Plasma Science and Technology Division
Room A106 - Session PS+MS-TuA

Modelling of Plasmas and Plasma Driven Processes

Moderators: Mingmei Wang, Lam Research Corporation, **Jinyu Yang**, University of Notre Dame

2:20pm **PS+MS-TuA-1 Towards Completing Chemistry Sets for Plasma Simulations***, **Sebastian Mohr**, G. Armstrong, K. Lemishko,* Quantemol Ltd., UK*; A. Owens, W. Wu, J. Tennyson,* University College London, UK

Plasma simulations are widely used in both academic and industrial settings to gain insights into fundamental plasma physics and optimise plasmas processes. Their success not only hinges on a robust physical model but also on the availability of data describing the chemical processes in a discharge. These data can be in the form of

Collision cross-sections, mostly for electron processes

Rate coefficients, mostly for heavy particle processes

Lifetimes and de-excitation channels of excited states

Probabilities for surface reactions

Species properties such as the enthalpy of formation

For rather simple or common gas mixtures such as argon or oxygen, sufficient data can usually be found in existing publications or databases; however, for more complex gas mixtures, especially ones including gases which have not been extensively studied yet, these data are usually not available for all species and reactions of interest. Furthermore, even in quite well known gas mixtures so far unknown or neglected phenomena can become important under specific process conditions. Hence, it is of vital importance to generate new data in a timely fashion.

We have developed a series of software tools to address the issue of missing data for plasma simulation purposes and to give easy access to existing data. These include:

The calculation of missing electron – molecule collision cross sections [1].

An online database QDB [2] of existing plasma chemistry data including both cross-sections and rate coefficients as well as some surface chemistry data

Machine learning algorithms for the quick estimation of species and reaction data [3]

A database of radiative lifetimes for excited states tailored to the needs of plasma modellers [4].

A global plasma model with additional tools such as a chemistry set reduction [5] to tailor a chemistry set to specific process conditions.

A collisional-radiative model to calculate the emission spectrum of a plasma discharge based on the densities of the excited states and the neutral gas temperature.

We will present the latest additions to these tools and examples to showcase their use and their impact on plasma simulations such as adding reactions with formerly unknown cross-sections or rate coefficients to chemistry sets or the impact of adding the radiative decay of vibrational states to a plasma model.

[1] B Cooper at al 2019 *Atoms***7** 97

[2] J Tennyson et al 2022 *Plasma Sources Sci. Technol.***31** 095020

[3] M Hanicinec at al 2023 *J Phys D*, in press, doi:10.1088/1361-6463/acd390

[4] A Owens et al 2023 *Plasma Sources Sci. Technol.*, submitted

[5] M Hanicinec et al 2020 *Plasma Sources Sci. Technol.***29** 125024

2:40pm **PS+MS-TuA-2 Particle-in-Cell Monte Carlo Collision Modeling of Low-Pressure Plasma Discharges***, **Ken Hara**, Y. Yamashita,* Stanford University

Predictive modeling of partially ionized gases plays a critical role for applications such as semiconductor manufacturing, plasma processing, spacecraft propulsion, hypersonic flows, and high-energy density plasmas. However, plasma modeling remains challenging due to the nonlinear coupling of different physical and chemical processes. In particular, when operating the plasma sources at low pressure, the plasma constituents are not in equilibrium and their velocity distribution functions may become a non-Maxwellian due to the lack of collisions. Conventional fluid approaches cannot capture such rarefied flow physics and thus kinetic methods are needed. In this talk, we will present the development of particle-in-cell (PIC) Monte Carlo collision (MCC) models for low-pressure plasma discharges. The in-house PIC/MCC models are applied to various phenomena, including DC/RF breakdown, cylindrical sheath, capacitively coupled plasmas, and plasma instabilities. In particular, the effects of macroparticle (MP) weights on the plasma behavior are studied using a cylindrical (axisymmetric) PIC/MCC model. As the cell center volume is small near the symmetry line compared to the periphery, the numerical noise due to the lack of MPs can artificially generate plasmas near the centerline, leading to numerical plasma nonuniformity. The numerical heating is mitigated by modifying the MP weight. Acceleration of the PIC/MCC simulations and applications to DC/RF breakdown will be discussed in the talk.

