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Book of Abstracts

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Field Emission / 2

Theoretical study of field emission from a "real" metal surface

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A mathematical model of the electrode surface morphology was proposed and constructed, considering submicron irregularities on its surface. It is shown that the theoretical decrease in the field electron emission current density with an increase in the electron yield work from the metal does not agree well with the breakdown field experiments for different materials. It is shown that the presented model of the metal surface makes it possible to simulate the field emission current and to agree the theoretical model with the experimental results.

Topic:

Field Emission

Modelling & Simulation / 3

Numerical study of dark current dynamics and reflection and transmission phenomena in a High-Gradient Backward Traveling Wave accelerating cavity using the electromagnetic simulation software CST Studio.

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High-Gradient accelerating cavities are one of the main research lines in the development of compact linear colliders. However, the operation of such cavities is currently limited by non-linear effects that are intensified at high electric fields, such as dark currents and radiation emission or RF breakdowns.

A new normal-conducting High-Gradient S-band Backward Travelling Wave accelerating cavity for medical application ($v=0.38c$) designed and constructed at Conseil Européen pour la Recherche Nucléaire (CERN) is being tested at Instituto de Física Corpuscular (IFIC) High Power RF Laboratory. The objective consists of studying its viability in the development of compact linear accelerators for hadrontherapy treatments in hospitals.

Due to the high surface electric field in the cavity, electrons are emitted following Fowler-Nordheim equation, also known as dark currents. The emission and dynamic of these electrons are of fundamental importance on different phenomena such as RF Breakdowns or radiation dose emission.

In this work, 3D electromagnetic numerical simulations have been performed using the computer simulation technology software CST Studio Suite. Then, the resulting EM field maps are used to study the emission and electron dynamics inside the cavity.

In addition, numerical results of the reflection and transmission phenomena have been performed when the cavity is partially filled with a plasma-like material, to simulate RF breakdowns conditions.

The simulation results are compared with experimental data and first conclusions discussed.

Topic:

Modeling and Simulations

Modelling & Simulation / 4

Simulation of High-Field Conditioning and Operation

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To synthesize the experimental results and theory pertaining to high-field phenomena, a Monte Carlo model has been developed to simulate the conditioning and operation of high-field systems. Using a grid-based approach, any arbitrary geometry and surface field distribution may be simulated in spatially resolved fashion for both RF and DC devices alike. The probabilistic behaviour of breakdown and the inhomogeneous distribution of breakdown sites are among the phenomena described by this approach. An outline of the model is presented and several results are discussed.

Topic:

Modeling and Simulations

Experiments & Diagnostics / 5

Update on High-Field Research Activities at CERN

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Alongside the numerous operational accelerators on the CERN site, several radio frequency (RF) and DC test facilities have been established to support the development of novel prototypes and investigate high-field phenomena. In these facilities, copper RF cavities are regularly operated at surface electric fields in excess of 200MV/m while DC electrodes of various materials have been tested to field levels in the tens of megavolts range. An update of these and other high-field research activities at CERN will be provided and the plans for the future detailed.

Several other activities which will be briefly featured include the application of Machine Learning analysis techniques to experimental data, the development of a novel framework for simulating the

operation of high-field devices, and breakdown studies in an operational radio frequency quadrupole (RFQ).

Topic:

Experiments and Diagnostics

Modelling & Simulation / 6

Thermal runaway and the Pre-breakdown characteristics of FCC, BCC and HCP metal nanotips under the high electric field using PIC-ED-MD simulations

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The most important physical parameter that determines the microstructure evolution in the thermal runaway and the subsequent electric pre-breakdown behaviors of nano-size metal field emitters and micro-protrusions on the metal surfaces is yet to be elucidated. In this work, we conduct a systematic multiscale-multiphysics simulations for FCC (Cu, Au and Al), BCC (Mo, W and Zr) and HCP (Ti, V and Zn) metal nano-tips (R0=1 nm and H0=100 nm) based on the latest developed PIC-ED-MD computational methodology. The structural evolution and thermal runaway mechanism are found to be decisively determined by the thermal conductivity and boiling point of metal. The nano-tip made of metal with low thermal conductivity and high boiling point (Mo, W, Zr, V and Ti), the field emission induced heating processes (Joule and Nottingham heats) lead to formation of nano-protrusion because of the continuous thinning and sharpening of the molten region at the apex of the tip, and the thermal runaway usually occurs at the tip of atomically sharp nano-protrusion. Meanwhile, the metal nanotips made of Cu, Al, Au and Zn are prone to the melting and recrystallization. The high electric-field stress exerted on the surface of nanotip strongly deforms the whole molten region, and the detachment of the large liquid droplet from the nano-tip base is prevalent during the thermal runaway process. We further apply the multi-variable linear regression method to analysis the influences of some intrinsic physical properties of metals (boiling/melting point, work function, crystal structure, surface crystallographic orientation and thermal/electric conductivity) on the pre-breakdown characteristics including on-set pre-breakdown time and the critical E-field strength. The results strongly support the use of boiling point of metals as the most decisive descriptor to indicate the pre-breakdown resilient of various metal nano-tips. A quantitative expression is also obtained between the pre-breakdown E-field and boiling point, based on the current PIC-ED-MD simulations for nine metal materials.

Topic:

Modeling and Simulations

Field Emission / 7

Field emission of nanoprotusions, from its nucleation to quantum dot physics

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Metallic surfaces under an intense electric field tend to form nanoprotusions leading to very localized electron field emission and eventually a current runaway and the destruction of the emitter. The sharply pointed geometry of the protrusions strongly enhances the applied field over the top-most atoms which then permits all of the field emission to often come from only few atoms. This mechanism is very general and has been extensively studied for example with W [1], Pt [2], tungsten carbide-coated W, HfC and ZrC emitters [3]. Independently of the chemical composition of the emitter and the residual gas molecule in the UHV environment, it has been shown that these nanoprotusions have a peculiar voltage dependence of the electron energy spectrum compared to standard metallic emitters and can also be considered as interesting electron sources [1].

Although these protrusions can appear spontaneously, we will show that a controlled formation of nanoscale protrusions on the top of macroscopic tips can be obtained by the field-surface-melting mechanism in UHV environment [1,4]. Then, we will present experimental conditions where nanoprotusions can be considered as promising collimated, coherent and stable electron emitters [2]. These properties are made possible because nanoprotusions tend to form quantum dots with discrete electronic energy levels giving rise to resonant tunneling or Coulomb blockade phenomena [5]. Finally, our recent results concerning the illumination of nanoprotusions with an intense femtosecond laser will highlight the stability of their physical properties at higher energy and ultra-low time scale [4].

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Topic:

Field Emission

Modelling & Simulation / 8

Concurrent multi-scale modelling of vacuum arc plasma initiation

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The complex physical mechanisms involved in the formation of vacuum arcs have been of interest for many decades. Vacuum arcs are relevant in many engineering disciplines, but the physics behind them is not yet fully understood. In recent years, there have been many experimental and computational studies focused on understanding aspects of vacuum arcs.

Our work focuses on further development of a simulation model to describe the physical processes starting from electron emission and leading to the formation of an ionized plasma. The FEMOCS code

is extended to include plasma simulation based on previous work on ArcPIC. Emission of electrons and heating of the cathode is simulated using the finite element method, while plasma simulation is performed using the particle-in-cell method with Monte Carlo collisions. We add evaporation of neutral atoms from the cathode, as well as ionization processes for multiple species of ions, notably impact ionization and direct field ionization.

A static nanotip is simulated with different parameters to study local field thresholds leading to thermal runaway. We find that our simulations are largely in agreement with experimental results. The most significant interactions contributing to initial formation of vacuum arcs are identified. The most important collision for plasma formation is found to be impact ionization of neutrals into Cu⁺ ions, while higher-order ions are found to play a lesser role. Direct field ionization of neutrals is also found to be significant at high fields.

Topic:

Modeling and Simulations

Experiments & Diagnostics / 9**Recent results from the CERN pulsed DC systems****Author:** Ruth Peacock¹**Co-authors:** Walter Wuensch²; Graeme Campbell Burt¹; Alessandra Lombardi²; Alexej Grudiev²; Giulia Bellodi²; Ana Teresa Perez Fontenla²; Sergio Calatroni²; Edgar Sargsyan²; Suitbert Ramberger²; Catarina Serafim³; Stefano Sgobba²¹ *Lancaster University (GB)*² *CERN*³ *University of Helsinki (FI)***Corresponding Author:** ruth.peacock@cern.ch

There have been several pulsed DC system experiments ongoing including recent measurements of field emission current fluctuations associated with dislocation motion showing a variation in the number of events per pulse and a dependence on breakdowns. Also, results of a study comparing the optical spectra obtained during field emission experiments without breakdown from different materials, showing a dependence of light intensity on the voltage and the spectra for different materials. As part of the different material tests, a study of the effects of H- irradiation on different materials, giving values for the field reached during conditioning for irradiated and non-irradiated electrodes and the locations of breakdowns.

