Chemical Analysis and Imaging of Interfaces Focus Topic
Room A105 - Session CA1+AS+LS+NS+SS+VT-MoM

Modeling, AI, and Machine Learning Applied to Interfaces

Moderators: J. Trey Diulus, NIST, **Kateryna Artyushkova**, Physical Electronics

8:20am **CA1+AS+LS+NS+SS+VT-MoM-1 Topological and Geometric Descriptors of Complex Self-assembly at Liquid Interfaces***, **Aurora Clark**,* University of Utah **INVITED**

Amphiphilic surfactants at liquid/liquid interfaces can form complex self-assembled architectures that underpin interfacial reactivity and transport. This has been demonstrated by surface sensitive spectroscopies and molecular dynamics simulations within the domain of liquid/liquid extraction, which involves solute adsorption, complexation reactions and transport across the phase boundary. Being able to quantify surfactant organization is a significant challenge because the distribution of species is broad and highly heterogeneous. As such, in the analysis of molecular dynamics data, there is significant need to develop descriptors that allow statistical analysis of surface organization. This work presents recent developments based upon geometric measure theory and topological data analysis that are able to identify surface assemblies and their dynamic evolution. These methods are revealing intricate dependencies of surface assembly upon solution composition and the impact this has upon transport mechanisms.

References:

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Alvarado, E.; Liu, Z.; Servis, M. J.; Krishnamoorthy, B.; Clark, A. E. A Geometric Measure Theory Approach to Identify Complex Structural Features on Soft Matter Surfaces, *Journal of Chemical Theory and Computation*, **2020**, *16,* 4579-4587.**DOI:** 10.1021/acs.jctc.0c00260,

9:00am **CA1+AS+LS+NS+SS+VT-MoM-3 Machine Learning and the Future of Surface Analysis***, J. Jones, M. Caouette,* ***Kateryna Artyushkova,*** Physical Electronics **INVITED**

Machine learning can potentially revolutionize all areas of material science and engineering, including surface analysis, by automating and accelerating data acquisition and analysis. The application of machine learning and artificial intelligence (ML/AI) has been actively evaluated and used in scanning probe microscopic methods[1-2], while the application of AI in surface analysis methods such as AES, XPS, and TOF-SIMS is in the very early stages.[3] In this talk, I will discuss the potential areas where AI will change how we do surface analysis.

With recent instrumental development yielding improvements in sensitivity and throughput, the data acquisition stage of surface analysis has become much faster than the experimental planning or data analysis stages, which bothrequire significant operator time and human-based decisions. Using a spectrometer still requires a human operator with instrument-specific knowledge and experience in how to operate it. More importantly, the operator uses physical and chemical knowledge to decide on what specific data must be obtained and from which locations on the sample, depending on the analytical question being addressed by the experiment. Experienced scientists make these decisions effortlessly during the experiment, but it is a very challenging task for ML algorithms that rely on training data with explicit descriptors.

Initial AI applications to analytical surface analysis will focus on instrument optimization and performance inherent in the analytical workflow. Unlike acquisition parameters based on chemical or material science requiring broader context, tuning, and standardizing the spectrometer can be easily cast into numerical terms processable by AI.

Machine learning can also be utilized as a live data integrity monitoring service during acquisition, recognizing and rejecting "bad data". Systemically erroneous data caused by charging or sample damage are often not discovered until the experiment is complete and the data analyzed by a human. Catching it automatically during the experiment saves valuable operator and instrument time. Here, I will present an initial application wherein ML was used to identify whether ToF-SIMS spectra were correctly calibrated.

1.S.V.Kalinin, *ACS Nano*2021, 15, 8, 12604–12627.

2. S.V.Kalinin, arXiv:2304.02048

3. G Drera *et al* 2020 *Mach. Learn.: Sci. Technol.*1 015008

9:40am **CA1+AS+LS+NS+SS+VT-MoM-5 Complexity to Clarity: Detecting, Identifying and Analyzing Complex Materials with Machine Learning***, **Paul Pigram**, W. Gardner, S. Bamford, D. Winkler, B. Muir, R. Sun, S. Wong,* La Trobe University, Australia

Our ability to analyze and understand any physical, chemical, or biological material relies on accurately determining its structure, characteristics, and responses. Contemporary analytical techniques produce large volumes of data from pointwise sample analyses (one dimensional (1D) data), maps of compositional distributions (two dimensional (2D) data), and depth profiles showing composition throughout a sample volume (three dimensional (3D) data).

Correlative analyses linking data from the same sample, obtained by different analytical techniques or different operating parameters, are becoming critically important. Different analytical perspectives on the same sample enhance the richness and depth of the conclusions that can be drawn from it.

Recent advances in analytical science have resulted in an overwhelming avalanche of data – the “big data” problem. In our lab a single time-of-flight secondary ion mass spectrometry (ToF-SIMS) experiment might collect a map (512 x 512 pixels) with 2000 mass spectral peaks of significant intensity in 2 – 10 minutes. These half a billion data points all have differing degrees of significance.

In many cases, only a small number of peaks, 10 – 200, may be judged to be characteristic of a specific sample, and the rest of the data may be discarded. However, there are significant risks that such analyses are biased, and may miss important but subtle trends.

There is a very substantial knowledge gap in our ability to find and make full use of the information and knowledge contained in large scale data sets. This gap is driving rapid international progress in the application of materials informatics and machine learning to analytical surface science.

This presentation will highlight our work on applying artificial neural network approaches to analysis of a variety of very large hyperspectral data sets to better understand complex materials and their interactions.

Vacuum Technology Division
Room C120-122 - Session VT-MoM

Vacuum Measurement, Partial Pressure, and Gas Analysis

Moderators: James Fedchak, National Institute of Standards and Technology, **Yev Lushtak**, Lawrence Berkeley Lab

8:20am **VT-MoM-1 30 Years of Active and Combination Cold-Cathode Gauges***, **Martin Wüest**,* INFICON Ltd., Liechtenstein

It is 30 years since the first high vacuum active total pressure gauges appeared on the market.

Previously the sensors were operated via a cable by a controller. Due to miniaturization of electronics, it became possible to reduce the size of the electronics box such that it could be mounted directly on the feedthrough of the sensor. Not long after the active gauges, the first high vacuum combination sensors appeared on the market, where two different sensors were combined in one package.

We will trace the development of inverted magnetron gauges from their invention in the 1950s, to the active and combination sensors available since 1993/1994 to today’s self plasma optical emission spectroscopy gauges.

8:40am **VT-MoM-2 Enabling Vacuum Process Monitoring with Time-of-Flight Spectroscopy***, **Kristian Kirsch**,* VACOM Vakuumkomponenten & Messtechnik GmbH, Germany

The increasing complexity of industrial vacuum processes requires broader and deeper knowledge of the vacuum itself. A crucial aspect for increasing quality demands is the necessity of in-situ monitoring and control of pressure and residual gas composition within vacuum processes. A consequence of advanced process control is the reduction of production errors, prevention of failures or major damage in combination with increased operating time. Traditional monitoring devices like hot cathodes or quadrupole mass spectrometers are both only able to measure either pressure or residual gas composition. Therefore, these devices are only conditionally suited for complete process control of vacuum processes. With our novel wide-range vacuum monitor NOVION® industrially available pressure and gas analyzation is possible.

In this talk we present the fundamental principles of the novel vacuum monitor and explain the compact combination of well-known time-of-flight spectroscopy with our own patented ion trap. Within different application cases we discuss advantages and limits of this technology and demonstrate with one single device wide range gas analysis, simultaneous measurement of total and partial pressures, leak detection for Helium and detection of air leaks. With these combined capabilities the novel vacuum monitor is able to quickly capture the complete pressure and gas composition measurement at various stages of the vacuum process chain.

9:00am **VT-MoM-3 Remote (100 meters) RGA Operation for High Energy Physics Experiments***, W. Fletcher, A. Nikitin, D. RioPousa, M. Aitken, J. Leslie, S. Johnson, G. Jennings,* MKS Instruments, Inc. Mass Spectrometry Solutions Group, UK*; **Gerardo Brucker**,* MKS Instruments, Inc. Mass Spectrometry Solutions Group

Residual gas analyzers(RGA) are widely considered essential vacuum monitoring instrumentation for both high and ultra-high vacuum processes. High Energy Physics vacuum installations sometimes place RGA sensors within ionizing radiation environments, which can degrade the semiconductor and other components of their control/analysis subsystems. To protect all vulnerable components from such harsh conditions, the electronics control unit (ECU) must be remotely located with respect to the quadrupole mass filter (QMF) subsystem. In such a configuration, the QMF and ECU may be connected via long transmission cables. Bridge cable assemblies include mixed communication paths for conveying (1) information (mass and ion currents), (2) control signals (electrode biases) and (3) power (filament current supply and quadrupole RF drive). The cable assembly must also comprise a coaxial transmission line as required for efficient RF delivery. Critical to the operation *is the delivery of* precisely controlled two phase RF supply signals to the quadrupole subsystem, as required to generate repeatable mass spectra. The RF supply signal amplitude is of the order of hundreds of volts peak (V_{pk}) and its frequency is typically a few MHz. With modern vacuum installation projects demanding cable lengths exceeding 50 meters, our engineering team recently developed a patented methodology for (1) conveying a time-varying voltage signal from ECU to QMF including (2) monitoring and adaptively controlling an amplitude of the time-varying voltage signal at the QMF. A physical length of the transmission line configured to correspond to an electrical length substantially equal to a positive integer multiple of one-half wavelength of the time-varying voltage signal allows the transmission line to operate resonantly and adaptively control the amplitude of the time-varying voltage signal from the ECU for cable lengths exceeding 100 meters.

9:20am **VT-MoM-4 Prospects for Wide-Range, Primary Pressure Sensing with Tethered Optomechanics***, **Daniel S. Barker**, Y. Bao, J. Lawall, J. Gorman, J. Scherschligt,* National Institute of Standards and Technology

We present our initial tests of the pressure sensing performance of silicon nitride membranes and trampolines. The damped motion of these micromechanical systems is calculable using the kinetic theory of gases and can be measured with optical interferometry. We assess the accuracy at which kinetic theory predicts the sensor response via comparison with a capacitance diaphragm gauge transfer standard. The intrinsic thermomechanical damping of our current devices restricts their linear operation to the medium vacuum range (0.1 Pa to 100 Pa). Refinements to both the device design and optical readout system will allow field-deployable, chip-scale sensors with range extending below 10^{-4} Pa.