3:00pm **PS+MS-TuA-3 Radio-frequency Hollow Cathode Discharge Characterization using Plasma and Machine Learning Models***, **Kallol Bera**, A. Verma, S. Ganta, S. Rauf,* Applied Materials, Inc. **INVITED**

Low to moderate pressure radio-frequency (RF) hollow cathode discharges (HCDs) have gained significance for advanced plasma processing in the semiconductor industry. HCDs form in cylindrical cavities in the cathode. One can use an array of such HCDs to create uniformly dense large-area plasma. In the HCD, RF sheath heating as well as secondary electron acceleration play an important role. For modeling low-pressure RF HCDs, where kinetic effects are important, particle-in-cell Monte Carlo collision (PIC-MCC) modeling scheme has been used. In this PIC-MCC model, using charge density of particles, Poisson equation is solved for electric potential, which yields the electric field. Using this electric field, all charged particles are moved. The code considers particle collisions with each other and with neutral fluid using a Monte Carlo model. The single HCD behavior is studied over a range of pressure, RF voltage, frequency, and secondary electron emission coefficient. A strong positive power deposition region is observed within the hollow-cathode hole. The plasma penetrates inside the hollow-cathode hole with an increase in pressure and frequency, leading to plasma density enhancement. Higher secondary electron emission coefficient has a stronger impact on the plasma penetration into the hole at higher frequency. However, the effect of increasing RF voltage on plasma penetration into the hole is limited. Large area plasma using an array of HCDs is coupled to electromagnetic fields in the process chamber. Multiphysics modeling of an array of RF HCDs is difficult due to the geometrical complexity, which makes the simulations computationally prohibitive. This precludes development and utilization of these models in scenarios where the computations need to be performed rapidly and repeatedly. To overcome these challenges, we developed a deep learning based non-linear model order reduction method for plasma process in HCDs. A space-filling method is used to design computational experiments at different voltages at the fundamental frequency and at the second harmonic along with their phase difference. The temporal voltage-current characteristics of the HCD are used to train the reduced order model based on modified recurrent neural network. Our model predictions match well with the plasma simulation results within and outside the training range at a significantly smaller computational time. Further, an electromagnetic model is developed with coupled non-linear voltage-current characteristics from the neural network model. The coupling of electromagnetic field to non-linear discrete discharges characterizing an array of HCDs for large area plasma is in progress.

4:20pm **PS+MS-TuA-7 Experimental Characterization and Modeling of the Spatial Afterglow of Plasmas***, **Nabiel Hilmy Abuyazid,*** University of Illinois at Urbana Champaign*; N. Uner,* Middle East Technical University, Turkey*; S. Peyres, R. Sankaran,* University of Illinois at Urbana Champaign

There has been recent interest in the spatial afterglow of plasmas because of its potential role in charging and agglomeration of aerosol particles as well as neutralization and dosing of surfaces. In general, the spatial afterglow is analogous to a temporal afterglow, characterized by a decay of charge resulting from a change in the applied power, except that the charge decay occurs in space rather than in time. However, the nature of the charge decay has been much less studied than temporal afterglows, perhaps because of the challenge of performing experiments at higher pressures and in smaller dimensions.

Here, we performed double Langmuir probe (DLP) measurements, which enable spatial measurements of the plasma density, and developed a one-dimensional advection-diffusion-recombination model that describes the charge decay in the spatial afterglow. Our results show excellent agreement between experimental measurements and model outputs over different pressures. Experimental measurements were limited to a pressure of 300 Torr at which point the DLP traces no longer exhibited known shapes and could not be analyzed to extract plasma parameters. By validating the model at the lower pressures, we were then able to extend the model to predict behavior at higher pressures, up to atmospheric. At pressures above ~75 Torr, the rate of charged species decay is primarily influenced by pressure, as three-body recombination becomes increasingly dominant over diffusional losses, and is secondarily influenced by gas flow velocity and temperature. Importantly, our findings reveal a transition from ambipolar diffusion to free diffusion at some distance from the bulk plasma within the spatial afterglow. First studied in temporal afterglows, apparent diffusivities of charged species vary as the plasma decays, eventually reaching a critical point where the ambipolar field becomes too weak and charged species begin to diffuse freely. The shift to free diffusion could lead to negatively-charged electrons being lost and positively-charged ions remaining, which has been previously reported to explain how aerosol particles that leave a bulk plasma negatively charged become neutralized or even positively charged after their transit through the spatial afterglow.

4:40pm **PS+MS-TuA-8 Circuit-based Reduced Order Model for Fluid Plasma Simulation of Capacitively Coupled Plasma Reactors***, **Sathya Ganta,** A. Verma, K. Bera, S. Rauf,* Applied Materials, Inc.