The pulsed DC systems are dedicated to the study of vacuum electrical breakdown phenomenon in relation to high gradient RF applications as part of the Compact Linear Collider (CLIC) project at CERN. These systems consist of 2 high precision machined electrodes placed parallel to one another with gap of up to 100µm. A high-voltage feedthrough supplies a voltage of up to 10kV at pulse lengths between 1µs and 1ms.

Topic:

Experiments and Diagnostics

Field Emission / 10**Joule heating of an emitter on the cathode surface by field electron emission current with account of the non-isolation of the**

vertex

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The physical nature of the high-voltage breakdown in vacuum that can occur in particle accelerators, particularly in the CLIC (Compact Linear Collider, CERN), is quite complex and, despite numerous studies, a complete theory of the process does not yet exist.

The emission of electrons from the cathode surface is usually local, due to the existence of tips on the surface. Increasing the voltage in the vacuum gap leads to an increase in the density of the field emission current and, accordingly, to the heating of the emitter due to Joule energy dissipation. It is usually assumed that heating the local area leads to breakdown. In this paper, we use the hypothesis that the breakdown occurs due to the heating of the cathode tips by the field electron emission current.

Therefore, we consider the nonstationary problem of the thermal conductivity of a nanoemitter on the surface of a massive metal cathode when the field emission current passes through it. The cases of different values of the applied electric field strength are considered, the influence of temperature and dimensional effects, as well as the sublimation process are considered.

Topic:

Field Emission

Applications / 11

Open Issues in a Self Consistent RF Vacuum Arc Model

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We find that a general vacuum arc model seems to require four stages: a trigger, ionization, plasma evolution, and surface damage. Within this framework, a large number of mechanisms operate, involving field emission, surface failure, ionization, plasma interactions with the surface and surface interactions with plasma. Field emission is complicated by the duty cycle, space charge, nearby plasma and the geometry of field enhancements. RF field emission is uniquely slow and inefficient, but enhanced by nearby plasma. Surface failure can involve electromigration, diffusion, exploding wire physics, explosive electron emission and an ordinary Coulomb explosion. During the ionization stage, image charge can collect ions near the metallic surface, and sputtering can increase the plasma density from a few atoms to a system that produces Amps of current. We find that sputtering yields increase when the surface melts. Surface instabilities may limit the plasma density and can produce macro particles and dust. Both Maxwell stress and plasma pressure act on the surface. After the plasma is gone, surface tension and capillary waves dominate the micro-surface, while differential cooling and cracking dominate the macro-surface. In the RF case, a unipolar arc, confined by image charges and fueled by sputtering and instabilities, seems to determine the evolution of the surface. A wide range of variables is involved in arcs with many surface micro-geometries, ns to ms timescales, possible pre-existing plasma and magnetic fields. This work seems relevant to arcing in tokamaks, accelerators, micrometeorite impacts, HVAC transmission lines and dielectric breakdown.

Topic:

Modeling and Simulations

Modelling & Simulation / 12

Mechanistic understanding of material evolution under electric fields during Rf breakdown

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High-gradient electric-fields are inevitably encountered in technologies ranging from accelerating structures to miniaturized electronic devices. It is now well understood that material functionality under extreme field conditions can heavily depend on the coupling between electro-thermal loading and microstructural deformation, but the fundamental mechanisms underpinning this coupling remain poorly understood. While they are difficult to explicitly access experimentally, relevant nanoscale deformation mechanisms can in principle be directly probed by atomistic simulations. We include electric-field-induced Lorentz forces using a charge-equilibration molecular dynamics framework that allows for the dynamical evolution of atomic charges. Using this tool, we explore the joint effect of electric-fields-induced stresses and thermo-mechanical stresses on the plastic deformation of fcc metals. We explore the motion and multiplication of dislocations in both the bulk and at free surfaces and discuss the various regimes of electric fields and pulsed heating as they couple with the plastic deformation and surface diffusion. These results inform possible mechanisms of breakdown precursor formation in accelerating structures.

Topic:

Modeling and Simulations

Field Emission / 13

Optical Excitation Response Times for Field Emission from an Individual p-type Si Nanowire

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There has been extensive research on optically modulated and optically pulsed tip electron sources for new high field physics in the ultrafast laser community [1], electron microscopy [2] and ultrafast electron diffraction [3]. This is mostly the excitation of metallic tips or surfaces for which the quantum efficiency is extremely low eg. 10⁻³-10⁻⁴. This means that the high current emission will be

limited by temperature effects. Another route is to exploit the photo-excitation of p-type semiconductor tips for which very high photon-electron conversion rates can be obtained (>10%), though at the expense of much slower time responses.

In contrast to the exponentially increasing current as a function of applied voltage common for metal emitters, semiconducting emitters can reveal strong current saturation related to a field-induced depletion zone originating at the emitter apex. The saturation current is highly sensitive to light and temperature. The basic behavior [4] and rough theory [5] were worked out many years ago followed by many experimental results with cursory analysis. However there is a dearth of in-depth measurements and concomitant understanding of the phenomenon in terms of semiconductor physics. We have shown that SiNWs can serve as an excellent platform for exploring FE from semiconductors with the added advantage for future applications that they can be mass produced. Our principal present goal is to understand the optical time response and eventually apply this knowledge to higher current, faster, cone-like Si emitters.

Our optical response to square wave laser pulses reach the μsec time scales which are among the fastest for semiconducting nanowires in the literature and are postulated to be controlled by the reservoir of defect states in the gap. Note that the literature is almost exclusively made on double-clamped nanowires without field emission. In contrast, the response time to electrical pulses reach the highest we can apply currently (100 MHz) which means that the two transport stimulations do not access defect reservoir populations in the same way.

The rather original measurement techniques will be explained.

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Topic:

Field Emission

Field Emission / 14

THE SWITCH-ON MECHANISM OF THE CURRENT EMISSION

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The Switch-On effect of the current emission is known since long time. This effect is usually attributed to the existence of a Switch-On Voltage, after which the electrodes in the vacuum switch from a non-conductive to a conductive condition. Once reached the Switch-On Voltage the changes in the electrodes are permanent and the electric current can be measured even at lower voltages. In our experiments we find that when a constant electric field, not too intense (≤ 40 kV/mm), is applied to smoothed, unconditioned new brand electrodes, the current output is initially negligible (certainly below our current measurement sensitivity $\approx 10^{-9}$ A). After a long-lasting (in the order of tenths of hours) constant dc voltage has been applied, a sudden increase in current is observed.

By then decreasing and/or increasing the voltage around the constant value, we found regular and reversible Fowler-Nordheim type diagrams. These transitions are interpreted as changes in the electrode surface structure. Our research aims to characterize these transitions (transition time, current and voltage levels) for electrodes made of different materials and/or with different surface treatments. Considerations are finally exposed to explain this Switch-On effect as a consequence of the accumulation of electric charge at the metal-insulator cathode interface.

Topic:

Field Emission

Poster Session / 15

An influence of the cathode surface morphology on the dark current and high-gradient high-vacuum breakdown of the accelerating structures.

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One of the main directions of development of acceleration technology is to increase the acceleration rate to 100 MV / m, as, for example, in projects Compact Linear Collider (CLIC), International Linear Collider (ILC), which will reduce the linear dimensions of modern electronic accelerators, make them more compact and achieve record acceleration energies of charged particle beams (of the order of several TeV). Since each breakdown leads to a loss of the charged particles beam density and damage to the surface of the material, various methods of increasing the resistance to high-gradient breakdown of the accelerating structure are investigated. One way to solve the problem of high-vacuum high-gradient breakdowns is to reduce the field emission current density. A model of field emission current which constructs considering the morphology of the cathode surface and the influence of metal surface modification on the field emission current in the case of multilayer metal-metal-vacuum systems is theoretically investigated at this work.

Topic:

Field Emission

Field Emission / 16

Modeling of Quantum Tunneling in Terahertz Scanning Tunneling Microscopes

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The tip-sample bias of a Scanning Tunneling Microscope (STM) is modulated by coupling THz pulses to the tip in order to get high transient tunneling current. This non-linear tunneling current and its

parametric dependence need to be studied thoroughly to achieve efficient imaging of the sample surface. In this theoretical study, we investigate the basic scaling of rectified electrons in a THz-STM junction. We use a self-consistent quantum model [1-3] that includes both space charge potential and exchange-correlation potential, which were ignored in previous studies. Among these two important effects, the exchange-correlation potential, in particular, become crucial in THz-STMs since they are operated at high transient voltage in field emission regime [1][2]. We validate our calculation with recently reported experimental data and study the rectification property of the tip-sample junction for different parameters. We find that the time dependent tunneling current and the electron transport can be manipulated by varying the d.c. bias voltage (polarity, amplitude), incident THz field (polarity, shape, peak amplitude), work functions of STM tip and sample - especially their difference ΔW , and the tip-sample separation. Our study provides an important framework to characterize, control, and improve probing techniques at nanometer scale over subpicoseconds time periods.

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Topic:

Field Emission

Experiments & Diagnostics / 17

Performance of electrical vacuum breakdown under cryogenic temperatures

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The cryogenic high-voltage pulsed DC system in FREIA laboratory continues the test series of copper electrodes to establish peculiarities of BDs craters occurred at low temperature down to 4K.

