methods to study far from equilibrium Statistical Physics problems at surfaces and interfaces. The applications to be presented include: deposition of semiconductor films from vapor; metal electrodeposition; mineral (especially calcite) growth and dissolution in laboratory and natural conditions; anomalous diffusion and infiltration (if time permits).

The author's research is supported by FAPERJ, CNPq, and CAPES.

Field Electron Emission Theory and Its Future

R. G. Forbes

Quantum Foundations and Technologies Group, School of Mathematics and Physics,
University of Surrey, Guildford, Surrey GU2 7XH, UK

Field electron emission (FE) is a quantum tunnelling process in which electron tunnelling is induced by a high negative electrostatic (ES) field, typically about –3 V/nm. FE has scientific importance in its own right, but also has important technological applications. This presentation relates to the theory of field electron emission, with a focus on the theory of current-voltage characteristics and on the theory of electron transmission probability. For those with limited familiarity with FE, the initial part of the presentation will provide a brief introduction to the theory, applications and significance of FE.

Then, after a brief survey of where we have got to after about 100 years of investigation, the intention is to present and discuss a high-level roadmap for what (in the author's view) needs to be done in order to put the basic principles of FE theory onto a more sophisticated and complete scientific basis.

In general terms, the author has already suggested four immediate priorities: (1) work on removing entrenched errors and weak practice from FE technological literature; (2) systematic research on aspects of FE systems engineering [i.e., effects (*other than* emission theory) that influence measured current-voltage [$I_m(V_m)$] characteristics]; (3) further research on how to make reliable comparisons between FE theory and experiment; (4) further development of emission theory and of related issues concerning $I_m(V_m)$ data analysis for electronically ideal emitters, taking so-called "Extended Murphy-Good (EMG) FE theory" as the starting point.

Although there is an important need to understand the theory of FE from non-metallic materials such as complex semiconductors and carbon materials (particularly nanotubes and graphene), and from "rough surfaces", and from two-dimensional materials, the best route forwards seems to lie in better understanding of FE from metal surfaces.

As regards item (4) above, the route forwards seems to have two main branches: (a) consolidation of emission theory and validity tests for sharply curved smooth-surface emitters, based on the existing work of Kyritsakis [1] and others; and (b) "getting atoms into the theory" for atomically flat metal surfaces (for example, see [2]). For (a) a necessary preliminary for $I_m(V_m)$ data analysis is to move from the use of data-analysis plots (such as the Fowler-Nordheim plot) to the use of numerical multi-linear regression. For (b) first steps are: to move away from the use of JWKB formulae to the use of completely numerical procedures, both for the evaluation of transmission probabilities and for integration with respect to normal-energy; to consolidate comparisons of the two types of theory; and to deal with detailed technical issues relating to smooth-planar-surface models.

Beyond this, one needs to explore the details of "getting atoms into the theory", in particular how to choose "paths of numerical integration", how to carry out the integrations, and how to "sum over paths". But, before attempting this for "atoms in charged surfaces", it seems advisable to look again at the related (but simpler) problem of the theory of the field ionization of hydrogenic ions, both in free space and when close to a metal surface.

Fundamental problems seem to arise if one seeks to model exchange-and correlation effects in a manner that is more sophisticated than use of the image potential-energy approximation within the context of the usual quantum-mechanical approaches to evaluating transmission probability. Some apparent problems will be indicated.

[1] KYRITSAKIS, A; DJURABEKOVA, F. A general computational method for electron emission and thermal effects in field emission nanotips. *Computational Mater. Sci.* 2017, 128: 15.

[2] LI, Y.-M.; MANN, J.; ROSENKREITZ, J. Modeling field electron emission from a flat Au (100) surface with density-functional theory. *Instruments* 2023,7: 47.