Fluid plasma simulations are essential for the design of radio frequency (RF) driven capacitively coupled plasma (CCP) reactors used for plasma-based deposition/etching processes. One can assess on-wafer performance using the computed ion/neutral fluxes, sheath potentials, and ion energies. These plasma parameters are directly related to process parameters like deposited film thickness, film stress, wet etch rate, uniformity etc. Hence, the fluid plasma simulations are vital to the semiconductor industry. To predict the ideal process parameters required to meet the on-wafer specifications, one needs to run a large number of simulations in the multi-dimensional process space, which requires enormous computational resources. A key aid in such scenarios would be fast and reliable reduced-order surrogates to the computationally cumbersome plasma fluid simulations. This paper explores one such reduced-order surrogate model based on a circuit-based estimation of the RF sheath. Here, the RF sheath is estimated to be a circuit consisting of a constant current source predicting ion current, a diode predicting electron current and a capacitor predicting the displacement current where these three circuit elements are in parallel to each other. First, a small set of 1D plasma fluid simulations are run corresponding to a set of process parameters that span the entire process space. The results from these plasma simulations, specifically the sheath voltage and current characteristics, are used to fit the parameters of the current source, diode and capacitor that form the RF sheath using a non-linear regression model. Once the circuit parameters are fitted, the resulting RF sheath circuit is coupled to an electromagnetic finite difference time-domain (FDTD) simulation making it a reduced-order surrogate of the plasma fluid simulation. The reduced order model is finally run corresponding to a new set of process parameters within the process space and its performance is compared to that of fluid plasma simulations and analyzed.

5:00pm **PS+MS-TuA-9 Fully Kinetic Modeling of Wafer Processing Chambers in CCP and coupled ICP/CCP Systems Using VSim***, **Daniel Main,** E. Lanham, J. Cary, T. Jenkins, J. Leddy, S. Kruger,* Tech-X Corporation

Inductively Coupled Plasmas (ICPs) are extensively used for materials processing in the semiconductor industry, typically with the addition of an RF bias [1]. For these reactors, it is assumed that the majority of plasma generation comes from the inductive power while the bias can independently control the flux and energy of ions needed for processing. In reality, the interaction between the multiple power sources is difficult to isolate and computational modeling becomes a necessity. Typically ICPs are modeled using a fluid approach, which does not correctly model the collision processes at lower pressures (~1-10 mTorr) nor the sheath that forms near the wafer. In this work, we discuss multiple techniques using the particle-in-cell software package VSim [2,3] that can be used for reactor-scale modeling of mixed inductive and capacitive discharge systems to accurately characterize the ion energies impacting a wafer for processing. One method is to use a global model to first compute a near-steady-state system composed of neutrals and plasma. The fluxes and densities from the global model serve as initial conditions for a high-resolution electrostatic capacitively coupled plasma (CCP) simulation to correctly model the sheath near the wafer and ion fluxes onto the wafer. Another approach is to model both the inductive and capacitive power sources in one simulation using a newly developed implicit electromagnetic scheme. We discuss differences between the CCP-only and coupled ICP/CCP systems found in ion energies, ion fluxes and the ion distribution function impacting the wafer, as well as the computational costs of the two methods.

[1] M. A. Lieberman and A. J. Lichtenberg, Principles of Plasma Discharges and Materials Processing, John Wiley & Sons, Inc. (2005).

[2] C. Nieter and J. R. Cary, J. Comp. Phys. 196, 448 (2004).

[3] www.txcorp.com

5:20pm **PS+MS-TuA-10 Hybrid Particle-in-Cell + Fluid Model of Multi-Frequency Capacitively Coupled Plasma with Tailored Voltage Waveform Bias***, **Shahid Rauf,** X. Shi, T. Wang, S. Ganta,* Applied Materials, Inc.