The system uses parallel plate 40 mm diameter anode and 62 mm diameter cathode with a tens micrometers inter-electrode space. 1 μ s high-voltage rectangular dc pulses with a repetition rate up to 1 kHz were used for the conditioning test at 30 K temperature. Microscopic post-mortem observation was performed for the tested samples.

We found the size ratios for anode and cathode breakdown features that link the results from several microscopic techniques. The difference between morphology of breakdown features on anode and cathode will be presented. We will also clarify the experimental conditions for specific star-like BD features.

Topic:

Experiments and Diagnostics

Poster Session / 18

HV Discharges Monitoring at HVPTF: Perspectives from X-ray Spectroscopy

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MITICA is an experiment located at Consorzio RFX which aims to create a prototype for ITER's Neutral Beam Injector (NBI). Since its design features an unprecedented potential difference (1 MV) there is an interest in researching means to prevent discharges in vacuum, which might prove fatal to the structure of the machine. In this context, High Voltage Padova Test Facility (HVPTF) is an experimental device with the aim of studying the processes leading to such undesirable discharges. HVPTF features a vacuum chamber containing two electrodes which can achieve an HV difference up to 800 kV. Both the vacuum (pressure, gas composition) and the electrodes (shape, distance) can be controlled in order to produce different conditions. Supplied voltage, current and pressure are monitored, as well as the bremsstrahlung hard X-rays produced by the free charges accelerated by the HV interacting with the electrodes.

The aim of this work is to show X-ray spectroscopy to be a promising monitoring mechanism, allowing for various insights in the physics of discharges. This contribution details the scintillators used to collect data (one LYSO and one LaBr), the development of the analyzing software, the resolution of issues like pile-up discrimination and time calibration, and some of first results obtained from the data acquired during the period between 2019 and 2022. Future perspectives will be also drawn, in particular related to the recent installation of a new Gas Electron Multiplier (GEM) detector on HVPTF.

Topic:

Experiments and Diagnostics

Experiments & Diagnostics / 19

High Voltage Conditioning in high vacuum on concave electrodes. Developments and possible applications associated to accumulation points on electrode surfaces

Author: Nicola Pilar^{None}

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Counterintuitive experimental evidences have been observed during High Voltage Direct Current (HVDC) tests of two concave, axial-symmetric, electrodes insulated by large vacuum gaps of 3 and 7 cm with voltages from 150 to 370 kVdc. The dissipation of microdischarge power during the conditioning procedure occurs mostly on the anodic side in a region close to the axis of the system where the electric field is at a minimum, far from the positions where the breakdowns have been observed. Numerical simulations, based on ray-tracing algorithm, correctly identify the positions where the power dissipation of microdischarges occurs. A mutual exchange of charged particles in the electrostatic field between electrodes seems a reasonable physical mechanism to interpret the observations. The areas with the most intense electric field, typically located on the surfaces of the electrodes under test, are not necessarily the sole surfaces involved in the HVDC conditioning in high vacuum. Drift of charged particles toward accumulation points on the electrode surfaces can focus the microdischarge power, possible developments and applications based on this effect are analysed and discussed

Topic:

Experiments and Diagnostics

Applications / 20

Control of erosion and ignition of pulsed vacuum arcs

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We will present recent results related to control of vacuum arc ignition and erosion in pulsed vacuum arc devices. As a particular example, we will consider vacuum arc microthruster devices. To this end, we will discuss breakdown process in the case of a micro-vacuum arc thruster. In these devices ignition analysis includes effects of insulator material, cathode material deposition and cyclic nature of insulation of the inter electrode layer. One example of plasma thruster is two stage device. The first stage is a short micro-second pulsed vacuum arc while the second stage is a long duration vacuum arc. Longer milli-second pulses of the second stage are formed in the presence of initial plasma formed during the first stage. This arrangement leads to enhanced cathode erosion.

Topic:

Applications

Poster Session / 21

Resistivity Measurement of Metal Surfaces to Track Down Dislocations Caused by Surface Conditioning

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Conditioning of a metal surface in a high-voltage system is the progressive development of resistance to vacuum arcing over the operational life of the system.

This is relevant for accelerator cavities where high level of performance is only achievable after long conditioning period. Beyond the accelerator research field, this is an important topic for any technology where breakdowns can cause device failure, either by directly disrupting device operation or by causing cumulative hardware damage.

We are developing a direct method to measure the surface resistivity of a metal surface that is being conditioned by inducing a high frequency (GHz) radio-frequency current in the parallel-plate electrode system. If the system can function as a resonant cavity, the surface resistivity data would be encoded in its quality factor (Q-factor). The changes in the resistivity measured in cryogenic conditions would indicate a formation of dislocations under the surface, something that has been speculated as an important process behind the conditioning.

We will present the algorithms used to extract the Q-factor from experimental data and the results of experiments done using copper electrodes and test cavities. Small changes in resistivity (less than 0.6%), induced by temperature changes, were measured. We also show the preliminary results of the 3D EM simulations, where the electrode system in the cryogenic setup in FREIA laboratory is modified to act as a resonant cavity.

Topic:

Experiments and Diagnostics

Experiments & Diagnostics / 22

X-RAY MEASUREMENTS REVEAL THE FINE DYNAMICS OF CURRENT MICRO-DISCHARGES IN A VACUUM HIGH VOLTAGE EXPERIMENT

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The High Voltage Padova Test Facility (HVPTF) is an experimental device for investigating High Voltage (HV) insulation in vacuum, in support of the realization of MITICA, the prototype of a neutral beam injector for ITER. Inside a high vacuum chamber, two stainless steel electrodes, separated by a few centimetres gap, can achieve an HV difference up to 800 kV. During the conditioning process of the electrodes, current micro-discharges and the presence of associated X-rays are observed, along with a global increase of gas emission (H₂ and CO₂ are detected by the Residual Gas Analyser). Different X-rays detectors have been installed during the last five years on HVPTF, with the aim to

investigate the physical processes behind the conditioning by means of X-rays analyses.

In this contribution, new information provided by the different devices are presented: in particular, the identification of a fine dynamics in the micro-discharge phenomenon is shown. Moreover, the growing contribution of the vacuum chamber during the electrodes conditioning, operating as a third electrode, is investigated. A possible physical interpretation of the micro-discharge dynamics is sketched.

Finally, the new set of LYSO scintillators is described and preliminary results about the recent electro-polished electrodes campaign is introduced.

Topic:

Experiments and Diagnostics

Modelling & Simulation / 23

Vacuum Insulator Flashover

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In this presentation we describe a new effort at Sandia National Laboratories and Texas Tech University to better understand the key physics involved in vacuum insulator flashover. In many pulsed power applications, the transmission lines from the capacitor bank to the target load move from a region of water insulation (separation) to vacuum insulation (separation). In this transition region an insulator stack is utilized to separate the two stages. The undesired breakdown across an insulator, i.e., flashover, during the rising time of a pulse is a key failure mode. Although field emission and secondary electron cascade processes, which account for breakdown initiated at the cathode triple junction, have detailed explanations, the processes involved for anode-initiated breakdown are much less understood. Here we will describe modeling and experimental efforts to investigate the hypothesized mechanisms.

This work was supported by the Laboratory Directed Research and Development program at Sandia National Laboratories, a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Topic:

Modeling and Simulations

Applications / 24

Fundamental Study on Conditioning of a Vacuum Gap with Low Breakdown Energy

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Conditioning experiment of a commercial vacuum interrupter was carried out with a gap distance of 1~3 mm. Energy of the vacuum arc following a breakdown has been controlled to be as low as

several hundred mJ with a 100 k Ω current-limiting resistor. Breakdown voltage and field emission current was measured during the conditioning process. The Murphy-Good plot was employed to further study change of field enhancement factor β and the field emission area A_e . The conditioning process was proceeded if no higher breakdown voltage was observed during the last 100 breakdowns. Results showed that at 1 mm gap distance, breakdown voltage increased smoothly as β decreased. The local breakdown electric field $\beta U/d$ remained almost constant. However it was out of expectation that the maximum field emission current before each breakdown increased from several mA to over 100 mA during the conditioning process. At gap distance of 2~3 mm, the conditioning process consists of two stages. The first stage was the same as the case with gap distance of 1 mm, with breakdown voltage increased and β decreased smoothly. But when β decreased to a certain value, the conditioning process turned into the second stage, with abnormal field emission current increase sometimes observed before breakdown. A microparticle approaching the cathode surface could be responsible for the current increase. β usually gets higher after such a breakdown. Then during the next few shots, with no abnormal field emission current rise before breakdown, β decreases again till the certain value, and a breakdown with abnormal field emission current shows again. This process loops throughout the second stage, with breakdown voltage fluctuated around a certain value, which is often called "saturation". Results in this paper could be partially explained by a model proposed by Chatterton's.