9:40am **VT-MoM-5 Novel Diaphragm Vacuum Gauge: Q'zGauge (QZG)***, **Masatoshi Ono**, S. Goto, H. Motoyama, H. Hojoh,* Vacuum Products Co., Japan **INVITED**

Among practical gauges, only diaphragm gauges give the pressure independent of gas species. Highly accurate (error of 0.2 %) capacitance diaphragm gauges (CDG) are used for process control of semiconductor fabrication, for example. The gauges have several problems, such as (a) Limited pressure range of two decades, (b) Possible measurement error of about 3% in molecular flow region due to thermal transpiration effect, (c) Startup time of a few hours, and (d) Necessity of stable room environment.

For overcoming these problems, we developed an accurate diaphragm gauge for wider pressure range, by using twin diaphragms and a quartz crystal oscillator, and named Q'zGauge (QZG). The head of the gauge, alike a drum in shape, consisted of a hollow metal barrel with a Inconel diaphragm welded at each end. The diaphragms, of 12 mm in diameter and 100 µm in thickness, were bridged at their centers with the oscillator, called "dual tuning fork resonator" , which showed large frequency change for longitudinal stress caused by deflection of the diaphragms. The inside of the head was kept at high vacuum. The resonant frequency was about 40 kHz without stress, and changed about 6% for the stress corresponding to pressure of 100 kPa which gave 3.5 µm of deflection of the diaphragms.

Through optimized design, taking into account of the temperature characteristics of the oscillator and gage head material, the sensitivity of the gauge, the ratio of change in pressure reading to that of the frequency, was almost constant, but shows slight temperature dependence. This dependence was measured with a thermistor attached to the head and used in the pressure calculation which made it possible to give an accurate pressure without a constant temperature oven.

The uncertainty of reading was 0.001 Pa for pressure range of 100 kPa to 0.1 Pa. This range was equivalent to that of more than two CDGs gauges.

Problems:

(a) Pressure range of QZG was more than four decade,

(b) and (c) problems peculiar to a constant temperature oven were unrelated to QZG.

(d) Influence of AC circuits of the controller in the ambient temperature and humidity was negligibly small on QZG's resonant frequency.

These performances of QZG were realized mainly by extremely high Q of the oscillator.

The deflection of the diaphragm was far smaller than the plastic deformation. This fact eliminated necessity of a cut off valve for protecting the damages of the diaphragms. This valve was essential to CDGs with maximum pressure of less than 10 kPa.

The similar tuning fork quartz oscillators have been used widely for wrist watches. This fact also made us expect reliable long life of Q'z Gauges.

10:40am **VT-MoM-8 A Demonstration of the Portable Cold Atom Vacuum Standard as a Pressure Sensor***, **Stephen Eckel**, D. Barker, J. Fedchak, J. Scherschligt,* NIST

We will demonstrate, live, the use of the portable cold atom vacuum standard as a pressure sensor. Cold atom vacuum standards use the loss rate of cold atoms from a conservative trap to measure the vacuum pressure. Because the collision cross section between a cold atom and a background gas particle can be calculated from first principles, such gauges are also primary standards. We will describe and show how these pressure readings are taken, including the preparation of the cold atom cloud, readout, and the conversion between loss rate and pressure. We will also describe the known specifications of this cold-atom-based vacuum gauge, including its range of operation, readout time, and overall precision.Our live demonstration will hopefully convince a skeptical audience of the ability of the portable cold atom vacuum standard to supplant ionization gauges for pressure sensing in the ultra-high vacuum.

11:00am **VT-MoM-9 Update on Construction of the Vacuum Fixed Length Optical Cavity Pressure Standard***, **Jacob Ricker**, K. Douglass, J. Hendricks,* NIST

Over the past few years, NIST has constructed and tested several Fixed Length Optical Cavity (FLOC) Pressure Standards for measuring gas pressure using refractometry. This refractometry technique has been shown to have similar uncertainty to the best primary standards in the world. NIST is currently constructing the next generation FLOC which will aim to have a resolution of below 5e-8 Torr. This FLOC will help span the gap in quantum traceable pressure standards between the Cold Atom Vacuum Standard and the existing FLOC performance.

Critical to our goals is construction of a high reflectance/narrow linewidth optical cavity. This presentation will update on the construction and fabrication of components for this next generation FLOC. Additionally, we will discuss the temperature control systems and temperature stability as it directly relates to our ultimate performance. Lastly, the goals and next steps to this project will be outlined.

11:20am **VT-MoM-10 Mfig a Mass Filtered Ion Gauge***, **Freek Molkenboer**, H. Bekman, T. Mechielsen, D. Elstgeest, Y. Westland, J. Emmelkamp, M. Haye, H. Lensen,* TNO Science and Industry, the Netherlands

In 2008, TNO introduced a sensor capable of detecting heavy hydrocarbons in vacuum systems at extremely low concentrations. In 2019, TNO embarked on the development of the third generation of this sensor, known as the Mass Filtering Ion Gauge (MFIG). To optimize the MFIG sensor's design, COMSOL modeling was utilized. The modeling allowed for the precise optimization of specific elements' geometric layout and size within the sensor, making it unique in its performance capabilities.

Through this approach, a highly sensitive sensor has been developed that is capable of measuring volatile organic compounds (VOC) contamination in high vacuum systems. The sensor operates in both transient and continuous regimes, outperforming state-of-the-art RGA technology in detecting a wide range of contamination. Additionally, the MFIG sensor exhibits the ability to detect ultra-short bursts of VOC contamination. These unique selling points offer distinct advantages that are valuable to industries where VOC contamination is a critical concern. Ultimately, this advanced sensor technology has the potential to increase yield and productivity in such sensitive fields.

To validate the performance claims of the MFIG sensor, extensive testing was conducted in laboratory environments both internally at TNO and by external companies, as part of the European ECSEL MADEin4 program which facilitated the development of this third generation sensor.

During the presentation, a detailed overview of the MFIG sensor's general concept will be provided, followed by a presentation of the experimental results obtained from the testing process.

Chemical Analysis and Imaging of Interfaces Focus Topic
Room A105 - Session CA+AS+LS+NS+SS+VT-MoA

Environmental and Energy Interfaces

Moderators: Musahid Ahmed, LBNL, **Xiao-Ying Yu**, Oak Ridge National Laboratory, USA

1:40pm **CA+AS+LS+NS+SS+VT-MoA-1 In situ Spectroscopies of Interfacial Reactions and Processes in Batteries***, **Feng Wang**,* Argonne National Laboratory **INVITED**

The performance and lifetime of batteries, whether they are traditional lithium-ion, solid-state, or other types, strongly depend on the effectiveness and stability of electrochemical interfaces within the devices. To design battery materials and interfaces with desired functionality, it is crucial to have a mechanistic understanding of the interfacial reactions and processes occurring during battery operation. This necessitates developing advanced techniques capable of characterizing local structures and capturing *non-equilibrium* dynamics at electrochemical interfaces, with the relevant spatial, time resolution and chemical sensitivity, both to light elements (H, Li, O) and heavy ones. Herein, we present the development and application of *in situ* spectroscopies specialized for probing interfacial reaction and processes in lithium-ion and solid-state batteries. With specific examples from our recent studies, we will show how to correlate the structure and function of electrochemical interfaces through *in situ* spectroscopy characterization, thereby gaining insights into the design and processing of battery materials, electrolytes and other components. Towards the end of this talk, we will discuss emerging opportunities in data-driven experimentation, analysis, and modeling for closed-loop battery development to accelerate the transition from lab discovery to commercial deployment.

2:20pm **CA+AS+LS+NS+SS+VT-MoA-3 Novel Strategies for the Characterization of the Next-Generation Energy Storage Materials by ToF-SIMS: From an in-Situ Exploration to an Operando Measurement***, **Tanguy Terlier**, Q. Ai, S. Sidhik, A. Mohite, J. Lou,* Rice University **INVITED**

Recently, advances in instrumentation and sample preparation have permitted a rapid development for characterizing a wide range of applications such as next-generation energy storage materials. Developing new materials is one of the most crucial topics for emerging technologies. However, the complexity of these materials in their structures makes them particularly challenging for numerous characterization and analytical techniques. Exploring chemical composition and the potential chemical reactions such as degradation, diffusion, or doping is crucial to understand advanced materials and to transfer the new technologies to the industry. Among the most suitable characterization tool, time-of-flight secondary ion mass spectrometry (ToF-SIMS) is a very sensitive surface analytical technique providing detailed elemental and molecular information about the surface, thin layers, interfaces, and full three-dimensional analysis of the samples.

Thanks to the advances in ToF-SIMS characterization, understanding of the chemical composition and the different components in the complex structures, permit a deeper exploration and a better knowledge in the next-generation energy storage materials such as batteries, perovskites, and 2D materials.

Firstly, we will focus on the characterization of batteries. Initially, we will discuss the sample preparation and our specific setup for transferring the specimens from the inert atmosphere in the glovebox to the ultra-high vacuum chamber of our instrument. We will illustrate the possibility to study the reversibility of the chemical composition between pristine, charged, and discharged batteries using surface mass spectrometry by ToF-SIMS in operando conditions. Then we will compare three methods of cross-sectioning used to identify the interfacial species in a composite cathode.

Secondly, we will show a study of an in-depth distribution of the 3D/2D heterostructures for perovskite solar cells where we have been able to identify individually the 3D and 2D heterostructures along with the depth of the film. Then, we will illustrate the characterization of interdiffusion in quasi-2D perovskite light-emitting diodes as a function of the organic ligand layer inserted into the perovskite crystals.

Finally, we will demonstrate how the retrospective analysis using ToF-SIMS can be very powerful and useful for exploring any single feature in 2D materials. Typically, ToF-SIMS acquisition is recording a full mass range spectrum per pixel (or voxel), which permits to isolate and to decorrelate specific regions of interest for resolving interfaces, diffusion, and doping in thin 2D structures. We will present how to treat a 3D volume image of a multilayer perovskite device for extracting useful information.