Multi-frequency capacitively coupled plasmas (CCPs) are widely used for thin film etching and deposition in the semiconductor industry. When operated at low pressures, kinetic effects dominate electron dynamics and, therefore, fluid assumptions are inaccurate for electrons in plasma models. Most industrial applications are, however, done using complicated gas mixtures with a variety of ions and neutral species. These plasmas are often electronegative with large concentrations of negative ions. Kinetic modeling for all the species, e.g., by solving the Boltzmann equation or using particle-based techniques, is impractical due to the high computational cost. A hybrid model for multi-frequency CCPs is described in this paper where the electrons are modeled as particles (using the particle-in-cell technique) while the ions and neutral species are treated as a fluid. The equations governing the kinetics of electron pseudo-particles, continuity and momentum equations for ions, Poisson equation for the electric field, and the continuity equations for neutral species are coupled at each time-step, with the time-step typically governed by the light electrons. This model is used to examine plasmas of Ar/CF_4 and $c\text{-}C_4F_8/O_2$ in a parallel plate CCP reactor with a high frequency (40 MHz sinusoidal) and a low frequency (400 kHz tailored voltage waveform) source. A combination of 1-dimensional, 2-dimensional (2D) Cartesian geometry, and 2D axisymmetric cylindrical geometry simulations is used to examine the effect of the low-frequency duty cycle on plasma chemistry and spatial structure of the plasma. The relative flows of the gases in the mixture are varied to understand the dynamics of both electropositive and electronegative discharges. Due to the long electron mean free path (relative to the inter-electrode gap), the plasma spreads out far from the region where the electrons absorb energy. This has major consequences on plasma uniformity in the 2-dimensional model. It is also found that, at a lower duty cycle, the time-averaged sheath at the powered electrode is thinner and the plasma occupies a larger volume. Consequently, for a given HF power and LF voltage, charged and neutral specie densities are higher at a lower duty cycle.

5:40pm **PS+MS-TuA-11 Wafer Edge and Focus Ring Effects on Ion Energy Distributions and Har Features During Plasma Etching Using Low Bias Frequencies***, **Evan Litch,*** University of Michigan*; H. Lee, S. Nam,* Samsung Electronics Co., Inc., Republic of Korea*; M. Kushner,* University of Michigan

Current microelectronic device architectures are continuing to trend towards 3-dimensional devices for higher functionality.A consequence of

fabricating 3D devices is the need to plasma etch high aspect ratio (HAR) features of ARs > 100.An example of HAR plasma etching is deep trench isolation (DTI) which is used to isolate 3D logic structures and imaging cells from interfering with each other.These DTI etches are performed in halogen-based mixtures (e.g., HBr/Cl_2) for a Si wafer in inductively coupled plasma (ICP) reactors.

At HARs, the primary etch mechanisms deep within the profile are ion/hot neutral chemical and physical sputtering. In-order to reduce the etch time for these features while maintaining critical dimensions, plasma etching with narrow-angular distributions of incident ions is required.By lowering the bias frequency (100s kHz), ion transit through the sheath is in the thin-sheath limit.(The thin sheath limit refers to ions being able to transit the sheath in a fraction of the RF period.) While this is helpful for ions incident across the majority of the wafer, ion distributions are typically broader and perhaps skewed at these lower frequencies near the edge of the wafer.This is primarily due to charging of the focus ring (FR) due to the longer period exceeding the RC time constant for such charging leading to greater sheath curvature at the edge of the wafer. To maintain critical dimensions of HAR structures at the wafer edge, modifying the FR geometry and/or electrical properties may be necessary to take advantage of lower bias frequencies.

In this work, results from a computational investigation of an ICP using very low bias frequencies for different FR parameters will be discussed.The simulations were conducted with the Hybrid Plasma Equipment Model (HPEM), investigating an ICP sustained in $Ar/O_2/Cl_2$.IEADs, uniformity of fluxes to the wafer and sheath structure for these systems will be discussed.Consequences on etch profiles will also be discussed.

Work was supported by Samsung Electronics Co. and the US National Science Foundation.

6:00pm **PS+MS-TuA-12 Plasma Dynamics During Synchronous RF Pulsing in Dual Frequency Capacitively Coupled Plasma***, **Abhishek Verma**, S. Rauf, K. Bera,* Applied Materials, Inc.*; D. Sydorenko,* University of Alberta Edmonton, Canada*; A. Khrabrov, I. Kaganovich,* Princeton Plasma Physics Laboratory