Topic:

Applications

Poster Session / 25

Multi-scale modelling of electrical breakdown in vacuum: Influence of electromagnetic power

Author: Tauno Tiirats¹**Co-authors:** Andreas Kyritsakis ; Roni Koitermaa²; Veronika Zadin³¹ *University of Tartu*² *University of Helsinki*³ *University of Tartu (EE)***Corresponding Author:** tauno.tiirats@gmail.com

Vacuum arcs –also known as breakdown–, i.e. electric discharges appearing in vacuum, are a major limiting factor for various applications such as particle accelerators, fusion reactors, vacuum interrupters, X-ray sources, and space applications. However, the physical mechanisms underlying the very initiation of the phenomenon still remain unclear. Recent experimental evidence indicates that the distribution of electromagnetic power is actually the main limiting factor of the arc initiation, instead of applied electric field and the cathode material as previously assumed. This project aims to understand the physics underlying the power supply limitations on the vacuum breakdown initiation by developing computational models that predict its behavior. A direct comparison with experimental results shall result in the exact determination of the desired design characteristics for structures that suffer from vacuum breakdown.

Topic:

Modeling and Simulations

Applications / 26

The role of alumina coating porosity on the electrical insulation in a weakly ionized plasma atmosphere

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The design of the RFX-mod2 experimental fusion device requires a copper shell close to the plasma to aid in stability and magnetic confinement of the plasma [1,2]. This conductive structure, only 3mm thick, placed around the plasma, must have electrical discontinuities in both the poloidal and toroidal directions, so as to allow the penetration of electromagnetic fields into the plasma region. These gaps are conceived to avoid the formation of net poloidal and toroidal currents in the copper shell during the experiment phases. Furthermore, the shell was designed with an overlapped region at the poloidal gap in order to minimize induced field errors.

The loop voltage, that is the electromotive force induced by external coils which sets up and supports the plasma current, can reach values up to 400 V, during operations in the Reversed Field Pinch magnetic configuration. Besides, if a fast termination occurs, i.e. rapid loss of the plasma magnetic confinement, these values can rapidly rise up to 1.5 kV. Therefore, intense electric fields can be generated between the shell edges, only a few millimetres apart, along the overlapping region. Furthermore, considering that the stabilizing copper shell, placed inside the vacuum chamber, is exposed to low temperature weakly ionized plasma, the formation probability of harmful electric arcs is high.

In order to avoid the formation of arcs, the copper shell will be coated with a ceramic layer made of aluminium oxide (alumina), applied by means of atmospheric plasma spraying.

An experimental apparatus was prepared with the aim of reproducing the conditions expected at the plasma edge close to the copper shell. It consists of a vacuum chamber in which a helium plasma is produced, generated by an incandescent tungsten filament and a DC power supply. The alumina-coated copper samples are polarized, applying a pulsed voltage up to approximately 2 kV. The electrical tightness of the insulating layer and the possible formation of electrical discharges on the alumina surface were verified.

It was observed that in some samples, in which the breakage of the dielectric layer occurred, the thickness of the ceramic layer was less than that required (100 µm) and was characterized by an irregular structure with high porosity and large cavities of tens of microns. Moreover, these cavities generate a network of interconnected fractures forming an almost continuous porosity, thus reducing the effective thickness of the alumina.

The electrical insulation has been significantly improved by creating alumina deposits with better compactness and reduced porosity. The latter parameters have been validated for having an effective electrical insulation in the presence of plasma.

In this contribution, we present the electrical insulation performance of alumina coated samples with different thickness and porosity levels. Furthermore, the copper samples with alumina coating were analysed, both in section and on the surface, by means of a scanning electron microscope (SEM).

References

- [1] Peruzzo S., et al. "Technological challenges for the design of the RFX-mod2 experiment." *Fusion Engineering and Design* 146 (2019): 692-696 <https://doi.org/10.1016/j.fusengdes.2019.01.057>.
- [2] Marrelli L. et al. "Upgrades of the RFX-mod reversed field pinch and expected scenario improvements" *Nuclear Fusion* 59 076027 (2019)

Topic:

Applications

Modelling & Simulation / 27**Monte Carlo simulation of vacuum breakdown occurrence statistics including the electromagnetic power flow dependence****Authors:** Andreas Kyritsakis^{None}; Juri Volodin^{None}**Co-author:** Veronika Zadin¹¹ *University of Tartu (EE)***Corresponding Authors:** akyritsos1@gmail.com, juri.volodin@ut.ee

One of the most extensively studied characteristics of vacuum breakdown (VBD) is the conditioning process and the VBD occurrence statistics, in various systems, including Radio-Frequency (RF) accelerators and pulsed-DC large electrode systems. Despite the abundant data on the VBD statistics, drawing useful conclusions regarding the physical processes that determine various patterns within those data (e.g. long-term and short-term conditioning, pulse duration dependence, pulse width dependence, VBD separation distribution, etc), is extremely challenging. One of the main reasons is that the existing VBD models focus on the low-level physical mechanisms which render them unable to produce direct quantitative predictions that are comparable to the aforementioned experimental data.

In this work, we attempt to bridge this gap between theory and experiment by developing a Monte-Carlo model that simulates the occurrence of VBD in any high-field system, based on a few general assumptions. We model VBD occurrence as a two-step Markov chain process. The electrode surface is separated into small elements, each of which is described by a local field E , a power coupling impedance parameter Z , and a surface state parameter β . On each pulse, each surface element is randomly tested for the occurrence of thermal runaway. The probability of thermal runaway (TR) is a sharply increasing function of βE . The points for which TR occurred are randomly selected on whether this TR will develop into full VBD, which depends on E and the power coupling parameter Z of each point. The surface state parameter β of a point is updated after each pulse in a different manner, depending on whether nothing, TR, or VBD occurred.

Finally, we test the above method for various distributions of the simulation parameters, fitting them to reproduce well-known experimental conditioning curves and other VBD statistics.

Topic:

Modeling and Simulations

Experiments & Diagnostics / 28**Microscopy investigation on different materials after pulsed high field conditioning and low energy H- irradiation.****Author:** Catarina Serafim¹**Co-authors:** Alessandra Lombardi²; Alexej Grudiev²; Ana Teresa Perez Fontenla²; Edgar Sargsyan²; Flyura Djurabekova³; Ruth Peacock⁴; Sergio Calatroni²; Stefano Sgobba²; Walter Wuensch²¹ *University of Helsinki (FI)*² *CERN*³ *University of Helsinki*⁴ *Lancaster University (GB)*

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During operation the LINAC4 RFQ (Radio-Frequency-Quadrupole) is exposed to high electric fields which can lead to vacuum breakdown. It is also subject to proton beam loss that can cause surface modification, including blistering, which can result in reduced electric field handling and an increased breakdown rate. An experimental study has been made to identify materials with high electric field capability and robustness to low-energy proton irradiation. In this presentation we briefly discuss the selection criteria and we analyze these materials investigating their metallurgical properties using advanced microscopic techniques such as Scanning Electron Microscope, Electron Back Scattered Diffraction, Energy-dispersive X-ray Spectroscopy and conventional optical microscopy. The different materials are observed and characterized on a micro and a nano-scale, and are compared before and after irradiation and breakdown testing.

Topic:

Applications / 29

High Gradient CrYogenic Brightness-Optimized Radiofrequency Gun (CYBORG) Test Bed

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Producing higher brightness beams at the cathode is one of the main focuses for future electron beam applications. For photocathodes operating close to their emission threshold, the cathode lattice temperature begins to dominate the minimum achievable intrinsic emittance. At UCLA, we are designing a radiofrequency (RF) test bed for measuring the temperature dependence of the mean transverse energy (MTE) and quantum efficiency for a number of candidate cathode materials. We intend to quantify the attainable brightness improvements at the cathode from cryogenic operation and establish a proof-of-principle cryogenic RF gun for future studies of a 1.6-cell cryogenic photoinjector for the UCLA ultra compact XFEL concept (UC-XFEL). The test bed will use a C-band 0.5-cell RF gun designed to operate down to 45 K, producing an on-axis accelerating field of 120 MV/m. The cryogenic system uses conduction cooling and a load-lock system is being designed for transport and storage of air-sensitive high brightness cathodes.

Topic:

Applications

Experiments & Diagnostics / 30

High Power RF Breakdown Test for Cryo-cooled Reentrant C-Band Copper Structure

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High gradient RF structures capable of maintaining gradients in excess of 250 MV/m are critical in several concepts for future electron accelerators. Concepts such as the ultra-compact free electron laser (UC-XFEL) and the Cool Copper Collider (C3) plan to obtain these gradients through the cryogenic operation (<77K) of normal conducting copper cavities. Breakdown rates, the most significant gradient limitation, are significantly reduced at these low temperatures but the precise physics is complex and involves many interacting effects. High-power RF breakdown measurements at cryogenic temperatures are needed at the less explored C-band frequency (5.712 GHz) which is of great interest for the aforementioned concepts. On behalf of a large collaboration of UCLA, SLAC, LANL, and INFN the first C-band cryogenic breakdown measurements will be made using LANL RF test infrastructure. The 2-cell geometry designed for testing will be modifications of the distributed coupled reentrant design used to efficiently power the cells while staying below the limiting values of peak surface electric and magnetic fields.