3:00pm **CA+AS+LS+NS+SS+VT-MoA-5 Advanced In-Situ and Ex-Situ S/TEM Probing of Interfacial Process in Rechargeable Batteries***, **Chongmin Wang**,* Pacific Northwest National Laboratory

In-situ diagnosis appears to be one of the essential methods for gaining insights as how an electrode material failure, therefore feeding back for designing and creating new materials with enhanced battery performances. In this presentation, I will highlight recent progress on ex-situ, in-situ and operando S/TEM for probing into the structural and chemical evolution of interfacial process in energy storage materials. Both ex-situ and In-situ high resolution imaging enables direct observation of structural evolution, phase transformation and their correlation with mass, charge and electron transport, providing insights as how active materials failure during the cyclic charging and discharging of a battery. In perspective, challenges and possible direction for further development of the in-situ S/TEM imaging and spectroscopic methods for energy storage materials and other field will also be discussed. Most importantly, integration of different analytical tools appear to be the key for capturing complementary information.

3:20pm **CA+AS+LS+NS+SS+VT-MoA-6 Investigating sp^2 and sp^3 Carbon Ratios by XPS: A Study of the D-Parameter and a New Second Plasmon Loss (2PL) Parameter***, **Alvaro Lizarbe**, G. Major, B. Clark,* Brigham Young University*; D. Morgan,* Cardiff University, UK*; M. Linford,* Brigham Young University

The D-parameter provides a useful estimate of the ratio of the sp^2 and sp^3 carbon in a sample. It is the energy difference between the maximum and minimum of the derivative of the C KLL Auger peak. The D-parameter can be an important analytical resource for diamond samples, as the quality of diamond depends on the sp^3 to sp^2 carbon ratio and any lattice impurities. For example, the highly sought after type 2a diamonds, which are colorless and free from impurities, consist almost entirely of sp^3 carbon. According to the universal curve for XPS, electrons with different kinetic energies have different mean free paths. Thus, electrons with different kinetic energies sample materials at different depths. In the case of carbon, the KLL Auger peak comes shallower in a material compared to the C 1s signal, which is a result of electrons with much higher kinetic energies. That is, a limitation of the D-parameter is that it is based on the C KLL Auger peak, found at around 1220 eV, while it is often related to the C 1s peak located at approximately 284.8 eV. Thus, the D-parameter is much more sensitive to adventitious carbon contamination. In an effort to derive a parameter that will be more representative of the amounts of sp^2 and sp^3 carbon in a material, we have examined the plasmon loss peaks of the zero-loss C 1s peak of direct current chemical vapor deposition (DC-CVD) diamonds, carbon nanotubes, and graphitic materials such as HOPG. By analyzing the second plasmon loss signal of the C 1s narrow scan, we obtain a new parameter for analyzing carbonaceous materials: the 2PL parameter. The 2PL parameter is the difference in energy between the second plasmon loss signal and the C 1s peak. We compare the traditional D-parameter with the 2PL parameter for various materials. They correlate quite well. We have also investigated various mathematical methods of deriving the 2PL parameter, including via a weighted average of the second plasmon loss and C 1s signals. Ultimately, because the 2PL parameter involves signals that are closer to the C 1s photoemission binding energy, we believe it may be more representative of the full chemistry of carbonaceous materials.

4:00pm **CA+AS+LS+NS+SS+VT-MoA-8 Solid-Liquid Interfaces for Energy-efficient Chemical Separation of Critical Minerals and CO_2 Conversion***, **Manh-Thuong Nguyen**, V. Prabhakaran, D. Heldebrant, G. Johnson,* Pacific Northwest National Laboratory **INVITED**

Chemical separations consume around 15% of the energy used by industry today. It is thus critical to develop energy- and material-efficient approaches for large-scale separations. In the first part of this presentation, I will illustrate how we employ modified 2-dimensional materials and solvents to separate critical minerals including rare earth elements. Polar functional groups present at the interface of graphene oxide laminate membranes are demonstrated to improve the selectivity of metal cations separated by both adsorption and sieving. Hydrophobic ionic liquid molecules including 1-ethyl-3-methylimidazolium chloride, when used as a minor solvent component, are shown to increase the energy efficiency of the desolvation of aqueous lanthanide cations in electrochemical separations. In the second part, I will present studies exploring the use of functionalized hexagonal boron nitride (h-BN) membranes to separate CO_2

from multicomponent gas mixtures. Strategies for improving CO_2 separation selectivity and efficiency, such as chemical functionalization and engineering the dimensions of interlayer transport channels, will be discussed. Finally, I will present studies on the electrochemical conversion of CO_2 into value added chemical feedstocks such as methanol on membrane-supported catalysts. Insights into the effects of local structure modification and confinement on catalytic processes will be presented.

4:40pm **CA+AS+LS+NS+SS+VT-MoA-10 Buried Interfaces of Ir Photodetector Devices Analyzed with Lab-Based Xps/Haxpes***, **Roman Charvier**, M. Juhel,* STMicroelectronics, France*; O. Renault,* Univ. Grenoble-Alpes, CEA, Leti, France*; A. Valery, D. Guiheux, L. Mohgouk Zouknak,* STMicroelectronics, France*; B. Domenichini,* ICB UMR 6303 CNRS-Université de Bourgogne, France

The development of new IR photodetectors should respond to challenges in order to reach best performances. A major objective is to understand critical interfaces that play an important role in the final device properties. This work addresses to chemical analysis of molybdenum oxide (MoO_{3-x}) used as hole transport material which is deposited between a photosensitive material and top electrode often made of indium-tin oxide (ITO). Such critical interfaces are typically located under 20 to 50 nm under the surface.

In the case of MoO_{3-x}, the stoichiometry is generally controlled by X-ray photoelectron spectroscopy (XPS) which is well-known to obtain chemical data close to the material surface (analysis depth < 10 nm). Two methods can be used to analyse deeper buried layers: (i) the use of hard X-rays to perform Hard X-ray PhotoElectron Spectroscopy (HaXPES) and thus generate photoelectrons having a kinetic energy able to go through several tens of nm; (ii) the etching of the surface by means of an Ar^+ beam (having an energy from 0.5 to 3 keV) in order to remove the superficial layers giving access to the underlying layers. In the former case, the analyzed thickness remains far below 100 nm while in the latter case, the chemistry of the surface atoms are often modified by argon ion beam. It is then necessary to mix the two approaches to allow the chemical analysis of buried interfaces. This analysis way is used here to characterize the stoichiometry of MoO_{3-x} thin films buried under 50 nm of ITO using chromium Kα hard-X-ray from lab-based HaXPES.

5:00pm **CA+AS+LS+NS+SS+VT-MoA-11 Detection and Discrimination of Aquatic Toxins Targeting Voltage Gated Sodium Channels Using Static ToF-SIMS Imaging***, **Jiyoung Son**, K. Engbrecht, J. Mobberley,* PNNL

Neurotoxins from aquatic microorganisms, such as cyanobacteria and algae, have been a public health concern due to their harmful impacts on the nervous systems of animals, including humans. A subset of these neurotoxins, including saxitoxin and brevetoxin, bind to and alter the function of voltage-gated sodium channels, which are essential to generating the cell membrane action potential. Existing detection and categorization methods, such as PCR and antibody-based enzyme-linked immunosorbent assays, are too specific and they require live animals like the mouse bioassay. They also require time-consuming and expensive sample preparation for analysis using LC-MS/MS and HPLC. In this project, we developed a method to detect the activity of the aquatic sodium channel neurotoxins, brevetoxin and saxitoxin, using a cell-based process. We specifically examined the impact of these two neurotoxins on HEK-293 cells, a robust cell line that has been transfected with a voltage-gated sodium channel gene, SCN1A, in order to better study neurotoxins. We cultured a layer of cells onto disinfected silicon chips, exposed the cells to neurotoxins, performed chemical fixation, and then air-dried the chips. We also prepared mock exposed samples where the cells on the silicon chips were not exposed to neurotoxins, but just the solutions each neurotoxin was resuspended in, either a 3mM HCl solution (mock saxitoxin) or a 50:50 ACN: water solution (mock brevetoxin). Control samples, which just exposed cells to cell culture media only, gave us a baseline reference. Dried samples were analyzed with mass spectral imaging using time-of-flight secondary ion mass spectrometry (ToF-SIMS). After collecting a series of spectral data, we utilized an in-house MATLAB tool to run principal component analysis (PCA) as previously described (Yu et al., 2020). Our initial statistical analysis of SIMS spectral data using PCA shows a noticeable difference in peak trends between neurotoxin and mock-exposed cells as well as neurotoxin-exposed and control cells. Our approach utilizes chemical imaging to develop a threat-agnostic model system for detecting and classifying neurotoxin activity. The technology and protocols developed from this work could transition to other rapid cellular assays for pathogenic and chemical threats.

Reference

Yu, J., Zhou, Y., Engelhard, M. *et al.In situ* molecular imaging of adsorbed protein films in water indicating hydrophobicity and hydrophilicity. *Sci Rep***10**, 3695 (2020). https://doi.org/10.1038/s41598-020-60428-1

Vacuum Technology Division
Room C120-122 - Session VT-MoA

Leaks, Flows, and Material Outgassing

Moderators: Giulia Lanza, SLAC National Accelerator Laboratory, **Chandra Romel**, Consultant

1:40pm **VT-MoA-1 Cesium Intercalation of Graphene: A 2D Protective Layer on Alkali Antimonide Photocathode***, **Mengjia Gaowei**,* Brookhaven National Laboratory **INVITED**

Alkali antimonide photocathodes have wide applications in free-electron lasers and electron cooling. The short lifetime of alkali antimonide photocathodes necessitates frequent replacement of the photocathodes during a beam operation. Furthermore, exposure to mediocre vacuum causes loss of photocathode quantum efficiency due to the chemical reaction with residual gas molecules. Theoretical analyses have shown that covering an alkali antimonide photocathode with a monolayer graphene or hexagonal boron nitride protects it in a coarse vacuum environment due to the inhibition of chemical reactions with residual gas molecules. Alkali antimonide photocathodes require an ultra-high vacuum environment, and depositing a monolayer 2D material on it poses a serious challenge. In the present work, we have incorporated a novel method known as intercalation, in which alkali atoms pass through the defects of a graphene thin film to create a photocathode material underneath. Initially, Sb was deposited on a Si substrate, and a monolayer graphene was transferred on top of the Sb film. Heat cleaning around 550–600 °C effectively removed the Sb oxides, leaving metallic Sb underneath the graphene layer. Depositing Cs on top of a monolayer graphene enabled the intercalation process. Atomic force microscopy, Raman spectroscopy, x-ray photoelectron spectroscopy, low energy electron microscopy, and x-ray diffraction measurements were performed to evaluate photocathode formation underneath the monolayer graphene. Our analysis shows that Cs penetrated the graphene and reacted with Sb and formed Cs_3Sb.