Field Emission Microscopy as a Tool for Characterizing Scanning Probe Microscopy

A. Knápek, D. Burda, M. Allaham, Z. Košelová, L. Dupák and D. Sobola

Institute of Scientific Instruments of the Czech Academy of Sciences
Královopolská 147, Brno, 612 00, Czech Republic

This talk will present the design and construction of a customized field emission microscope for the analysis of scanning probe microscopy (SPM) probes, namely AFM (atomic force microscopy) and STM (scanning tunneling microscopy) [1,2]. The field emission current from the probe is used here to characterize the probe and to express the formal emission surface area parameter (AFSN), which can be directly correlated to the probe quality [3,4]. For a scanning probe tip, the parameter reflects the size and shape of the region from which electrons tunnel to the sample surface. If this area is larger than expected or desirable, it may indicate problems with tip function or wear [4]. Since scanning probes typically have a functional layer on the surface that fundamentally affects the function of the probe [4,5], the discussion will cover three key areas of comparative analysis in scanning probe microscopy:
(1) the enhancement of tungsten STM probes with graphite coatings, which significantly improve conductivity and sensitivity even under non-ideal vacuum conditions; (2) the benefits of gold coatings applied to non-conductive AFM probes, resulting in improved surface conductivity and more linear field emission characteristics; and (3) the challenges faced by platinum-coated conductive AFM probes, in particular the destructive failures caused by excessive current and overheating. The presentation will emphasize how strategic coating choices can enhance the functionality and reliability of SPM probes and provide deeper insights into their applications in modern microscopy.

[1] D. Burda, Daniel *et al*., "Conductively Coated 3D Printed Emitters for Electron Devices," in Proceedings of IEEE 37th International Vacuum Nanoelectronics Conference (IVNC), 2024 Brno, Czech Republic, 2024, ISBN: 979-8-3503-7975-4.
[2] A. Knápek, *et al.* Programmable set-up for electrochemical preparation of STM tips and ultra-sharp field emission cathodes. Microelectronic Engineering, 2017, 173: 42-47.
[3] M. M. Allaham, *et al.* Interpretation of field emission current–voltage data: Background theory and detailed simulation testing of a user-friendly webtool. Materials Today Communications, 2022, 31: 103654.
[4] A. Knápek, *et al.* Comparative analysis of surface layer functionality in STM and AFM probes: Effects of coating on emission characteristics. Journal of Electrical Engineering, 2024, 75.4: 268-274.
[5] Z. Košelová, *et al.* Cleaning of tungsten tips for subsequent use as cold field emitters or STM probes. Journal of Electrical Engineering, 2024, 75.1: 41-46.

The described research was supported by the Czech Technology Agency (FW03010504) within the infrastructure provided by the Czech Academy of Sciences (RVO:68081731).

Multi-scale simulations for electron emission and diffusion from metal surfaces under high electric field

A. Kyritsakis

Institute of Technology, University of Tartu, Nooruse 1, 50411 Tartu, Estonia

Helsinki Institute of Physics and Department of Physics, University of Helsinki, PO Box 43, 00014 Helsinki, Finland

Applying a high electric field changes the electronic and the inter-atomic dynamics of surfaces, inducing electron and ion emission, biased atomic diffusion and evaporation, and, in extreme cases, the initiation of plasma. Although these effects can be exploited (e.g. electron and ion sources), they can become uncontrollable, leading to detrimental effects such as vacuum breakdown. The reliable function of high-electric-field devices such as electron sources, particle accelerators, high-voltage equipment, etc, requires an accurate understanding of the electron emission physics and the dynamics of surfaces under high electric fields.

This talk gives an overview of recent advances in the theory and simulation capabilities in three directions. First, the accurate calculation of electron emission from complex surfaces, based on first principles; second, the dynamics of atomic diffusion and evaporation on metal surfaces under high electric fields; and third, the dynamics of intensively emitting tips, their thermal runaway, and plasma ignition based on concurrently coupled Electrodynamics, Molecular Dynamics, and Particle In Cell simulations. These advancements are based on the development of a constellation of highly interlinked multi-scale multi-physics computational models and corresponding software, based on our software "FEMOCS," which concurrently couples finite element-based computations of electrodynamics and thermal effects with particle-in-cell plasma simulations as well as molecular dynamics. FEMOCS also provides the basic framework for ab-initio based simulation of the atomic diffusion on metal surfaces under field, and is also connected with the general tool for electron emission calculations, "GETELEC".