Topic:

Experiments and Diagnostics

Field Emission / 31

Why using the Nordheim parameter y in the mathematics of the special mathematical function “ v ” used in field emission theory should now be regarded as mathematically perverse

Author: Richard Forbes¹¹ University of Surrey**Corresponding Author:** r.forbes@surrey.ac.uk

This presentation forms part of my efforts to modernise the theories of field ion and electron emission and to encourage more consistent use of basic theory as between different groups of users. It primarily concerns the correction factor “ v_F ” that appears in the Murphy-Good (MG) theory of field electron emission (FE), which is based on the planar-image-rounded “Schottky-Nordheim” (SN) barrier. In MG FE theory, one can write the following expression for the emission current I in terms of the emitter local work function w (for simplicity, assumed uniform) and a characteristic local field-magnitude F_C (usually interpreted as the field magnitude at the apex of an emitting protrusion):

$$I = A (a/w) (F_C)^{-2} \exp[-(v_F) b w^{3/2} / F_C]$$

Here a and b are the Fowler-Nordheim constants, A is an area-like parameter, and (v_F) is an appropriate particular value of a special mathematical function (SMF) often just called “ v ”.

It has been known since 2008 that the SMF “ v ” is a very special solution of the Gauss Hypergeometric Differential Equation (HDE); consequently, it is now considered best mathematical practice to take “ v ” as a function of the independent variable in the Gauss HDE, which I denote by “ x ” and call the Gauss variable. Hence, I now write $v(x)$. This convention replaces the older convention of expressing “ v ” as a function of the Nordheim parameter y , which is given by $y = +\sqrt{x}$.

In recent years I have been arguing that we should make a separation between the mathematics of “ v ” and the use of this SMF in modelling FE and related phenomena. This separation would be analogous to the separation made between (a) the mathematics of the “abstract” SMF “ $\sin x$ ” and (b) its use in trigonometry, by setting x equal to an angle θ .

I have also been arguing that continued use of the Nordheim parameter y in the mathematics of “ v ”

should be considered mathematically perverse. The mathematics of “v” should now use the variable “x”. Several examples will be presented to underline what I mean by mathematically perverse, and to show that “x” is a “better mathematical variable” than “y”.

The SMF $v(x)$ finds uses, not only in MG FE theory, but also in other scientific contexts, for example field ionization of inert gas atoms, as in gas field ion sources and field ion microscopy.

When applying the SMF $v(x)$ to modelling FE via the MG FE equation, there are two possible conventions: (a) the “legacy convention” of setting $x=y^2$; and the modern “21st Century convention” of setting x equal to the “scaled-field f ” defined by

$$f = F/(F_R)$$

where F_R is the reference field needed to pull the top of the SN barrier down to the Fermi level.

It will be argued that, for experimentalists and technologists, the “21st Century convention” of using f has several significant advantages (which will be detailed) over the legacy convention of using y . The question of a suitable name for “v” will be discussed.

Much of the FE theory used in vacuum breakdown contexts is in fact based on an approximation for “v” developed by Charbonnier and Martin in 1962. In modern mathematical form this is written:

$$v(x) \approx (v_{CM})(x) = 0.956 - 1.062 x .$$

This appears to have originally been derived (as a function of y) by fitting to a table of values generated by Burgess et al. in 1953 (Phys. Rev. 90, 515). A modern method of deriving this formula, based on a form of linear expansion, will be presented.

A more complete account of a modern theory of “v” can be found in [1]. A tabulation of values of $v(x)$ and related functions, in terms of x (or equivalently f) can be found in [2].

[1] R.G. Forbes, Chap. 9 in: Modern Developments in Vacuum Electron Sources (Springer 2020).

[2] R.G. Forbes and J.H.B. Deane, J. Vac. Sci. Technol. B 28, C2A33 (2010).

Topic:

Field Emission

Field Emission / 32

Enabling Bright Carbon Nanotube Fiber Field Emission Cathode

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In this work, we introduce a new technique which improves emittance of the carbon nanotube fiber field emission cathode (CNT fiber FEC) many-fold. CNT fibers remain of high interest for next generation electron source research and development as they have low turn-on voltage, high conductivity, durability, and flexibility. However, control over its emission properties is a challenge. Our previous studies showed that formation of stray emitters due to thermal and field stress during emission causes spatially non-coherent beam, which means large emittance and low brightness. It was also shown that the emission over the surface was confined to small number of stray spots, which makes most of the surface useless and leads to local hot spots, arcs, and failure of the cathode.

To prevent formation of stray emitters, we electroplated fiber ropes, made of multiple twisted CNT fibers, with nickel, then cut its top with a femtosecond laser to minimize surface ablation, and welded it on a metal base. The final structure has 150 μm fiber core, 50 μm thick Ni shell, and is 4.8 mm in height. Our emission test results showed that emission from the cathode forms a single spot comparable to the entire size of the cathode fiber core and high output current. This is an indication of high brightness and emission uniformity over the surface. Detailed results and brightness estimations will be presented.

Topic:

Field Emission

Modelling & Simulation / 33**Investigation of electrical breakdown phenomena: multiscale-multiphysics simulations and experimental aspirations****Author:** Veronika Zadin¹**Co-authors:** Andreas Kyritsakis ; Flyura Djurabekova ²; Sergei Vlassov ; Ye Wang ¹¹ *University of Tartu (EE)*² *Helsinki Institute of Physics (FI)***Corresponding Author:** veronika.zadin@ut.ee

Many high electric field applications, for example, Compact Linear Collider in CERN are significantly limited by the presence of the phenomenon of electrical breakdowns. In case of sufficiently high applied electric field, even in ultra high vacuum conditions, electrical discharge appears, induces disturbances into the operating regime of the device, causes material damage and generally, limits significantly operation of the device. Phenomenon itself is known for long time, however, it's exact initiation mechanisms still remain elusive. Current hypotheses suggest, that electric field influence leads to a formation of field enhancing nanoscale tip. This tip will initiate significant field emission currents, evaporation of neutral atoms, formation of plasma and finally – complete electrical breakdown. In current talk we explore these hypotheses of electric field assisted surface diffusion as the initiation mechanism of the field emitters by the studies conducted using multi-physics-multi scale simulation framework FEMOCS and DFT calculations with nanoscale materials exposed to high field. We consider investigations of the machine learning algorithms to enable computationally practical incorporation of electric field influence to electron structure. The theoretical investigations are complemented by in situ electron microscopy experimental outlooks for confirmation and validation of computational studies.

Topic:

Modeling and Simulations

Applications / 34**Coherent Arc behavior in the VAR process****Author:** Abdellah Kharicha¹¹ *CD Lab for metallurgical applications of MHD***Corresponding Author:** akharicha@hotmail.com

Vacuum Arc Remelting (VAR) is typically the final melting process in the production of a wide range of metallic alloys. The process consists in applying during days a DC current of up to 40 000 A over large electrodes (~1m diameter). A strong DC arc takes place under vacuum between an electrode and a water-cooled copper crucible. For low applied current, high-speed video observation showed that spots formed preferentially in the centre, then moved with retrograde motion to the edge of the electrode. However for higher current it is reported the observation of a slow ensemble arc motion around the axis of the furnace with a time period of 20 to 40 seconds. Depending on the applied current and on the electrode dimension the path follows a butterfly pattern or a circle pattern. When an axial magnetic field is applied, the spots ensemble motion is stabilized at certain off centred position. We will present a numerical model able to explain and predict such coherent arc behaviour.

Topic:

Modeling and Simulations

Poster Session / 35

The field emission current density from a metal in the presence of field emitting nanotips on the surface in accelerating structures

Authors: Ihor Musiienko¹; Yuliia Lebedynska¹

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Field emission is one of the main factors, which leads to the loss of electrical insulating properties of the interelectrode vacuum gap. Solving the problem of reducing the field emission current value in accelerating structures is necessary to obtain gradient-stable materials before the occurrence of dark currents and, as a consequence, the possibility of overcoming high-vacuum high-gradient breakdowns.

The increasing of the field emission current value in high-gradient accelerating structures is due to the following main factors: suppression of the work function of metal; irregularities on the metal surface in the form of nanoscopic tips.

In the presence of an electric field strength E near the nanoscale tip on the metal surface, the local electric field strength increases, which leads to an increasing of the field electron emission current value. Therefore, it is important to substantiate the parameters of the metal surface roughness using the generalized enhancement factor β of the electrode surface.

The purpose of this study is to calculate the field emission current density from the surface of high-gradient accelerating structures, taking into account the model of continuous uniform distribution of hemispherical nanotips on the copper surface.

Topic:

Field Emission

Modelling & Simulation / 36

#2011287 Cu Surface Diffusion Bias under Electric Field Gradient - Accelerated Molecular Dynamics, Finite Elements Method, and Density Functional Theory

Author: Jyri Kimari^{None}

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Vacuum-facing metal surfaces are exposed to strong electric fields in many devices, such as particle accelerators, free-electron lasers and fusion reactors. Under sufficiently strong fields, current can arc through the vacuum, disrupting and damaging these devices. Despite decades of research, the

precise mechanisms of the vacuum arc breakdowns are still unknown. The interplay of different physical phenomena, as well as their associated length and time scales, pose numerous challenges in experiments and simulations.