2:20pm **VT-MoA-3 On Ground and In-Orbit Decontamination Strategies for Space Hardware***, **Delphine Faye**,* Centre National d'Etudes Spatiales, France **INVITED**

Lessons learnt from the past have led to anticipating space equipment failures that may be caused by the presence of chemical contaminants resulting mainly from outgassing of polymer materials under vacuum[1].

Nowadays, when on-board instruments are becoming more and more sophisticated, when constraints are becoming more and more stringent in terms of quality and reliability for an extended mission duration, controlling both molecular and particulate contamination levels is a necessity and must be applied throughout the various phases of development and operation of a spacecraft. In order to maintain optimum performance of all equipment until the end of the mission, it is of paramount importance to mitigate the risks of degradation. This requires basic precautions not only in design and manufacturing but also and above all in integration and testing where a clean environment is highly recommended[2].

However, if there are very strict rules for selecting space materials, if thermal pre-treatments under ultra-high vacuum are performed at different stages of assembly, a residual outgassing potential of some materials often remains to be considered. As a result, undesirable matter may be deposited on sensitive surfaces and evolve depending on in-orbit environmental conditions. Thus decontamination strategies must be foreseen whether on ground or in orbit, at the very beginning of life or when anomaly occurs. To do this, there are conventional cleaning processes but interesting alternatives are also being studied e.g. for cleaning especially with non-contact techniques or for trapping contaminants under vacuum[3].

After a brief reminder of contamination issues for space sub-systems, this talk will present feedback from several use cases on specific projects. Different methodologies and associated techniques will be described as preventive or corrective actions as well as recent Research and Technologies developments[4].

references

1.A.C. Tribble, “fundamentals of contamination control”, SPIE Press, 2000

2.ECSS-Q-70-01C, “Space Product Assurance, Cleanliness and contamination control”, 2008

3.ECSS-Q-70-54C, “Space Product Assurance, Ultracleaning of flight hardware”, 2017

4.D. Cheung, D. Faye, “Evaluation of decontamination processes adapted to large optical components” International Symposium on Contamination Control 2018, The Hague, Netherlands, 23-26/09/18

3:00pm **VT-MoA-5 Helium Permeation Through Zerodur Glass*, Sefer Avdiaj*,** University of Prishtina, Albania

In the pursuit of a new optical pressure standard [1], Ultra-Low Expansion (ULE) glass cavities were proposed as a means of measuring helium refractivity. However, the utilization of ULE glass gave rise to certain complications, with the pumping effect on helium being a significant issue [2]. As a solution, Zerodur glass was suggested as an alternative material for the cavity. To estimate the flow of helium gas through Zerodur glass, knowledge of the permeation constant K and the diffusion constant D is necessary. These parameters are related through the solubility S of helium in glass, as $K = S \cdot D$. In this research work, we experimentally measured the permeation of helium gas in Zerodur over a temperature range of 27 – 120 °C. Our results indicate that Zerodur has potential as a material for the new quantum standard of pressure.

3:20pm **VT-MoA-6 Improvement and Verification of Modified Knudsen Equation to Calculate the Gas Flow Rate through a Cylindrical Tube in Various Flow Regimes*, Hajime Yoshida,*** AIST, NMIJ, Japan

Calculating the gas flow rate through a cylindrical tube of known geometry might seem to be a simple problem but is actually rather complicated. This is because the characteristics of the gas flow depend on pressure, gas species, temperature, tube diameter, and tube length. There are at least six flow regimes to explain the characteristics of the gas flow, such as molecular flow, viscous laminar flow, turbulent flow, critical flow, subcritical flow, and their intermediates including slip flow.

In recent, we have developed the modified Knudsen equation which is applicable to the whole flow regime for arbitrary length of the tubes [1,2]. This equation has two advantages; one is that this equation is used without considering Knudsen number, Reynolds number, Mach number and the length-to-diameter ratio of tube, and the other is that it can be solved in straight forward without an iterative procedure although the other equations sometimes need it. This equation is especially useful when one does not know which flow regime the gas flow is in.

The solution of the modified Knudsen equation agreed with typical previous studies within 20 % - 30 %, but more study was still needed to confirm if this equation would be truly used for “whole” flow range. 70 literatures reported so far were compared with the modified Knudsen equation. The results reveal the conditions that the relatively large differences between them were observed. The author improved the modified Knudsen equation so that the agreements became within 20 % by introducing the effective length of turbulent flow. On the other hand, it was also found that significant differences around 50 % were observed at the high Reynolds number flow of short tubes. The improvement of modified Knudsen equation and comparison of the calculations of improved modified Knudsen equation with 70 literatures will be presented.

[1] H. Yoshida, Y. Takei and K. Arai, Vacuum and Surface Science 63 (2020) 373.

[2] H. Yoshida, M. Hirata, T. Hara, Y. Higuchi, Packag Technol Sci. 34 (2021) 557.

4:00pm **VT-MoA-8 Dirty Vacuums - To Contamination and Beyond*, Rod Boswell,*** *C. Charles, M. Davoodianidalik, J. Richmond, M. Shadwell,* Australian National University, Australia

With the recent global interest in space centred around the moon and Mars there is a real need for environmental test facilities that closely mimic lunar and Martian conditions. The challenges centre around two phenomena: vacuum and dust and both challenge mechanical sliding and rotating mechanisms, thermal control, space suits, interaction with charged particle and photon radiation.

Our group and Boswell Technologies has embarked on a number of projects aimed at investigating the basic physics and engineering problems posed by these environmental conditions and also to make available large dirty vacuum systems for research and industry to test systems in a dirty aggressive environment. In particular the lunar regolith comprises sharp edged dust with dimensions down to micrometres what can wreak havoc with moving systems especially human space suits where the dust apparently “burrows” into the material spurning all attempts to remove it. It is considered that photo-electrons generated by Lyman Alpha from the sun results in charged dust levitating from the surface and coating everything.

We have constructed a 3 metre diameter concrete dome and successfully vacuum tested it down to conditions close to that found on Mars. The design was inspired by habitats fabricated for those who, believing the arrival of imminent Armageddon, desired to protect themselves in these structures buried in the Australian sub-soil........ Smaller vacuum systems of a few hundred litres are being used to approach lunar conditions with pressures around 10^{-6}Torr. For both chambers care needed to be taken with the structural integrity, dust and vacuum pumps and the onerous conditions of Work Health and Safety…….

A Lyman Alpha source has been developed and tested using rf energised hydrogen plasmas and magnesium fluoride windows. Initial tests have demonstrated the generation of photo-electrons by VUV radiation and absolute calibrations are being carried out with a commercially available VUV spectrometer and a VUV Deuterium source.

4:20pm **VT-MoA-9 Outgassing Studies of A36 Mild Steel*, James Fedchak,*** *E. Newsome, D. Barker, S. Eckel, J. Scherschligt,* NIST-Gaithersburg

We present our most recent outgassing results for A36 mild steel. Mild or low-carbon steel is commonly used for structural applications and for piping. Modern secondary refining processes reduce the hydrogen content in mild steel, thus making these steels excellent candidates as low-outgassing materials for the construction of ultra-high vacuum chambers. Indeed, results from a 2016 paper by Park et al.[1] show H_2 outgassing rates for three Korean mild steels to be much lower than those from untreated stainless steel. Stainless steels such as 316L or 304L are commonly used for vacuum chamber construction, but for ultra-high vacuum or extreme-high vacuum applications, these steels must typically be heat-treated by vacuum-firing (nominally a 950 °C bake under vacuum for several hours) or subjected to a medium heat treatment (>400 °C bake in vacuum or air for several days) to achieve the required H_2 outgassing rate. However, untreated mild steel has the potential to achieve similar outgassing rates as heat-treated stainless steel. This could significantly impact the construction of future gravity wave detectors and other large vacuum systems because of the potential to reduce the cost compared to vacuum systems constructed of stainless steel which is both more expensive and must be heat-treated. We present results for both H_2 and H_2O outgassing. The former is measured after most of the water has been removed from the vacuum system by low-temperature bake (150 °C or less) with the system under vacuum. The water outgassing rate is measured during the system pump down prior to the baking the system to remove water, and is critical to many large vacuum system users as this affects the time and cost of commissioning.

[1] C. Park, T. Ha, and B. Cho, J. Vac. Sci. Technol. A Vacuum, Surfaces, Film. **34**, 021601 (2016).

Vacuum Technology Division
Room C120-122 - Session VT-TuM

Particle Accelerators and Large Vacuum Systems

Moderators: Julia Scherschligt, National Institute of Standards and Technology, **Steven Wulfsberg**, SAES Getters USA

8:00am **VT-TuM-1 Study on a Pressure Anomaly Detection Method Applying Machine Learning in SuperKEKB Accelerator Vacuum System***, **Yusuke Suetsugu,*** High Energy Accelerator Research Organization (KEK), Japan

A large-scale vacuum system of the SuperKEKB accelerator has been running well since the first commissioning in 2016. However, owing to the large beam currents and the high frequency of beam loss and re-injection, air leaks from connection flanges due to thermal cycles caused by the intense synchrotron radiation etc., and irregular pressure rises due to discharging etc. have been often observed. Sometimes, they resulted in serious troubles which interrupt the beam operation. If any signs of abnormal pressure are detected before a usual alarm is issued or before machine operators notice the abnormality, quick countermeasures can be taken before the major troubles occurs. We are proposing and studying an anomaly detection method applying machine learning to detect the signs of pressure anomalies and call attention to operators as early as possible. First, a typical beam-filling cycle is defined as the period from the beam (re-)injection, storage, and abort. For each of the approximately 600 vacuum gauges in the main ring, the measured values for three days from eight days before the beam-filling cycle to be checked are defined as the "standard data", which include several beam-filling cycles. Then the regression curve for the behaviors of pressures during a beam-filling cycle is derived using the standard data against beam current (beam injection and storage) or time (just after beam abort). Second, for every beam-filling cycle to be checked, the standard errors are calculated from the measured pressure values during the cycle ("measured data") using the obtained regression curves. Using the ratio of the standard error of the measured data to that of the standard data and so on as feature quantities, the behavior of pressure is judged to be "normal" and "abnormal" (2 class classification) utilizing a two-layer neural network. The classification criteria are previously learned from actual abnormal behaviors of pressures when vacuum troubles occurred since 2016. A simulation test using the actual beam abort events from May 2022 showed that signs of pressure anomalies can be detected. Here we report on the status of the study on this pressure anomaly detection method.