Low-pressure multi-frequency capacitively coupled plasmas (CCP) are used for numerous etch and deposition applications in the semiconductor industry.Pulsing of the radio-frequency (RF) sources enables control of neutral and charged species in the plasma on a millisecond timescale.In this work, the synchronous (i.e., simultaneous, in-phase) pulsing of both power sources in a dual frequency CCP is examined.To resolve kinetic effects at low gas pressure, modeling has been done using the electrostatic Particle-in-cell/Monte Carlo collision method.The objective of this work is to investigate the sensitivity of the plasma properties to small changes in timing during synchronous pulsing of the 2 RF sources.It is demonstrated that small deviations in the on and off times of the 2 RF sources can lead to major changes in the plasma characteristics. In the simulations, the pulsing parameters (on and off times and ramp rates) are varied and the temporal evolution of plasma characteristics such as electron density,ion energy, ion energy flux, species current at the electrode, and electron temperature are examined.It is demonstrated that if the low-frequency (LF) source is turned on (or off) a few µs before (or after) the high-frequency source, plasma density during the off-state (or on state) undergoes sharp variations due to the frequency coupling effect. Similarly, turning on the LF source with a small delay results in a sharp increase in the plasma density when the HF source is turned on. The study demonstrates the importance of synchronization of RF pulsing in dual frequency CCPs and discusses methods to finetune plasma properties further.

Applied Surface Science Division
Room B117-119 - Session AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM

Multi-Modal & Multi-Dimensional Analysis

Moderators: Gustavo Trindade, National Physical Laboratory, UK, **Paul Mack**, Thermo Fisher Scientific, UK, **Tim Nunney**, Thermo Fisher Scientific, UK

8:00am **AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-1 Growth and Characterization of Large-Area 2D Materials*, Glenn Jernigan,*** US Naval Research Laboratory **INVITED**

Nothing could be more coupled than Growth and Characterization. When two dimensional (2D) materials appeared on the radar of the scientific community (with the amazing properties of graphene), it was immediately obvious that large area samples would be needed. Exfoliating flakes was insufficient for the demands of scientific studies, in addition to not being viable should a commercial application be developed. Thus, the search began for growth methods to produce large-area 2D materials for large scale testing and development.

The Naval Research Laboratory has, over the past 15 years, pursued research programs in producing large areas of graphene, transition metal dichalcogenides (TMDs), boron nitride (BN), and other 2D materials. In every one of those programs, they began with surface analysis of composition, chemistry, and morphology of the grown films. The uniquely sensitive nature of x-ray and ultraviolet photoelectron spectroscopy (XPS and UPS) and scanning tunneling and atomic force microscopy (STM and AFM) to 2D materials was necessary to measure the electrical, chemical, and physical properties obtained in the large area films and to understand what was observed in the exfoliated flakes. The production of large areas allowed "mass-scale" optical and electrical characterization, which then became a feedback loop in the search for new and interesting properties and relevant applications. In this presentation, I will show how we developed large-area graphene, by both epitaxial growth and chemical vapor deposition methods, TMDs, and other 2D materials for characterization and device utilization.

8:40am **AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-3 Using a Correlative Approach with XPS & SEM to Measure Functionalized Fabrics for Antimicrobial Applications*, Tim Nunney,*** *H. Tseng,* Thermo Fisher Scientific, UK*; D. Marković, M. Radetić,* University of Belgrade, Serbia

Medical textiles are an indispensable component for a wide range of hygienic and healthcare products, such as disposable surgical gowns and masks, or personal protection equipment, with opportunities to provide further protection by engineering textiles with suitable medical finishing. While antibiotics are considered a viable option for their efficiency in treating bacterial infections, their abuse can result in adverse effects, e.g., bacteria resistance. Nanocomposites have emerged as a promising alternative to antibiotics, as the large surface-to-volume ratio and high activity helps attain the targeted antimicrobial efficiency by using tiny amounts of nanocomposites, and their biocompatibility and scalability are particularly advantageous for medical applications [1]. Thus, developing processing methods to integrate nanocomposites in the fabrics is essential for exploiting their properties for medical textiles.

In this study, polypropylene fabrics, alginate and copper oxides, were selected to develop novel antimicrobial nanocomposites based on various surface treatments, i.e. corona discharge and alginate impregnation, which led to improved fabrics hydrophilicity with functional groups introduced as binding sites for Cu(II), a precursor that formed Cu nanoparticles when reacted with reducing agents, i.e. NaBH4 and ascorbic acid. The composition of the fabrics after being treated with corona discharge and impregnation observed by XPS indicates the materials formed mainly consisted of C and O, attributed to the presence of a thin, hydrophilic layer and alginate, respectively, consistent with depth profiling measurements. Following Cu reduction, XPS mapping of the fabrics finds that, reacting with ascorbic acid resulted in formation of nanocomposites containing a mixture of Cu and Cu (II) oxides across the surface, which could be visualised by using SEM in the same locations. Excellent anti-microbial activity against Gram-negative bacteria E. coli, Grampositive bacteria S. aureus and yeast C. albicans was observed for the treated fabrics[2]. This result not only demonstrates a cleaner, and healthier approach for developing novel nanocomposites, but more importantly highlights the role of surface techniques in uncovering challenges in designing and engineering functional textiles.