In our earlier study [1], we showed in simulation that a runaway process of Cu nanotip melting and evaporation can produce the necessary material for the formation of plasma that will conduct the electric current through vacuum. An open question remains of the growth of these nanotips, as well as their sharpening for enhanced field emission and heating.

A proposed mechanism of biased diffusion under electric field gradient could contribute to mass transfer toward the extremities of any initial protrusions or roughness on the surface [2]. In the study at hand [3], we simulated Cu surface diffusion directly in these conditions using molecular dynamics (MD). The implementation of the electric field involves concurrently solving the Laplace equation of macroscopic electric field on a finite elements method (FEM) mesh that follows the discrete atomic system and extends beyond it. Furthermore, we extended the time scale of our simulations by the collective variable -driven hyperdynamics (CVHD) method for better collection of diffusion statistics. Finally, we estimated the surface polarization characteristics from our MD simulations, and compared them directly to density functional theory (DFT) calculations, finding good agreement.

In this talk, we will discuss the evidence we found for biased diffusion on Cu surface, as well as the practicalities of coupling CVHD-accelerated MD with FEM.

[1] Kyritsakis, Andreas, et al. *Journal of Physics D: Applied Physics* 51.22 (2018): 225203.

[2] Kyritsakis, Andreas, et al. *Physical Review B* 99.20 (2019): 205418.

[3] Kimari, Jyri, et al. In preparation.

Topic:

Modeling and Simulations

Field Emission / 37

A Computational Tool for Static Simulations of Semiconducting Field Emitters

Authors: Andreas Kyritsakis¹; Salvador Barranco Cárceles²

Co-authors: Aquila Mavalankar³; Ian Underwood²; Vahur Zadin¹

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Cold electron emission and vacuum breakdown are gaining popularity due to their significance in applications such as electron sources for mobile 3D medical imaging [1] and high-gradient particle accelerators [2]. The robust development of such devices is hindered by the lack of both effective computational models to engineer and optimise them through simulation and tools for the processing and analysis of experimental field emission results.

An initial model, GETELEC, has been reported for the computation and analysis of field emission and Nottingham heat [3] from metals. We expanded and generalized GETELEC to calculate the Nottingham heat and the field emission currents from semiconducting and insulating materials. Thus, providing the boundary conditions to calculate electron injection into vacuum from semiconductors, and the current and heat distributions in the emitting crystal.

Here we present our attempts to combine GETELEC with a commercial finite element method software (COMSOL) to resolve the band structure inside the semiconductor when a high field is applied and electron emission occurs. Our model aims to find solutions to the nested-self-consistent

problem of solving the Poisson and current continuity equations for 3D semiconducting geometries. Resulting in an accurate and user-friendly computational tool to design semiconducting field emitters

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- [3] A. Kyritsakis and F. Djurabekova, Computational Materials Science 128, 15 (2017).

Topic:

Field Emission

Experiments & Diagnostics / 38

Observations of dislocations in Soft Cu samples exposed to high fields

Authors: Ayelet Yashar^{None}; Enrique Rodriguez Castro¹; Iaroslava Profatilova^{None}; Inna Popov^{None}; Walter Wuensch²; Yinon Ashkenazy³

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It was proposed that breakdown nucleation can be explained as emanating from surface plastic activity due to collective dislocation dynamics within the surface layer of samples exposed to high electric fields. In the past, we have demonstrated that extensive mobile dislocation structures are routinely observed in soft large-grained OFHC copper. However, as of this day we are missing a clear characteristic that is modified due to exposure to high fields. Specifically, there are no clear indications linking conditioning under high fields to variations in dislocation structure. In this talk, I describe the status of current efforts to identify such an effect and establish constraints on the effects of high fields. I demonstrate that although there are no clear signs of a simple change in dislocation density with field exposure, further study is required to address other features of the observed structures. Initial results and challenges for this are described.

Topic:

Experiments and Diagnostics

Poster Session / 39

Effects of the series impedance on vacuum arc plasma onset

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The surface electric field has been regarded as the only parameter that determines the occurrence of a vacuum breakdown (VBD) for a given surface condition. However, recent studies have accumulated an increasing amount of evidence indicating that the ultimate limit depends strongly also on the electromagnetic power that is available to be delivered at the VBD site. Here we study this dependence both experimentally using a pulsed DC system and by numerical plasma simulations using the particle-in-cell (PIC) model ArcPIC [Timko et. al. *Contrib. Plasma Phys.* 55, 299(2015)]. By varying the series impedance, we controllably limit the power coupling from the source to the vacuum discharge gap. The experimental results show that the breakdown voltage increases with increasing impedance, i.e., with increasing circuit resistance and decreasing capacitance. The ArcPIC results showed that a minimum current is required to ignite the plasma, and the breakdown voltage is defined by the circuit impedance and the critical power loaded to the gap just before the breakdown.

Topic:

Modeling and Simulations

Modelling & Simulation / 40

Atomistic simulations of growth mechanisms of hydrogen blisters in copper

Authors: Alvaro Lopez Cazalilla^{None}; Flyura Djurabekova¹

Co-authors: Ana Teresa Pérez Fontenla²; Catarina Filipa da Palma Serafim²; Sergio Calatroni²; Walter Wuensch³

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Blistering is a process which usually takes place close to the surface of metals when they are irradiated, as can be seen in radio-frequency quadrupoles accelerating structures. This pronounced change of the surface morphology has been measured when the extended irradiation is done with energetic light ions.

The mechanism of continuous growth of a small bubble to a quantifiable size blister is not completely understood. Frequently, such process is associated to the prismatic dislocation loop punching, which takes place in very short timescale and cannot be covered by experimental techniques. In FCC metals, the pressurized voids yield emitting shear loops, which were suggested to provide explanation on the plastic growth of the bubbles. However, the detachment of these loops has not been demonstrated.

We use molecular dynamics to address the fast bubble growth in Cu, associated with blistering, when exposed to H- irradiation [1]. To do that, we employ a methodology which allows us to closely follow the formation of prismatic loops at different H concentrations. Moreover, we also analyze the interaction of these loops with the different surface orientations of copper. This study sheds light on the mechanism of blister production and, also, to its effect on the surface exposed to irradiation.

We observe the emission of a complete prismatic loop composed by several shear loops, which Burgers vectors are aligned with the gliding direction of the prismatic loop. We show that the prismatic loops are not necessarily smaller than the bubble cross-section. In addition to this, we note that these loops travel toward defects-sinks such as grain boundaries or surfaces, and in the latter case, are creating different shape protrusions. These protrusions' shapes are different depending on the grain orientation, as observed experimentally, and we verify it by our computational method.

[1] Alvaro Lopez-Cazalilla, Flyura Djurabekova, Fredric Granberg, Kenichiro Mizohata, Ana Teresa Perez Fontenla, Sergio Calatroni, Walter Wuensch Acta Materialia, 225 (2022) 12

Topic:

Modeling and Simulations

Field Emission / 41

New field emission dynamics in a 2D space charge dominated regime beyond Fowler Nordheim for high gradient injectors

Author: Mitchell Schneider¹

Co-authors: Benjamin Sims²; Emily Jevarjian ; Jiahang Shao³; Ryo Shinohara⁴; Sami Tantawi⁵; Sergey V. Baryshev⁶; Taha Posos ; Tanvi Nikhar²; Zenghai Li ; john power⁷

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The work presented here shows evidence of the diversions from classical Fowler Nordheim in the RF regime. At high gradients in excess of 100 MV/m, it was shown that the field emitter cathode (FECs) made from ultra-nanocrystalline diamond (UNCD) follows a two-dimensional space charge dominated regime. Field emission dynamics now must be considered in a 2D regime, combining the 1D longitudinal classical Fowler Nordheim and 1D transverse Child Langmuir limit. These cathodes were able to produce remarkably high charge of 300 nC/6 μ s pulse giving a beam current of 0.12 A. This cathode produced uniform emission with effective emission area of tens of microns which is three orders of magnitude higher than predicted by classical Fowler Nordheim. To explore this new n-dimensional space charge dominated field emission physics, we present the design of a new X-band field emission rf gun.

Topic:

Field Emission

Experiments & Diagnostics / 42

Status of High-Power Testing of X-band Parallel Feed Nb Accelerating Structures

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This talk will present the status for developing high gradient X-band bulk niobium accelerating cavities. We optimized the cavity design to maximize the shunt impedance and reduce the peak surface magnetic fields. This means that a much higher gradient can be produced for the same quench field limit of niobium (230 mT), increasing the power loss to gradient² ratio > 100 [mWm/(MV)²]. We provide an update on the status of testing X-band superconducting high gradient structures, in conjunction with our ongoing material science testing at cryogenic temperatures to develop accelerating structures and other high power rf components.

Topic:

Experiments and Diagnostics

Experiments & Diagnostics / 43

Dislocation structures of Cu electrodes exposed to high fields

Author: Inna Popov^{None}

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It was suggested that breakdown might result from collective dislocation effects within a surface of metal electrodes exposed to high electric fields. We applied scanning and transmission electron microscopy to check this assumption. In this talk, I present a picture of the lattice structural defects observed in soft and hard Cu – dislocation dipoles, stacking faults, twins, and grain boundaries.