8:20am **VT-TuM-2 NEG Coating for PETRA IV: Resistivity and Sticking Probability Measurements***, **Ruta Sirvinskaite**, L. Lilje, S. Lederer, R. Boespflug, N. Plambeck, S. Antipov, M. Schroeder, A. Winiarska,* DESY, Germany

Non-Evaporable Getter (NEG) development at DESY has been ongoing to accommodate PETRA IV machine requirements. While most of the PETRA IV beam vacuum chambers will be manufactured from oxygen-free silver-bearing (OFS) copper and coated with NEG, getter film performance on these substrates has not been tested as extensively as on the stainless-steel. In order to investigate pumping and impedance properties of the columnar NEG films, TiZrV and Zr layers with varying thicknesses were sputtered on four Cu-OFS tubes. The 1 µm films were activated at temperatures ranging from 140 to 250 °C to determine how the sticking probability as well as CO pumping capacity develops over time after multiple saturations prior to increasing the activation temperature. By measuring the attenuation of the RF signal along the four tubes, resistivity of both NEG materials was calculated. The results were then compared to previously reported findings for columnar NEG films.

8:40am **VT-TuM-3 Vacuum System for Cornell Brookhaven Energy Recovery Linac Test Accelerator***, **Yulin Li**, D. Burke,* Cornell University

A novel electron accelerator, Cornell Brookhaven Cornell Energy Recovery LINAC Test Accelerator (CBETA) has been successfully designed, constructed, installed and commissioned by collaboration between CLASSE and Brookhaven National Laboratory.Many unique accelerator technologies are implemented in CBETA, including photo-cathode electron injector, 4-turn superconducting RF (SRF) Energy Recover LINAC (ERL), non-scaling Fixed-Field Alternating Gradient (NS-FFAG) optics with 4x energy acceptance.The CBETA layout consists of an existing photo-cathode injector with an SRF cryomodule (ICM) as well as a main LINAC cryomodule (MLC), a NS-FFA return loop (that transports electron beams at four energies, 42, 78, 114 and 150 MeV in a single bore beampipe), and two splitter sections where the four energy beams are separated and combined. The total circumference of the CBETA loop is about 80-m.The basic requirement of the CBETA vacuum system is to achieve an adequate level of vacuum and physical aperture for transporting electron beams at four different energies.Furthermore, by the nature of this test accelerator, the vacuum system engineering must accommodate a very high density of beam diagnostics tools, such as over 150 beam position monitors, and insertable beam profile viewers.Beam path length change of up to 20° RF-phase are achieved in the splitter sections via one set of three RF-shielded sliding joints mounted on a pair of motorized stages in each of the eight-splitter beam lines.Aluminum alloy was chosen as primary beampipe construction material because of its good electric conductivity (resistive-wall), no residual radioactivity (from beam losses), low magnetization (from cold work and welding etc.) as well as its low cost of fabrication (machining, extrusion, etc.).Compact non-evaporable getter (NEG) pumps are used due to the space constraints.To preserve the high performance of the superconducting RF cavities in the MLC, all vacuum beam line components were constructed and assembled in strict particulate-controlled condition, and installed using portable clean rooms.The CBETA vacuum system installation was completed in the summer of 2019 and the entire CBETA accelerator system was commissioned shortly after.All CBTA milestones were successfully achieved, including full beam energy recovery after 8 turns of beam circulations through the SRF cavities and the NS-FFA return loop.We present the CBETA vacuum component construction and installation, and the vacuum system operational experiences.

9:00am **VT-TuM-4 Operational Experiences of NEG Dominated Pumping System at CHESS-U***, **Leila Aboharb**,* Cornell University

Successful operations of the Cornell High Energy Synchrotron Source Upgrade (CHESS-U) have proven the in-service reliability of the compact non-evaporable getter (NEG) pumps in a new experimental vacuum system predominantly pumped with distributed NEG-strips and modular high-capacity NEG pumps. The 80-meter section improvement in the Cornell Electron Storage Ring (CESR) is composed of 6 double-bend achromats operating with a single positron beam up to 200 mA. After a successful commissioning period, a vacuum level of 10^{-9} Torr was achieved with minimal maintenance and NEG re-activations.

The CHESS-U vacuum system experienced a catastrophic failure when a beam steering error created a pinhole leak in an undulator vacuum chamber (0.6-mm wall). The installed NEG-dominated pumping system had demonstrated an adequate pumping performance, which allowed a quick recovery and reconditioning of the affected 20+ meter vacuum section. With the hard work of the technical staff, X-ray user operations were able to resume after 10 days of recovery efforts (chamber fabrication and replacement, vacuum conditioning). The accidental air-exposure to the NexTorr pumps (combination of ion pump and NEGs) resulted in minor Argon instability issues that required mitigation. Corrective actions were developed in areas such as thermal monitoring, chamber construction, and beam steering while also granting the opportunity to test the pumping integrity of the effected NEG pumps after the exposure.

The 3-year operational experiences of the NEG pumping system will be presented.

9:20am **VT-TuM-5 ALS-U Vacuum Systems Production QA/QC Process***, **Sol Omolayo**,* Lawrence Berkeley Lab, University of California, Berkeley

The Advanced Light Source at Lawrence Berkeley National Lab is in the process of being upgraded to a 4th generation light source. The upgrade requires thousands of vacuum components to be procured, fabricated, inspected, assembled and installed. QA/QC is paramount concerned in ensuring the vacuum system meets requirement. A process was developed to manage QA/QC from the design phase to the installation and commissioning

9:40am **VT-TuM-6 Exploring Large Vacuum Systems at LIGO: A Brief Introduction to the Vacuum Challenges of the Cosmic Explorer***, **Melina Fuentes-Garcia**,* LIGO Laboratory, California Institute of Technology*; J. Feicht,* California Institute of Technology

The Laser Interferometer Gravitational-Wave Observatory (LIGO) consists of a set of multi-kilometer-scale gravitational wave detectors able to detect major events in our universe, such as black hole pair collisions. Because of stringent noise requirements, LIGO operates in an ultra-high-vacuum environment to minimize disturbance to the laser, optics, and other equipment inside the chambers. Factors such as material outgassing, contamination control, seal integrity, and pumping must all be optimized for minimal disturbance to the detectors. Cosmic Explorer (CE) aims to increase LIGO's sensitivity tenfold by scaling LIGO's 4 km long vacuum arms to 40 km, which amounts to a 90-million-liter vacuum system nominally sustained at 1E-9 Torr. This next-generation detector will significantly enhance our ability to detect gravitational waves, but will require greater challenges to the design and construction of its large vacuum system. Here we introduce some of the major challenges currently being studied, with an emphasis on the selection of alternate beam tube materials and elimination of high temperature bakeouts to reduce outgassing.

11:00am **VT-TuM-10 Exploring the Gravitational Wave Universe: Vacuum Systems for LIGO A+ and Beyond***, **Michael Zucker**,* LIGO Laboratory, Caltech and MIT **INVITED**

LIGO, the Laser Interferometer Gravitational-wave Observatory, recently completed the first phase of an upgrade called A+. This has improved sensitivity to gravitational waves from distant colliding black holes, neutron stars and other astrophysical phenomena by effectively circumventing the Heisenberg uncertainty principle, using a new quantum engineering technique called *Frequency-Dependent Squeezing* (FDS). An extension of both LIGO vacuum systems was required to enable this new technique. FDS is also an important step toward realizing vastly improved next-generation gravitational wave instruments, such as the *Einstein Telescope* and *Cosmic Explorer,* planned for the next two decades. These instruments will extend the realm of gravitational wave observations to the edge of the observable universe. Such new facilities will rely on ultrahigh vacuum at unprecedented scale, up to an order of magnitude larger than present instruments, presenting novel design and engineering challenges.

11:40am **VT-TuM-12 A Cryogenically Cooled Water Trap for ITER's Vacuum System***, **Jared Tippens**, C. Smith III,* Oak Ridge National Laboratory

The ITER project has the goal to demonstrate the feasibility of fusion and to advance the scientific and engineering understanding of fusion for future commercial reactors. The vacuum systems that are under development for the tokamak and supporting systems are expected to be dominated by one-of-a-kind devices due to their scale and varying operating environments.One specific challenge for these devices is the ability to process and recycle tritium, a radioactive hydrogen isotope in the fuel that is necessary for the fusion reaction to occur but is rare on Earth. Additionally, several of the vacuum systems are sensitive to water vapor which has the capability to inhibit pump performance if not removed from the gas stream. A custom designed water trap can enable both requirements to be met, and four of them are planned for the ITER vacuum system.

Due to vacuum operating pressures (as low as 1 Pa), a desiccant such as Zeolite cannot be efficiently used to adsorb and retain water vapor, so an alternative approach was chosen to utilize a cryogenically cooled water trap to desublimate water vapor from the process gas. The temperature must be lowered enough to remove the water vapor from the stream, but not so low as to remove the helium and gaseous hydrogen isotopes. With helium at a temperature of 80K available in ITER’s vacuum pumping room, this cooling load was selected as source for the water trap cooling.

To comply with the nuclear requirements, the tritium content inside the trap must be continuously monitored and removed to exhaust processing. The water trap must also be a double contained vacuum vessel with safety switches to mitigate the risk of tritium exposure to the vacuum pumping room. The tritiated water stored within must be removed batchwise to exhaust processing using heaters and inert purge gas. The capacity of the trap must be large (up to 5 kg of water) to account for the unlikely event of gross system water leaks, but in practice will accumulate water vapor at a low and steady rate of 1 Pa.m^3/s. Each trap must fit within a 1 meter diameter by 1 meter tall space reservation and include embedded tubes that enable heat transfer between the cryogenic helium and the process gas.