Improved Method of Calculating Apex Fields for an Array of Identical Carbon-Nanotube-Like Posts in Close Proximity to a Counterelectrode

T. A. de Assis[1,2], R. G. Forbes[3] and F. F. Dall'Agnol[4]

[1]Physics Institute, Federal University of Bahia, Campus Universitário da Federação,
Barão de Jeremoabo st., 40170-115, Salvador, BA, Brazil
[2]Physics Institute, Fluminense Federal University, Avenida Litorânea, 24210-340,
Niterói, RJ, Brazil
[3]Quantum Foundations and Technologies Group, School of Mathematics and Physics, Faculty of Engineering and Physical Sciences,Institute of Physics, University of Surrey GU2 7XH, UK
[4]Department of Exact Sciences and Education, Federal University of Santa Catarina, 89036-004,
Blumenau, Santa Catarina, Brazil

In cold field electron emission (FE), the applied electrostatic field is an important parameter to model an ideal FE device. It is necessary to define the local field enhancement factor (FEF), arguably the most analyzed parameter to assess the performance of an emitter. However, a consistent definition of the applied field is not straightforward, since the local field distribution is not uniform in the FE device due to the presence of the protruded emitter and its electrostatic interaction with other emitters and the counter-electrode. In this talk, we discuss a consistent definition of the applied electrostatic field that takes into account a weighed distance between the emitter plate and the counterelectrode that, in turn, accounts for the field penetration within the emitters in a regular array. We point out the advantages regarding the FEF and the issues with defining the applied field that does not consider the field penetration [1].

[1] T. A. de Assis, F. F. Dall'Agnol and R. G. Forbes "Alternative Definition of the Apex Field Enhancement Factor for a Regular Array of Electrostatically Interacting Post Emitters" in Proceedings of IEEE 37th International Vacuum Nanoelectronics Conference (IVNC), 2024 Brno, Czech Republic, 2024, ISBN: 979-8-3503-7976-1.

This work was supported by CNPq and CAPES.

Field Electron Emission: Modern Tasks and Open Challenges

S. V. Filippov[1], A. G. Kolosko[1], E. O. Popov[1], F. F. Dall'Agnol[2] and T. A. de Assis[3,4]

[1]Division of Plasma Physics, Atomic Physics and Astrophysics Ioffe Institute, Saint-Petersburg, Russia
[2]Department of Exact Sciences and Education, Federal University of Santa Catarina, 89036-004,
Blumenau, Santa Catarina, Brazil
[3]Physics Institute, Federal University of Bahia, Campus Universitário da Federação,
Barão de Jeremoabo st., 40170-115, Salvador, BA, Brazil
[4]Physics Institute, Fluminense Federal University, Avenida Litorânea, 24210-340,
Niterói, RJ, Brazil

Nowadays, many prototypes of vacuum devices, such as miniature mass spectrometers, disinfecting ultraviolet and mercury-free lighting lamps, as well as touch and pressure sensors, have been developed based on field electron emitters. The choice of a particular field emitter for a final device depends on its operational characteristics, including: the threshold field for the onset of emission, the maximum possible emission current, and the uniformity of the distribution of active emission sites over the surface. These characteristics, in turn, depend on three emission parameters that simultaneously affect the magnitude of the emission current: local work function, formal emission area, and the local field enhancement factor. All of these parameters are incorporated into the corrected form of Fowler-Nordheim field electron emission (FE) theory, initially developed by Murphy and Good in 1956 [1,2]. This talk reviews modern tasks and open challenges (both theoretical and experimental) that remain in FE science [3]. It addresses issues related to the experimental measurement of FE properties of large-area field emitters (LAFEs) and discusses methods for optimizing the FE properties of single-tip emitters and homogenizing the emitted current of LAFEs.

[1] R. G. Forbes, "Simple good approximations for the special elliptic functions in standard Fowler-Nordheim tunneling theory for a Schottky-Nordheim barrier," Appl. Phys. Lett., vol. 89, no. 11, pp. 113122-113122–3, 2006, doi: 10.1063/1.2354582.
[2] R. G. Forbes and J. H. B. Deane, "Reformulation of the standard theory of Fowler– Nordheim tunnelling and cold field electron emission," Proc. R. Soc. Math. Phys. Eng. Sci., vol. 463, no. 2087, pp. 2907–2927, 2007, doi: 10.1098/rspa.2007.0030.
[3] S. V. Filippov, A. G. Kolosko, E. O. Popov, R. G. Forbes, "Field emission: calculations supporting a new methodology of comparing theory with experiment," Roy. Soc. Open Sci. vol. 9, p. 220748, 2022, doi: 10.1098/rsos.220748.