Topic:

Experiments and Diagnostics

Modelling & Simulation / 44

Phenomenological description of vacuum breakdown

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\textbf{1. Potential mechanisms of vacuum breakdown. }The field electron emission (FE), where electrons are released from cold negative electrodes due to the applied electric field, is a necessary step in the development of vacuum breakdown. It is well known that the field emission current from cold electrodes in vacuum exceeds, by orders of magnitude, values given by the quantum mechanical Fowler-Nordheim formula, evaluated in terms of the applied electric field (which in the simplest case of a parallel-plate gap equals V/d , where V is the interelectrode voltage and d is the gap width). Various mechanisms for this enhancement of electron emission have been postulated.

The most popular mechanism is the amplification of the applied electric field by microprotrusions, pre-existing on the surface of the negative electrode or

resulting from the application of the electric field. The conventional problem with this hypothesis, as far as pre-existing microprotrusions are concerned, is that in order to explain values of the field emission current observed in the experiment, the microprotrusions have to be assumed to be quite slender (needle-like), and such protrusions are not normally seen on electrode surfaces; e.g., section 3.1 of \cite{Latham1991} and \cite{Descoeudres2009b,Zadin2014}. Still, this point is far from having been clarified; for example, analysis of deviations from the gas discharge similarity law, observed at high and very high pressures in experiments on discharge ignition and breakdown in corona-like configurations, appears to confirm the existence of the microprotrusions on the surface of the electrodes \cite{2021b}.

Another popular mechanism is a local reduction of the work function of the cathode material, caused by, e.g., lattice defects or adsorbed atoms. However, this effect seems to be insufficient to explain the observed values of the field emission current; e.g., \cite{Sinelnikov2014,Wuensch2019}. Other interesting hypotheses proposed in the literature include ‘nonmetallic’ electron emission mechanism \cite{Latham1991}, enhancement of field emission by waves confined to the metal surface (plasmons) \cite{Wuensch2019}, and mobile dislocations near the surface of electrodes \cite{Engelberg2020}. Thus, there is still no widely accepted understanding of the mechanism of enhancement of field electron emission from cold electrodes in vacuum, in spite of several decades of active research.

What other mechanisms may play a role at the initial vacuum stage of breakdown, apart from field emission, if any? The most popular mechanism is fast heating of cathode protrusions due to shape-related runaway process; works \cite{Kyritsakis2018, Veske2020, Barengolts2019a, Barengolts2019b, Mofakhmi2019,2021k} may be mentioned as recent examples. Other mechanisms mentioned in the literature (e.g., \cite{Descoeudres2009b}) include gas desorption at the anode caused by an intense FE current, melting of a spot at the anode by a heavy bombardment of FE electrons, macroparticles that are released from the electrodes by field induced stresses and subsequently partly evaporated by the FE current, direct field evaporation of surface atoms. The critical transition in the density of the mobile dislocations within a metal was proposed as a vacuum breakdown mechanism in \cite{Engelberg2018,Engelberg2019}.

Other mechanisms come into play as the breakdown develops, in particular, a transition from the field to thermo-field to thermionic emission, vaporization of the electrode material, production of plasma by ionization of the metal vapor, melting of the electrode material, and formation of a crater on the electrode surface with eventual droplet detachment.

\textbf{2. Difficulties in numerical modelling. }The initial stage of breakdown in high-electric field has been simulated in a number of works (e.g., \cite{Kyritsakis2018, Veske2020, Barengolts2019a, Barengolts2019b, Mofakhmi2019,2021k}), however it appears that the whole process, including the formation of craters, has not been simulated in a self-consistent manner up to now. This is in contrast with the cases of spot ignition in low-voltage vacuum arcs and unipolar arcs in fusion devices, where several works dedicated to the modelling of the whole life cycle of a spot have been published; e.g., \cite{2019d} and references therein. Apart from the uncertainty and diversity of the dominating physical mechanisms, the main difficulty lies in the presence of very different length scales. For example, microprotrusions simulated in \cite{Kyritsakis2018} have the tip radius of 3nm and a total height of 93.1nm, while the crater radius is typically a few micrometers or bigger.

\textbf{3. Phenomenological approach. }A phenomenological description of the field electron emission is used in practice: experimental current-voltage

characteristics of field emission from cold electrodes in vacuum are fitted by the Fowler-Nordheim formula with the applied electric field being multiplied by the so-called field enhancement factor β , which has to be of the order of 10^2 or higher; e.g., reviews \cite{Latham1991,Latham1995,Wuensch2019} and references therein.

A correlation of the vacuum breakdown field with the field enhancement factor β , determined by means of analysis of the measured field emission currents, was reported in \cite{Descoedres2009b}. It was found that the product βE_b , where E_b designates the applied DC breakdown field (and hence the product βE_b may be interpreted as an “effective” average microscopic local breakdown field inside the emission center), is a constant value only dependent on the material and not on β or the gap spacing. The value of βE_b around $1.1 \times 10^{10} \text{ V/m}$ was found for copper electrodes.

The existence of this correlation makes it natural to explore the possibility to describe the initial stage of vacuum breakdown within the framework of the same phenomenological approach, i.e., in terms of the field enhancement factor β without invoking any special mechanism for the breakdown apart from the mechanism responsible for the enhancement of field emission. Such an attempt is described in this contribution. A half-space filled with a metal is considered. A surface-directed electric field E_w exists at the half-space surface. The temperature distribution inside the half-space is uniform at 300K at the initial moment and evolves with time under the action of electron emission heating (the Nottingham effect) or cooling at the surface and the Joule heating inside the metal. The evolution of the temperature distribution is simulated by solving the heat conduction and current continuity differential equations in the half-space. The thermal and electrical conductivities of the half-space material are given functions of the local temperature; the dependencies for copper are employed. The electron emission current density at each point of the surface, which serves as a boundary condition for the current continuity equation, is evaluated by means of the Murphy-Good formalism in terms of the local value of the surface temperature and of the electric field equal to βE_w . The heat flux from the surface inside the metal is evaluated with account of electron emission heating or cooling; the boundary condition for the thermal conduction equation.

In the framework of this model, the parameter governing the temperature evolution inside the metal is the product βE_w , rather than β and/or E_w separately, in agreement with the above-mentioned experimental findings \cite{Descoedres2009b}. Two cases have been considered: β is the same at each point of the surface, and β varies along the surface. In the first case, the solution is 1D: heat propagation inside the metal is the same at each point of the surface. If βE_w is high enough, there is a very fast increase of the temperature and the current density at, or very near, the surface: the maximum temperature reaches the critical temperature of copper (8390K) within approximately 2ns for $\beta E_w = 10^{10} \text{ V/m}$ (and within 1 microsecond for $\beta E_w = 0.7 \times 10^{10} \text{ V/m}$, while there is virtually no heating on the microsecond time scale for βE_w below $0.5 \times 10^{10} \text{ V/m}$). At such applied electric field values, the Joule heating underneath the surface comes into play and overtakes the Nottingham effect. This is a manifestation of the so-called thermal runaway. This instability has been extensively studied in the context of low-voltage vacuum arcs (e.g., review \cite{Hantzsche2003}); its shape-related version was studied in the context of high-voltage vacuum breakdown initiated by microprotrusions (e.g., \cite{Kyritsakis2018, Veske2020, Barengolts2019a, Barengolts2019b, Mofakhami2019,2021k}).

Also considered in the modelling was the axially symmetric case where β varied along the surface as a Gaussian function of the distance from the origin with the height of the curve’s peak of 150 and the standard deviation

of 40nm. (Note that the latter value was chosen in accordance with the measurements \cite{Descoedres2009b}, which gave the diameter of the emitting area typically between 20 to 80nm). For $E_w = 10^8$ V/m, the critical temperature was reached within 8ns.

\textbf{4. Conclusions. }It appears to be possible to describe the initial stage of high-voltage vacuum breakdown within the framework of the phenomenological approach, i.e., in terms of the field enhancement factor without invoking any special mechanism for the breakdown apart from the mechanism responsible for the enhancement of field emission. It is of interest to exploit this option in the modelling of advanced stages of vacuum breakdown, which would take into account a transition from the field to thermo-field to thermionic emission, vaporization of the cathode material, production of plasma by ionization of the metal vapor, melting, and formation of a crater with eventual droplet detachment, on the level comparable to that reached in the modelling of the whole life-cycle of spots in low-voltage vacuum arcs and unipolar arcs in fusion devices (\cite{2019d} and references therein).

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Topic:

Modeling and Simulations

Experiments & Diagnostics / 45

Application of Machine Learning to Breakdown Prediction in CERN's High-Gradient Test Stands

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CERN has established several high-power RF test stands, to investigate high-field phenomena. Recently, a machine learning framework has been developed and applied to the high-gradient cavity test data from these facilities. The aim has been to search for the existence of previously unrecognized features related to the incidence of RF breakdowns. Preliminary results have shown two key features in the data which are associated with emerging breakdowns. A general overview of the methodology is provided, the found phenomena are presented, and the plans for future studies are discussed.