References:

[1] D. Marković, J. Ašanin, T. Nunney, Ž. Radovanović, M. Radoičić, M. Mitrić, D. Mišić, M. Radetić, Fibers. Polym., 20, 2317–2325 (2019)

[2] D. Marković, H.-H. Tseng, T. Nunney, M. Radoičić, T. Ilic-Tomic, M. Radetić, Appl. Surf. Sci., 527, 146829, (2020)

9:00am **AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-4 Multi-Modal Analysis in Photoelectron Spectroscopy: From High-Resolution Imaging to Operando Experiments*, Olivier Renault,*** CEA-Leti, France*; A. Benayad,* CEA, France*; N. Gauthier,* CEA-Leti, France*; R. Charvier,* ST Microelectronics, France*; E. Martinez,* CEA-Leti, France

Over the past years, the field of surface and interface analysis has been greatly expanded by new developments made possible by lab-scale instruments enabling higher excitation energies. These new developments are directly serving technological advances especially in the area of technologies in renewable energies and nanoelectronics, which are adressing more and more complex system requiring to go beyond traditional ways of characterizing surfaces and interfaces. Different dimensions are to be explored in multi-modal surface analysis : the depth dimension, the lateral dimension, and the dynamic dimension.

After a short review of some of the achievements towards enhancing the depth dimension by lab-scale hard X-ray photoelectron spectroscopy (HAXPES) and the lateral dimension using X-ray PEEM, we will present different application cases of *operando* HAXPES. Here, the material is analyzed as being part of a device operated *in situ* during the experiment, in conditions that are as close as possible to the final applications and where the interfaces can be studied in dynamic conditions. We will first review some results of *operando* HAXPES on resistive memories obtained with synchrotron radiation [1, 2] before presenting various lab-scale experiments [3, 4] and the current limitations to such approaches.

[1]B. Meunier, E. Martinez, O. Renault et al. *J. Appl. Phys*. **126**, 225302 (2019).

[2]B. Meunier, E. Martinez, O. Renault et al., *ACS Appl. Electron. Mater*. **3** (12), 5555–5562 (2021).

[3]O. Renault et al., *Faraday Disc*. **236**, 288-310 (2022).

[4]A. Benayad et al., *J. Phys. Chem. A* 2021, 125, 4, 1069-81.

9:20am **AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-5 Multi-Modal Analyses of Ultrasonic-Spray-Deposited Ultrathin Organic Bathocuproine Films***, J. Chen,* ***Juliet Risner-Jamtgaard****, T. Colburn, A. Vailionis, A. Barnum, M. Golding,* Stanford University*; K. Artyushkova,* Physical Electronics*; R. Dauskardt,* Stanford University

Bathocuproine (BCP) is a small organic molecule that is typically used as an ultrathin hole blocking interlayer (< 10 nm thickness) in organic solar cells and perovskite solar cells. The film is typically deposited via low-throughput vacuum thermal evaporation with an *in-situ* Quartz Crystal Monitor to measure film thickness. Open-air ultrasonic spray deposition for low-cost and large-scale deposition is an attractive alternative method for solution processing of BCP films, but the process lacks a comparable *in-situ* metrology. Given that the BCP film is transparent to visible light and ultrathin, it is important to utilize a multi-modal approach to evaluate optoelectronic and physical properties of the sprayed film.

A suite of characterization techniques that span a range of equipment complexity, measurement time, and measurement sensitivity are used to analyze the BCP films. We begin by demonstrating the limitations of the singular ellipsometry model[1] for BCP found in literature and motivate a need to rely on other techniques. Multi-modal analyses including X-Ray Reflectivity, Angle-Resolved X-ray Photon Spectroscopy (AR-XPS), Auger Spectroscopy, Scanning Electron Microscopy, and Transmission Electron Microscopy with EELS are then performed on the sprayed BCP film. The advantages and disadvantages of each characterization technique are compared and discussed. We conclude that AR-XPS provides the most distinctive determination of individual layer thicknesses for a sample architecture consisting of silicon substrate/native SiO_x/BCP across the applicable range of AR-XPS from ~ 1-10 nm.