In summary, a cryogenically cooled water trap has been designed to meet the unique requirements of ITER and its vacuum systems. Four of these traps will protect sensitive vacuum equipment from water vapor as well as enable the recycling of tritium back into the fuel.

12:00pm **VT-TuM-13 Photon Stimulated Desorption Beamline at NSLSII***, M. Ferreira,* ESS, Sweden*; S. Hulbert, P. Palecek, I. Saleh, M. Seegitz, T. Shaftan, O. Tchoubar, **Robert Todd**,* Brookhaven National Laboratory

Understanding the expected gas desorption of an accelerator is critical in the proper design of accelerator vacuum systems and can have a major impact on the machine design and cost. From some of the earliest work on the subject for the Cambridge Electron Accelerator up through and including LHC, desorption measurements have played an important role in predicting vacuum behavior of large accelerators susceptible to synchrotron radiation. Much of this early work served well the machines they applied to and other machines with similar parameters and material choices. But as machines continue to be developed with higher energy, beam current, stability and susceptibility to e-cloud, novel materials need to be investigated to improve vacuum, and in some cases reduce SEY (Secondary Electron Yield). Part of these investigations require careful study of their desorption yields. This would benefit future upgrades to the existing NSLS-II facility as well as other synchrotrons facilities with stringent design specifications. Additionally, such a beamline could have a major impact on the selection and validation of proposed materials and components for EIC, including possible coatings for the electron storage ring, IRs (Interaction Regions) and the beam screen of the Hadron/Ion ring. Desorption rates of these newly proposed materials would be used as inputs to advanced modeling tools such as Molflow and SynRad for accurate predictions of vacuum behavior. A beamline at NSLS-II, dedicated to the PSD/ESD study of novel and proposed vacuum materials has been constructed and commissioned to advance further research into desorption behavior. The PSD of stainless steel and OFHC copper to be used for the Rapid Cycling Synchrotron of EIC have been measured and compared to prior work to baseline the system, with plans to evaluate the NEG coated chambers for the EIC electron storage ring. The layout of the experimental line and the commissioning measurements will be presented.

Vacuum Technology Division
Room C120-122 - Session VT-TuA

Novel Vacuum Instrumentation

Moderators: Jason Carter, Argonne National Laboratory, **Yulin Li**, Cornell University

2:20pm **VT-TuA-1 Saving Energy of Subfab Equipment for Semiconductor Manufacturing***, **Yohei Yoda**,* EBARA, Japan **INVITED**

Since the semiconductor industry has achieved continuous high growth in terms of both technology and commerce due to the spread of IACC5 * 1, the market will be doubled to 100 trillion yen in 2030 is a consensus in that industry. To purse miniaturization of devices based on Moore's Law, nanometer-order processing technology and three-dimensional processing technology are being researched and developed in various fields. Therefore, the increase in load and complexity of processes accompanied by the evolution of semiconductor manufacturing technology is remarkable. On the one hand, with an awareness of packaging technology, the diversification of processes and the increase in the number of processes will be further promoted in the future. On the other hand, as long as the increase in the production volume of semiconductor manufacturing and the number of processes, energy reduction and high efficiency during the manufacturing process are necessary issues in order to achieve a sustainable society in 2030.

In this report, we will discuss environmental technology development trends and roadmaps for 2030, whichregarding exhaust systems centered on dry vacuum pumps for manufacturing equipment that uses a large amount of energy in semiconductor manufacturing and exhaust gas treatment equipment which is responsible for reducing greenhouse gases.

Environmental Technology Development Trends for Exhaust Systems and 2030 Roadmap

The energy consumption ratio in semiconductor manufacturing can be roughly divided into consumption in equipment such as air conditioning, DI water and cooling water in clean rooms, and equipment in manufacturing equipment. Among these, the energy consumption ratio in the exhaust system including the dry vacuum pump in the manufacturing equipment is about half, which accounts for a huge proportion. Furthermore, to consume greenhouse gases such as CF4 and NF3 which produced during semiconductor manufacturing, exhaust gas treatment equipment is used to reduce the gases emission. The equipment used in the exhaust system uses utilities such as electric power, circulating cooling water, nitrogen, city water, fuel, and oxygen. Technological development for reducing usage and recycling / reuse will be an important performance index for 2030, along with achieving process performance and improving equipment availability. The latest technological trends regarding energy-saving technologies and on-demand control for each device will be reported and our environmental technology roadmap for 2030 will be explained.

3:00pm **VT-TuA-3 The Transfer of R&D Vacuum Products to Series Production - When Cleanliness and Quality Control Becomes Critical***, **Klaus Bergner**, C. Worsch, F. Haidu, K. Marschall, M. Flaemmich,* VACOM Vakuum Komponenten & Messtechnik GmbH, Germany

Today's research in the field of vacuum technology is an essential enabler for lithography, measurement and correction of the smallest and most novel chip structures. This lays a foundation for future applications in medicine, communication or consumer electronics.

After a successful release, a market-driven transition from the R&D phase to volume production with short time-to-market cycles takes place. However, the ramp-up process can be challenging and could lead to several production errors or even destruction of substrates or modules. Troubleshooting is then often costly as personally supported prototypes leave the R&D status and obvious but uncommunicated details are overlooked. This is particularly crucial for ultra-clean vacuum systems, which require careful attention to design, production, cleaning, assembly and maintenance to prevent failure due to contamination.

Quality and process control of individual components and modules becomes critical to ensure the performance and reliability of the final system. In this talk, we will explore the challenges associated with ramping up individual components of ultra-clean vacuum systems and the measures that can be taken to reduce ramp-up time while maintaining quality.

We show how surface contamination can be reduced from a double-digit µg/cm^2 value to a single-digit ng/cm^2 value. We highlight the most essential steps in the design phase, the right choice of cleaning technologies, appropriate analyze methods and constant process monitoring.

In summary, we provide a decided insight into process chain for the realization of ultra-clean vacuum components in all stages of "cleanliness". True to the motto: Design clean, Plan clean, Make clean, Prove clean, Keep clean.

3:20pm **VT-TuA-4 High Temperature Inlet of Residual Gas Analyzers for Atomic Layer Deposition Process Monitoring***, **Chenglong Yang**,* MKS Instruments, Inc. Mass Spectrometry Solutions Group*; J. Leslie, G. Jennings,* MKS Instruments, Inc. Mass Spectrometry Solutions Group, UK*; U. Meissner,* MKS Instruments, Inc. Mass Spectrometry Solutions Group, Germany*; M. Aitken, A. Wallace,* MKS Instruments, Inc. Mass Spectrometry Solutions Group, UK*; G. Brucker,* MKS Instruments, Inc. Mass Spectrometry Solutions Group

Residual gas analyzers (RGA) are used widely in the semiconductor industry for in-situ leak detection. Although RGAs can monitor contaminants, precursors and process byproducts in Atomic layer deposition (ALD), they are just used for process optimization/troubleshooting and are not yet ready for in-situ process monitoring owing to their short lifetime and less persuasive value for process monitoring. As an example, RGAs for ALD are challenged by harsh physico-chemical conditions including (1) chemical compatibility, (2) sensor contamination, (3) sensitivity degradation and (4) high measurement speed requirements. Many ALD precursors are liquid or solid at room temperature and can condense on cold surfaces, leading to blockage of the gas inlet system if the sampling pipes and valves are not at the required temperature conditions. MKS recently redesigned the popular UniBloc™ inlet system featured in most of its Process Analyzers to address the specific requirements of ALD. In its latest design, inlet components are uniformly heated (up to 200 ^{o}C) in order to avoid undesired reactions and/or deposition of byproducts prior to mass analysis. High sample flow rates, via bypass pumping, reduce sample transfer lag and improve sampling speeds as required for short pulse monitoring. Field replaceable valve seats and sampling orifices improve the lifetime and serviceability of the inlet system. Built-in calibration bottles, localized pressure measurement (Baratron® capacitance manometer) and sniffer tubes complete the new design and provide the performance and compatibility demanded by modern ALD processes. The improved Unibloc™ RGA design offers the opportunity to monitor ALD process in-situ, increase throughput and yield valuable process insights that will unlock future efficiencies in thin film growth.

4:20pm **VT-TuA-7 Improved Reliability of High Sensitivity Leak Testing of Large Chambers***, **Brad Shaw**,* Leak Testing Specialists, Inc. **INVITED**

This paper will present practices that have been of great value in successful leak testing operations for very large high vacuum, and ultrahigh vacuum projects. *Successful* in this context refers to the delivery of technically reliable leak testing with consistent schedule durations at an efficient cost.

This list of practices is the accumulation of lessons learned through the leak testing of a number of large projects, including the leak testing of the Laser Interferometer Gravitational Observatory (LIGO) beam tubes, the development and implementation of the leak testing of the National Ignition Facility (NIF) beam path clusters, space simulation chamber shroud replacement, and a series of large, double wall, vacuum insulated spheres for liquid hydrogen.

Some practices described in this paper have been of sufficient value across an array of applications that they have been added to industry codes and standards for leak testing. Use of vacuum pumping the calibrated leaks for system calibration is an example of a practice developed on a large project, that is now included in ASTM Standard Practice E1603/1603M. Another example is the calculation of the Test Quality Factor (TQF) in each leak test and evaluating the test reliability against a double bound requirement. This refined TQF practice has been added to the revised ASME Mandatory Appendices for helium hood and helium filled object leak testing.

Some practices in this paper are “best practices” that are frequently neglected, but that have historically been of great value. One example is the neglect of leak testing new components at receiving inspection. Failing to perform leak testing upon receipt is a common source of project schedule and cost over-run. The successful builders of large high and ultrahigh vacuum systems are among the most consistent in leak testing components at Receiving, without regard to the source of the component or assurances that the product was leak tested by the manufacturer.

Many practices discussed in this paper offer innovative ways of doing common, but difficult leak testing tasks by simpler, faster, more consistent and reliable means. The use of helium receivers for rapid filling of large hoods is one example. There are also details for helium hood leak testing that are not commonly used but that can be a significant source of savings. Another example involves the use of the Test Quality Factor (TQF) as a sensor for predictive maintenance of leak testing systems.

For each of the practices discussed, we will present cases that illustrate the benefits derived from implementation, or cases of non-implementation and the resulting consequences.