Topic:

Field Emission / 46

The influence of carbon layer on the field emission properties of tungsten nanotip at nanogaps

Authors: Yimeng Li^{None}; Guodong Meng^{None}; Zhan Fuzhi¹

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With the rapid miniaturization and integration of electronic and electromechanical devices, especially for vacuum micro/nano electronic devices, it is urgent to study the influence of electrode surface condition on the field emission behaviors at nanoscale and explore its underlying principle. In this paper, the influence of surface carbon layer on field emission of tungsten nanotip was studied based on the in-situ transmission electron microscopy (TEM). Results show that compared to the field emission of nanotip without carbon layer, the presence of carbon layer depressed the field emission characteristics significantly, and during the field emission of nanotip with carbon layer, the soft breakdown (SBD) and hard breakdown (HBD) phenomenon was observed. The results presented in this paper would be of a great help for better understanding the physical mechanism of field emission at nanoscale.

Topic:

Field Emission

Poster Session / 47

Growth of Nb films on Cu substrates by direct current and high power impulse magnetron sputtering: a molecular dynamics study

Authors: Milad Ghaemikermani¹; Alvaro Lopez Cazalilla^{None}

Co-authors: Kostas Sarakinos²; Guillaume Jonathan Rosaz³; Sergio Calatroni³; Flyura Djurabekova¹

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The application of superconducting radio frequency cavities on particle accelerators has brought the need of coating Cu with Nb thin films. Two techniques have been widely used in this field: conventional direct current magnetron sputtering (DCMS) and high power impulse magnetron sputtering (HiPIMS). Experimentally, the application of both techniques has led to different surface morphologies and growth. While in HiPIMS, the surface grows evenly, in DCMS grows in islands or columnar structure forms. We use molecular dynamics to explore the differences between the deposited Nb films on Cu, by mimicking the conditions of each deposition technique. Our computational model reproduces accurately the quality of the Nb-deposited films, based on several features (e.g. surface roughness) when compared with experiments. Moreover, we explore the differences between the two simulated methods focused on the temperature of the sample and the deposition energy, at the atomic level. Our results show that the best temperature for growing the Nb on Cu substrate in the HiPIMS method can be 750 K which leads to a more compact film layer.

Topic:

Modeling and Simulations

Poster Session / 48**Ab initio Investigation of Cu Nanoparticle Behavior Under High Electric Field****Author:** Ye Wang^{None}**Co-authors:** Andreas Kyritsakis ; Tarmo Tamm ; Veronika Zadin**Corresponding Author:** yewang_@hotmail.com

Metal surfaces have inevitable defects, such as dust particles, scratches, and protrusions caused by manufacture. Such defects will generate local electric field enhancement, occur vacuum breakdown, give rise to great damage to metal devices. The Compact Linear Collider (CLIC) in CERN, is one of the important examples where vacuum breakdown may affect the performance efficiency of the entire machine. Based on this, it is necessary to investigate how high electric field affect metal surfaces. In this work, Cu, as a common cathodes material, is chosen to study its behavior under high electric field.

In our preliminary estimates, when increase the bond length between Cu pair and scan its total energy, we obtain a total energy curve with a potential well. Then the same process is operated under electric field, it is observed that the potential well disappeared. After that, external electric field also be added in Cu cell, it can be seen clearly that the surface bend because of the electric fields. Such phenomenon demonstrates that electric field affects the behaviour of Cu nanoparticles, and need to go deeper in further studies.

Topic:

Modeling and Simulations

Modelling & Simulation / 50**Exploring Dependencies of Work Function on Topography and the Application to Micron-scale Field Emission Model for PIC-DSMC Simulations****Author:** Chris Moore^{None}**Co-authors:** Ezra Bussmann¹; Morgann Berg¹; Taisuke Ohta¹; Matthew Hopkins¹ Sandia National Laboratories**Corresponding Author:** chmoore@sandia.gov

We present data from atomic-scale (nm) surface characterization using Scanning Tunneling Microscopy (STM), Atomic Force Microscopy (AFM), and Photoemission Electron Microscopy (PEEM) to show a connection between the surface's local (atomic-scale) work function on the local nanostructure and spatially varying atomic step density. Atomic step-terrace structure is confirmed with scanning tunneling microscopy (STM) at several locations on our surfaces, and prior works showed STM evidence for atomic step dipoles at various metal surfaces. From our model, we find an atomic step edge dipole $\mu = 0.12$ D/edge atom, which is comparable to values reported in studies that utilized other methods and materials. The local field emitted current density from the Fowler-Nordheim

equation has an exponential dependence on both the local E-field at the surface and the work function. Therefore, local variations in the work function can have a significant impact on vacuum arc initiation. Furthermore, here we argue that the existence of low work function regions on an otherwise pure/clean material surface occur due to large atomic step densities which also coincide with locally larger topographic field enhancement of the field and thus have an even larger effect on the field-emitted current density. We have taken the surface characterization data and generated a representative probability density function (PDF) of the work function and field enhancement factor (beta) for a sputter-deposited Pt surface. These PDFs are used in a model that generates stochastic, micron-scale field emission currents for use in Particle-In-Cell Direct Simulation Monte Carlo simulations of vacuum discharge at mm-scales.

Topic:

Experiments and Diagnostics

Excursion / 52

Bus to Chania

Excursion / 53

Guided tour to the archaeological museum of Chania

Excursion / 54

Guided tour to Chania old town

Excursion / 55

Free time in Chania

Excursion / 56

Bus back to OAC

Free discussions & Socializing / 57

FEMOCS collaboration meeting

Author: Tauno Tiirats¹

Co-authors: Andreas Kyritsakis ; Flyura Djurabekova ²; Jyri Kimari ; Roni Koitermaa ²; Veronika Zadin ³

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Open discussion on handling FEMOCS as an open source software

Poster Session / 58

Elemental Theory of Photoemission and Nanoplasmonics

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Photoemission is a widely known physical phenomena that occurs when an electron with sufficient energy strikes the surface of a material and releases an electron. Nanoplasmonics is the manipulation of absorption, scattering and near-field interactions using different materials, shapes and sizes in the nanometer domain.

Topic:

Poster Session / 59

Plasmonics manipulation of Photoemission

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Photoemission plays an important role in several branches of physics. Usually, the photocathodes are covered in layers of photoemissive material to increase the quantum efficiency. Using plasmonics, is it possible to fabricate pure metallic photocathodes that has an increase in the number of emitted electrons?

Topic:

Poster Session / 60

LARGE ELECTRODE SYSTEM MEASUREMENTS OF FIELD EMISSION INDUCED OPTICAL EMISSION SPECTRA

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Optical light spectra have been observed during field emission tests with Cu, CuCrZr, Nb and Ta electrode pairs in the CERN pulsed DC systems. Spectra for Cu and CuCrZr have been reliable and repeatable displaying an increase in light intensity proportional to the field-emitted current. The spectra obtained for Cu-based materials resemble the reflectance spectrum for Cu, which is likely the result of multiple reflections from the Cu surface between the emission point to the vacuum chamber window. Nb and Ta both emitted light for a limited duration of time which stopped after a breakdown, where the breakdown is identified by a spike in pressure. Analysis has shown a correlation between light intensity, detected by both the spectrometer and cameras, and the field-emitted current.

Topic:

Field Emission

Poster Session / 61

PULSED DC HIGH FIELD MEASUREMENTS OF IRRADIATED AND NON-IRRADIATED ELECTRODES OF DIFFERENT MATERIALS

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Beam loss occurs in H- RFQs, and has been observed for example in LINAC4 at CERN. To determine if such beam loss can induce breakdown, and to compare the robustness of different materials, tests have been done in pulsed high-voltage DC systems. Cathodes of different materials were irradiated with 1.2E19 H- p/cm², the estimated beam loss of the LINAC4 RFQ. The irradiated electrodes were tested to observe if the irradiated area had an impact on the breakdown locations. Tests were done using irradiated and non-irradiated electrodes of the same material for comparison. The main differences observed was an increase in the number of breakdowns during the initial conditioning for Cu OFE and TiAl6V4 with little to no difference to the field reached, and significant reductions in achievable field for CuCr1Zr, Ta and Nb.

Topic:

Applications

Poster Session / 62

Field Emission for Medical Imaging

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In a world with a fast-growing and rapidly aging population, where availability and accuracy of diagnosis is key to early detection and treatment of disease and injury, the development of enhanced medical imaging techniques will improve the wellbeing of unwell members of society. The unique features of field emitters can be exploited to develop portable systems for 3D X-ray imaging, that will combine the superior clinical diagnose of 3D with the lower running costs and radiation dose similar to traditional 2D radiography. My poster will showcase main engineering ideas hind this technology, the challenges that prevent its commercialisation and the ongoing research we are undertaking to overcome them.

Topic:

Poster Session / 63

Analysing Cu electrodes with AFM and SEM

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In this work Cu electrodes were characterized with AFM and SEM. The AFM topology map was used to create a field enhancement map of the surface. SEM images show different structures with multi-scale roughness. A hypothesis for CuO protrusion growth on the Cu electrodes is introduced.

Topic:

Experiments and Diagnostics