This work was partially supported by CNPq and CAPES.

Towards a New Class of AlGaN/Ga Vacuum Field Effect Transistors

N. Hernandez[1,3], M. Cahay[1,3], J. Ludwick[2,3], T. Back[2], J. O'Mara[4,5], H. Hall[4] and D. E. Walker Jr.[4]

[1]Spintronics and Vacuum Nanoelectronics Laboratory, University of Cincinnati, Cincinnati, OH, USA
[2]Air Force Research Laboratory, Materials Manufacturing Directorate,
Wright-Patterson Air Force Base, OH, USA and
[3]UES, 2179 12th St, Wright-Patterson Air Force Base, OH, USA
[4]Air Force Research Laboratory, Sensors Directorate, Wright-Patterson Air Force Base, OH, USA
[5]KBR, 4027 Colonel Glenn Hwy Suite 301, Beavercreek, OH, USA

In this work, we describe our recent work towards the development of AlGaN/GaN Heterostructure based Vacuum Field Effect Transistors (VacFETs). Our research aims to develop high current density VacFETs with applications in high-frequency and high-power systems, gas and chemical sensing, and devices operating in harsh environments. Our multifaceted approach combines simulation techniques, state-of-the-art fabrication methods, and rigorous experimental characterization. In the past, we have proposed a VacFET that consists of a modification of a conventional AlGaN/GaN high electron mobility transistor to include a nanogap near the gate on either the source (cathode) or drain (anode) side of the device [1]. When compared to other recently fabricated VacFETs, the proposed device has potential for much higher emission current densities and transconductance levels, of the order of several hundreds of mA/mm and tens of mS/mm, respectively. For similar material parameters and physical dimensions, the proposed VacFET has a turn-on voltage that depends on the location of the nanogap on either the source or drain side of the gate. It is shown that the current–voltage characteristics of VacFETs with a nanogap either on the drain or source side of the gate are highly sensitive to their physical parameters and biasing conditions, making them a very strong candidate for chemical or gas sensing applications. This is due to the sensitivity of the tunneling current to the effective barrier height and field enhancement factor of the nanogap.

Recently, we reported the design, fabrication, and measurement of the field emission (FE) characteristics of AlGaN/GaN nanoscale lateral vacuum diodes with triangular cathodes and cathode to anode spacings from 50 to 600 nm [2]. The FE characteristics of the AlGaN/GaN diodes with metallic or AlGaN/GaN anodes show successful rectification with forward bias FE current in the range of microamperes or milliamperes, respectively, when biased within a maximum range varying from 10 to 30 V. In the forward bias mode, the measured current Im vs applied anode to cathode bias Vm are well fitted to Murphy–Good profiles associated with FE at higher biases, and an Ohmic leakage profile below the threshold for FE. Our results are the first successful demonstration of FE of electrons between the two two-dimensional electron gases (2DEGs) present on both sides of a nanogap formed by electron lithography through an AlGaN/GaN heterojunction. A qualitative explanation of the loop-type FE characteristics of both AlGaN/GaN vacuum diodes, with either metallic or AlGaN/GaN anodes, is presented.

Finally, we will describe our current effort towards the fabrication of gated AlGaN/GaN FE devices, exploring both side-gated and top-gated configurations, including an optimization of the gate geometry and placement to achieve maximum emission current modulation and device efficiency.

[1] Nathaniel Hernandez, Marc Cahay, Jonathan Ludwick, Tyson C. Back, Harris Hall, and Jonathan O'Mara. Physics based model of an AlGaN/GaN vacuum field effect transistor. J. Vac. Sci. Technol. B, 40(5):053201, September 2022. doi:10.1116/6.0001959.

[2] Nathaniel Hernandez, Marc Cahay, Jonathan O'Mara, Jonathan Ludwick, Dennis E. Walker, Jr., Tyson Back, and Harris Hall. Field emission characteristics of AlGaN/GaN nanoscale lateral vacuum diodes. J. Appl. Phys., 135(20):204305, May 2024. doi:10.1063/5.0204235.