We hope the paper will contribute to future successful leak testing of large, high-vacuum and ultra-high vacuum systems.

5:00pm **VT-TuA-9 An Alternative to Helium Leak Checking*, Kieran Massey*,** *J. Brindley, V. Bellido-Gonzalez, D. Monaghan,* Gencoa Limited, UK

The vacuum leak detection market is dominated by helium detection using quadruple-based mass spectroscopy. These detectors offer high sensitivity and have become the industry standard. Helium, which enables these leak checkers to function so effectively, has an uncertain future with a critically short supply and prices on the rise. Leak checkers based on this technology are also costly to buy and have high ongoing maintenance costs.

What is required is a detector that functions with a cheap, readily available and safe gas but can still offer detection levels relevant for the particular industry. An alternative gas sensor built around plasma emission monitoring enables detection of gases using a small remote plasma which can be converted into a helium equivalent leak rate. This sensor is based on RPEM technology (remote plasma emission monitoring) which offers greater robustness and reduced maintenance relative to traditional mass spectrometer-based gas detection.

The presentation will cover the technology of RPEM and how it has been adapted for leak checking of vacuum systems and components using argon and carbon dioxide gas as opposed to Helium.

5:20pm **VT-TuA-10 Reference Leaks for Traceable Outgassing Rate Measurements of Hydrocarbons and Water*, Annas Bin Ali,*** *M. Bernien,* Physikalisch-Technische Bundesanstalt (PTB), Germany*; J. Setina,* Institute of Metal Technology (IMT), Ljubljana, Slovenia*; K. Jousten,* Physikalisch-Technische Bundesanstalt (PTB), Germany

Outgassing from components built into vacuum process chambers remains a pertinent issue for the semiconductor industry and has gained much attention as in Extreme Ultra-Violet Lithography (EUVL) where vacuum cleanliness is requisite. Too high outgassing can cause reflectivity loss in optical tools due to reactions of the light with adsorbed molecules stemming from outgassing of both photoresist and internal surfaces. Water and hydrocarbons are the major outgassing species affecting EUVL reflectivity as they trigger the diffusion and carbon growth on the optical surfaces resulting in lifetime issues of the optics. Quadrupole mass spectrometers are widely employed to identify such outgassing species and quantify outgassing rates. However, quantitative gas rate measurements using quadrupole mass spectrometers lack the necessary metrological quality, and the measured quantity is not traceable. This could result in either underestimation or overestimation of outgassing rates. In this work, samples are developed and characterized to serve as reference and transfer standard for water and dodecane outgassing rates. Dodecane serves as a model contaminant for hydrocarbon outgassing. Reference samples are realized by using a silicone rubber as a permeate sandwiched between two CF16-sized stainless-steel discs having a hole on both sides which define the open area. The outgassing flow can be tuned by choosing the permeate thickness and the open area of the holes. The partial pressure calibration system of PTB was used to characterize the reference samples. The gas flow from a reference sample was compared with a gas flow of dodecane/water generated by means of a calibrated capillary. In this way the outgassing rate can be measured traceable to the international systems of units. The reference samples demonstrated stable permeation rates of dodecane/water with a relative standard deviation of ~ 3 % over the period of a year. The design of the reference sample offers the possibility to refill the reservoir without completely disassembling the permeation part.

5:40pm **VT-TuA-11 Anti-Deposition Sensor Diaphragm Structures of Sapphire-Based Capacitance Manometer for Semiconductor Manufacturing Processes*, Takuya Ishihara,*** *Y. Mastugi, M. Soeda,* Azbil Corporation, Japan

Recently, various new manufacturing processes are put into practical use in the semiconductor industry. Especially, Atomic layer processes such as Atomic Layer Deposition (ALD) and Atomic Layer Etching (ALE) are essential in the fine pattern processing. These processes are mainly used in high aspect ratio holes, narrow trenches, or complex 3D structures with micro to nano meter scale orders because of the excellent uniformity or step coverage based on the surface chemical reactions. On the other hand, because the film deposition could occur in any surface inside the process chamber, capacitance manometers used for pressure monitoring receive bad influences from these process with undesirable film depositions on the sensor diaphragm. These depositions often cause sensor output drifts which can lead to the process halt and need zero-point adjustments or the replacement of manometers. In the viewpoint of the productivity, this is crucial for any device manufactures. Similar problems are sometimes occurred in some kinds of conventional CVD (chemical vapor deposition) processes.

Authors have developed entirely sapphire-based capacitive pressure sensor chips (Fig.1) utilizing MEMS (Micro-Electro-Mechanical Systems) processes, which are packaged in capacitance manometers for semiconductor manufacturing (Fig.2). In fact, most of troubles we have in these applications are above mentioned depositions on the sensor diaphragm. In this paper we will present some improvement on sensor structure to resolve these issues, in which sensor output drift could be depressed even if deposition on the sensor diaphragm is occurred.

We take two of measures to correspond to properties of deposited films.

Structure1: For soft or fragile films which is often deposited during conventional CVD process.

These films tend to deposit mainly on open surface and not so much on the side wall or bottom of narrow trench structures. We used this property to divide films, which can weaken mechanical influence on the sensor diaphragm. Fig.3 shows the actual trench structure we fabricated on the sensor diaphragm surface.

Structure2: For hard or unformal films deposited in atomic layer processes.

These films deposited on any surface on diaphragms, so above-mentioned trench structure cannot be effective. Therefore, we improved sensor diaphragm edge structures to suppress diaphragm deformations accompanied with unformal film depositions based on mechanical simulation (Fig.4).

Finally, we have confirmed the effectiveness of these improvements in actual process. Fig.5 and Fig.6 are sensor output signals of improved sensors during the CVD process and the ALD process respectively compared with which of conventional sensors. These exhibit excellent anti-depo property of the improved manometers.

6:00pm **VT-TuA-12 Overview of the Vacuum Pumping Systems for the SPARC Tokamak*, Matt Fillion,*** *A. Kuang,* Commonwealth Fusion Systems*; C. Day,* Karlsruhe Institute of Technology (KIT), Germany*; O. Mulvany, F. Ravelli,* Commonwealth Fusion Systems

Commonwealth Fusion Systems (CFS) is a spin-off of the Massachusetts Institute of Technology aiming to bring fusion energy to the grid. To accomplish this, CFS is developing and commercializing the ARC fusion power plant. To achieve this, CFS is currently building the SPARC tokamak—a superconducting, high-field, deuterium-tritium fueled tokamak that is designed for Q>1.

The Vacuum Pumping System of SPARC consists of three primary subsystems. The cryostat pumping system generates and maintains vacuum insulation of the cryostat to support the superconducting magnets. The leak detection system provides vacuum guarding for the tritium secondary interspaces and double seals in SPARC. Lastly, the torus pumping system is responsible for four main functions: the containment of tritium, reaching and maintaining the primary vacuum vessel base pressure, the recovery of the inter-pulse pressure, and providing particle control during the plasma discharge by pumping from the divertor. Each of the three vacuum pumping subsystems has an independent set of two dry screw pumps to provide rough vacuum and fore line pumping, mag-lev turbomolecular pumps for achieving ultrahigh vacuum, and a residual gas analyzer for leak detection and analysis of the plasma exhaust composition. The cryostat and torus pumping systems each contain custom tritium compatible closed loop refrigerator cooled cryogenic pumps to provide temporary enhanced pumping speeds.

Divertor pumping is a key aspect of tokamak particle transport control and an important area of study for ARC and other fusion power plants. The divertor is where neutral pressures are the highest ensuring the most efficient pumping for helium removal (a fusion byproduct). However, high divertor neutral pressure is crucial for divertor heat exhaust mitigation. To provide better control, CFS is developing a variable conductance louver system for active control over the divertor pumping speed. SPARC would provide much-needed data on desired neutral pressures and particles throughputs for steady state operations on next step devices.

The high throughputs required—along with the need to pump tritium—means a commercial solution for divertor pumping is unavailable. Thus, CFS is working with a commercial partner to develop an all-metal sealed cryogenic pump to meet the divertor pumping requirements. Utilizing added thermal mass on the lowest temperature stage, together with a proprietary charcoal, this pump can provide pumping at throughputs of 10.6 Pa m^3/s for the 10 second flattop duration of a SPARC pulse.

This talk will provide a general overview of the SPARC vacuum pumping systems and associated challenges, with a focus on the torus pumping system and the design of a custom cryogenic pump required by this system.

Vacuum Technology Division
Room Oregon Ballroom 203-204 - Session VT-TuP
Vacuum Technology Poster Session

VT-TuP-1 Measurements of NEG Pumping Performance at Cryogenic Temperatures*, **Sam Lodge**, P. Smith, A. Chew, N. Burch,* Edwards Ltd, UK*; D. Clement,* Gamma Vacuum*; P. Jones, P. Lamb, E. Lucchetta, P. Milner,* Edwards Ltd, UK*; T. Sinha,* Gamma Vacuum

Non-evaporable Getter (NEG) pumps are well established as a passive pumping technique in UHV and XHV applications. Recent studies comparing pumping speeds, sticking probabilities and capacities of Ti-V-Zr-Hf alloys at ambient and LN_2 temperatures will be reported.

Comparisons will be made with reported increased single element Ti and Ti alloy getters pumping performance at reduced operating temperatures.

VT-TuP-3 Boosting Pumping Speed Simulations of Sticky Vacuum Components*, **Stefan Kiesel**, A. Trützschler, K. Bergner,* VACOM Vakuum Komponenten & Messtechnik GmbH, Germany

Transmission probabilities of gaseous species through vacuum components are commonly studied using molecular flow Monte-Carlo simulation software, like Molflow+ [1]. Particle transmittance depends on the sticking coefficient between particle and wall. Since the sticking coefficient is only roughly known and varies e.g. with temperature, wall surface materials, and surface coverage, a simulation is typically repeated for different sticking coefficients. Our recent publication has shown, the amount of necessary simulations may be reduced to one by counting the amount of wall hits of transmitted particles [2].

In the presented study, we have employed this novel technique to several geometries and developed simple calculations to evaluate NEG coated tubes.