Characteristics from Bendable Single Tip Field Emitters

J. Ludwick[1,2], F. F. Dall'Agnol[3], N. Hernandez[4,2], G. Tripathi[4], T. A. de Assis[5,6], T. Back[1] and M. Cahay[4,2]

[1]Air Force Research Laboratory, Materials Manufacturing Directorate,
Wright-Patterson Air Force Base, OH, USA and
[2]UES, 2179 12th St, Wright-Patterson Air Force Base, OH, USA
[3]Department of Exact Sciences and Education, Federal University of Santa Catarina, 89036-004,
Blumenau, Santa Catarina, Brazil
[4]Spintronics and Vacuum Nanoelectronics Laboratory, University of Cincinnati, Cincinnati, OH,
USA
[5]Physics Institute, Federal University of Bahia, Campus Universitário da Federação,
Barão de Jeremoabo st., 40170-115, Salvador, BA, Brazil
[6]Physics Institute, Fluminense Federal University, Avenida Litorânea, 24210-340,
Niterói, RJ, Brazil

Field emission characteristics of emitters are influenced by their flexibility, as bending under applied electrostatic fields can significantly increase the characteristic field enhancement factor (FEF), and emission current. Recent experiments on carbon-based emitters reveal a systematic non-linearity in the Murphy-Good plot of their field emission data, suggesting significant bending under high applied electrostatic fields. However, this effect has not been thoroughly studied. In this talk, we numerically investigate the impact of electrostatic forces on the field emission properties of a flexible emitter as a function of the applied electrostatic field, the aspect ratio of the emitter, and its initial angle of inclination with the substrate. The characteristic FEF of a flexible emitter increases from while ramping-up the applied electrostatic field. Our analysis leads to a figure of merit, that quantifies the effect of the flexibility on the emission characteristics. Our analysis could potentially spark the development of new field electron emission technologies that explores the sharp emission current growth due to the variation in the characteristic FEF.

This work was partially supported by CNPq and CAPES.

Nanowire-, nanoring-, and crack-template-based transparent conductive films: Mean-field approach and computer simulations of effective electrical conductivity of random metallic nanowire networks

Yuri Yu. Tarasevich[1,2]

[1]Astrakhan State University, Astrakhan, Russia
[2]Institute of Physics, Fluminense Federal University, Avenida Litorânea, 24210-340,
Niterói, RJ, Brazil

Transparent conductive films (TCFs) are widely used for creating displays and touch screens, solar cells, transparent heaters, flexible and stretchable electronics, electromagnetic interference (EMI) shields, thermochromic devices, etc.

Widespread devices based on oxides, e.g., zinc oxide (ZnO), indium tin oxide (ITO), etc., have a number of significant disadvantages. For example, there are high material costs of ITO-based TCFs, indium deficiency, damage to organic substrates during sputtering, and fragility; an important disadvantage for their application in solar cells is the strong absorption of ITO in the UV and blue spectral ranges; brittleness is a serious obstacle to the use of such transparent electrodes for flexible and stretchable electronics. The listed disadvantages lead to the development of printing technologies and the creation of transparent electrodes based on templates, including natural templates and crack templates; metal nanowire-based TCFs, such as Cu, Ag, and Au nanowire electrodes, are considered to be a new generation of TCFs that are capable of replacing ITO electrodes.

As compared to regular periodic networks (square, honeycomb), the stray light energy from high-order diffractions by the random network is significantly less, which indicates the good optical performance of such random networks. In contrast to meshes with periodically aligned metal lines, random metal networks produce neither moiré nor starburst patterns.

When a potential difference is applied to two opposite boundaries of the TCF, the electrical potential varies almost linearly along the system. The main idea behind the mean-field approach (MFA) is the consideration of a sole nanowire placed in the mean electrical field produced by all the rest of the nanowires, rather than a consideration of the complete ensemble of nanowires.

The talk is devoted to application of the MFA to nanowire-based TCFs, to nanoring-based TCFs, to TCFs based on mixtures of rings and sticks, to TCFs based on curved wires, to crack-template-based TCFs, and to some artificial networks.