[1] Recent developments of Monte-Carlo codes MolFlow+ and SynRad+, M. Ady, R. Kersevan, 10th Int. Particle Accelerator Conf., Melbourne, Australia - doi:10.18429/JACoW-IPAC2019-TUPMP037, https://accelconf.web.cern.ch/ipac2019/papers/tupmp037.pdf

[2] Boosting sticking-dependent transmission studies to a single TPMC simulation, S. Kiesel et al., Vacuum, Volume 210, April 2023, 111744 – doi: 10.1016/j.vacuum.2022.111744

VT-TuP-4 Present Status of the SuperKEKB Accelerator Vacuum System*, **Yusuke Suetsugu**, K. Shibata, T. Ishibashi, M. Shirai, S. Terui,* High Energy Accelerator Research Organization (KEK), Japan*; M. Yao,* High Energy Accelerator Research Organization (KEK), Taiwan*; K. Kanazawa, H. Hisamatsu,* High Energy Accelerator Research Organization (KEK), Japan

The vacuum system of the SuperKEKB main ring (MR) consisting of 7-GeV electron ring (HER) and 4-GeV positron ring (LER), and the damping ring (DR) for 1.1 GeV positrons in the middle of the injector linac have been working well as a whole since the first commissioning in 2016. The maximum stored beam currents of MR are 1.46 A and 1.14 A for the LER and HER, respectively, and that of DR is approximately 30 mA, as of June 2022. The pressure rises per unit beam current are decreasing steadily. The new vacuum components developed for the SuperKEKB have been working as expected. No clear electron cloud effect has been observed in the LER so far after applying magnetic fields in the beam direction to the beam pipes at drift spaces in 2017. The recent behavior of the LER pressure against the beam current is explained by considering thermal gas desorption induced by the beam as well as photon-stimulated gas desorption. The beam lifetime is mostly limited by the Touschek effect due to a narrow dynamic aperture rather than the vacuum pressure, that is, the Rutherford scattering and Coulomb scattering. The challenges followed by high beam currents, such as damages of beam-collimator heads, excess heating of beam pipes at wiggler sections and so on, have recently become prominent. During the long shutdown time since July 2022 (called LS-1), we are installing a new non-linear beam collimator to reduce the beam impedances of collimator systems, exchanging the damaged collimator heads, replacing a beam pipe for the HER injection region to improve the injection efficiency, and installing the bellows chambers with photon masks in the wiggler section, together with maintenance works of the Belle II detector. The operation of the SuperKEKB will resume at the end of 2023. Here we will report the present status of the SuperKEKB vacuum system and the main works during the LS-1.

VT-TuP-6 Complex Bend Vacuum Chamber for NSLSII-U*, **Robert Todd**, M. Seegitz, P. Palecek,* Brookhaven National Laboratory*; M. Ferreira,* European Spallation Source, Sweden*; D. Hidas, A. Khan, V. Smaluk, T. Shaftan, S. Sharma,* Brookhaven National Laboratory

While the NSLSII synchrotron is a third-generation light source providing outstanding brightness and flux, there is a robust R&D program in place to upgrade to a fourth generation, or beyond, facility. Inherent in the so-called complex-bend magnet and lattice designs are significant limitations on the beam and exit slot apertures of the vacuum chamber. These restrictions and the need for the vacuum chamber to be mechanically aligned and decoupled from the magnets impose unique challenges. As part of the design process, a thorough survey of existing fourth generation machines was completed to look at existing design solutions for accommodating beam and for providing adequate conductance and pumping. For our chamber, the selected solution is not novel and utilizes an aluminum split clamshell design that has been done in many machines past and present. The adaptation of this design along with improved machining and welding should provide the most cost-effective solution. The geometrical and impedance solutions and structural and thermal modeling will be shown along with dynamic pressure simulations generated by Synrad and Molflow modeling code. With continuing changes in lattice and magnet parameters, a systematic, iterative approach to vacuum design has been implemented and will be presented.

Quantum Science and Technology Mini-Symposium
Room B110-112 - Session QS+VT-WeM

Vacuum Technology for Quantum Applications

Moderators: Ekta Bhatia, NY CREATES, **Freek Molkenboer**, TNO Science and Industry, the Netherlands

9:20am **QS+VT-WeM-5 Stand-Alone Vacuum Cells for Compact Ultracold Quantum Technologies***, **Oliver Burrow**, A. Arnold, P. Griffin, E. Riis,* University of Strathclyde, UK **INVITED**

Compact vacuum systems are key enabling components for cold atom technologies, facilitating extremely accurate sensing applications. There has been important progress toward a truly portable compact vacuum system; however, size, weight, and power consumption can be prohibitively large, optical access may be limited, and active pumping is often required. We have been developing centilitre-scale vacuum chambers with He-impermeable viewports and an integrated diffractive optic, enabling robust laser cooling with light from a single polarization-maintaining fibre. With these devices, a cold atom demonstrator based on the vacuum cell delivers 107 laser-cooled 87Rb atoms per second, using minimal electrical power.

Pressure measurements in these compact systems are made from cold-atom loading curves, and pressure evolution have been studied in a ceramic based vacuum chamber. With continuous Rb gas emission, active pumping yields a 10−7 mbar equilibrium pressure, and passive pumping stabilizes to 3×10−6 mbar with a 17 day time constant. With no Rb dispensing and only passive pumping, a ceramic based vacuum chamber has currently kept a similar pressure for more than 500 days. The passive-pumping vacuum lifetime is several years, which is estimated from short-term He throughput with many foreseeable improvements.

Progress is also reported, including new cell materials, mobile cold-atom demonstration and adaptation of the fabrication technique into a cold-atom gravimeter vacuum system. This technology enables wide-ranging mobilization of ultracold quantum metrology.

Oliver S. Burrow, Paul F. Osborn, Edward Boughton, Francesco Mirando, David P. Burt, Paul F. Griffin, Aidan S. Arnold, Erling Riis; Stand-alone vacuum cell for compact ultracold quantum technologies. Appl. Phys. Lett. 20 September 2021; 119 (12): 124002. https://doi.org/10.1063/5.0061010

11:00am **QS+VT-WeM-10 Hybrid Quantum-HPC Computing Clouds in Europe***, **Richard Versluis**,* TNO Science and Industry, the Netherlands **INVITED**

Quantum computing technology holds great promises for the long future but requires large investments in the near future as an enabler. Not only in terms of money and human resources such as talent, but also in infrastructure. This ranges from clean room infrastructure for QPU development, such as dedicated processing lines for quantum chip development to dedicated software and testing equipment for the screening and validation of quantum chips, to full stack system prototypes to demonstrate and validate crucial interfaces, but also to enable early adaptors to start implementing and exploring the potential of these new compute paradigms. Since a couple of years, some full stack demonstrators have been built, some in-house in a lab environment and some in an environment that is already a bit more market-orientated, such as a private cloud or a public cloud. Notably, some US companies like IBM, Google, Rigetti, IonQ and the Canadian company Dwave have set standards for online access to quantum computers. In Europe, the first publicly available cloud service for quantum computing, giving access to European quantum computers was Quantum Inspire, implemented by QuTech in The Netherlands. Since its launch in 2020, more online quantum computers have been launched in Europe, such as Quandela cloud.

With the necessity to get the most out of these early systems, hosting QPU's with still noisy and small numbers of qubits, a connection to HPC systems is crucial. It is anticipated that early advantage will be reached by combing classical and quantum algorithms, where the QPU could outperform an HC on some specific tasks, such as efficiency of the calculation in terms of wall clock time or energy used, the accuracy of the calculation, or simply by providing a different method of calculation that could not be done with a classical system. Integration of these, relatively immature systems, in an HPC workflow requires quite some effort. First of all, the language used to program quantum computers cannot be compared to high level classical programming languages like Python, C++, Rust etc. Secondly the integration of (runtime) compilers in the workflow is non-trivial. Hybrid classicll-quantum algorithms, therefore require systems that can handle multiple languages, compiler services. Thirdly, the workflow management is not-standard: where the integration of classical accelerators like GPU's is based on standard-predefined interfaces such as scrum, these workflow interfaces for QPUs have not been defined yet.

In this talk I will highlight the goals and some first results of European activities on the integration of HPC and Quantum Computers in European projects such as the EuroHPC projects, OpenSuperQ plus and Quantum Large Scale Integration.

11:40am **QS+VT-WeM-12 Design Considerations of an XHV System for an Ion Trap Quantum Computer***, **Paul Smith**, N. Burch, A. Chew, P. Jones, P. Lamb, E. Lucchetta, S. Lodge, P. Milner,* Edwards Ltd, UK*; D. Clement, T. Sinha,* Gamma Vacuum*; A. Abolghasemi, L. Earl, J. Randall,* Universal Quantum, UK

The design and configuration of an XHV system for an ion trap quantum computer is presented. A target operating pressure of 10^{-12} mbar has been identified to increase ion lifetime. Contributions to the residual gas load from leaks, permeation and outgassing will be evaluated as will the pumping strategies employed for each. The relative pumping performance of two combined NEG-IGP pumps will be reported. Other factors will be discussed including conductance optimization, limitations on component bakeout and NEG activation temperatures, vibrations, and shielding of magnetic fields and radiant heat loads.

12:00pm **QS+VT-WeM-13 Chances and Challenges: Aluminum Vacuum Components for Quantum Technology***, **Stefan Kiesel**, A. Trützschler, J. Hertel, K. Bergner,* VACOM Vakuum Komponenten & Messtechnik GmbH, Germany

Quantum technology currently experiences a huge push towards commercialization, since it promises a variety of attractive applications, including quantum sensors, quantum computers, and quantum clocks. Many of these systems require a vacuum to isolate quantum objects or devices from the surrounding environment and to create stable conditions. In addition, signal paths into the vacuum are necessary to manipulate quantum objects, facilitated by hermetically sealed electrical and optical feedthroughs. The most advanced modern systems are built up from large and expensive laboratory equipment. However, the needs of commercially usable applications drive the development of quantum systems towards transportable, durable, and standardized solutions. To meet these challenging demands, better materials, novel manufacturing technologies and innovative designs are issues of today's development projects. As an example, aluminum Con-Flat (CF) components offer the possibility of providing customized solutions with high geometrical accuracy, reduced weight, low outgassing rates as well as vanishing magnetic permeability. As a manufacturer of vacuum components, VACOM is actively collaborating in several publicly funded projects to promote the development of quantum technology. In this talk we show goals and results of these projects regarding the development of vacuum systems and vacuum components for quantum technology.

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