[1]Liu, Z.T., *et al*. The characterization of the optical functions of BCP and CBP thin films by spectroscopic ellipsometry. *Synthetic Materials*. 150(2):159-163. (2005)

9:40am **AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-6 Combinatorial Synthesis and High-Throughput Characterization of Pt-Au Thin Films Fabricated by Confocal Magnetron Sputter Deposition***, **David Adams**, R. Kothari, M. Kalaswad, C. Sobczak, J. Custer, S. Addamane, M. Jain, E. Fowler, F. DelRio, M. Rodriguez, R. Dingreville, B. Boyce,* Sandia National Laboratories

A few binary metal alloys are predicted to form thermally stable, compositionally segregated structures owing to the thermodynamic preference for minority species to collect and remain at grain boundaries established within the solid.(J.R. Trelewicz et al., PRB, 2009) When produced as a nanocrystalline thin film, these stable structures afford the potential to maintain excellent mechanical properties (e.g., high hardness) even after annealing to elevated temperature. Indeed, several systems, including $Pt_{.9}Au_{.1}$ thin films, are reported to develop thermally-stabilized, hard, nanocrystalline structures attributed to solute segregation at grain boundaries.(P. Lu et al., Materialia, 2019)

Future studies that seek optimal stoichiometry and/or preferred synthesis processes require access to a wide range of composition as well as an ability to vary key deposition parameters. Toward this end, our team reports on the challenges and the benefits of combinatorial synthesis for expediting the discovery of improved binary metal thin films. Our study utilized confocal sputter deposition wherein Pt and Au targets were individually sputtered via pulsed DC magnetron methods. Substrates (150 mm diameter wafers) were fixed in order to gain access to a wide compositional range for each deposition. The sputter power and cathode tilt orientation were then varied in subsequent depositions to access the nearly full binary metal compositional range. The binary collision Monte Carlo program SiMTra (D. Depla et al., Thin Solid Films 2012), which simulates the transport of sputtered atoms within the process gas, helped guide the selection of these process parameters in order to achieve compositional goals in relatively few depositions. Notably, the binary compositions predicted by SiMTra closely matched (within a few molar %) the measured compositions determined by Wavelength Dispersive Spectroscopy completed in 112 different areas across each wafer. The various combinatorial Pt-Au films were further characterized by high-throughput Atomic Force Microscopy, automated X-ray Diffraction, fast X-ray Reflectivity, mapping four-point probe sheet resistance, and automated nanoindentation. These studies reveal how hardness, modulus, film density, crystal texture, and resistivity of combinatorial films varied with composition as well the atomistics of film deposition. Attempts to correlate key film characteristics with the kinetic energies and incident angles of arriving metal species (estimated by SiMTra) are discussed with a goal of improving fabrication processes.

Sandia National Laboratories is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

11:00am **AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-10 Optical and X-Ray Characterization and Metrology of Si/Si(1-X)Ge(X) Nanoscale Superlattice Film Stacks and Structures***, **Alain Diebold**,* SUNY Polytechnic Institute **INVITED**

As traditional scaling of transistors comes to end, transistor channels and capacitors are being stacked to form new 3D transistor and memory devices.Many of these devices are fabricated using films stacks consisting of multiple Si/Si(1-x)Gex layers known as superlattices which must be fabricated with near atomic precision.In this talk, we discuss how Optical and X-Ray methods are used to measure the feature shape and dimensions of these structures.The use of X-Ray methods such as ω-2θscans and reciprocal space maps provide layer thickness and stress characterization. We will use simulations to show how a buried layer with a different thickness or Ge concentration alters the data. Recent electron microscopy studies have quantified the stress at the interfaces of these superlattices.We will also discuss how Mueller Matrix spectroscopic ellipsometry (MMSE) based scatterometry is used to measure feature shape and dimension for the nanowire/nanosheet structures used to fabricate nanosheet transistors and eventually 3D DRAM.The starting point for optical scatterometry is determining the optical properties of stressed pseudomorphic Si(1-x)Gex.MMSE can be extended into the infra-red and into the EUV.In addition, small angle X-Ray scattering has been adapted into a method knows as CDSAXS which can be used to characterize these structures.This talk will be an overview of these methods.

11:40am **AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-12 Non-Destructive Depth Differentiated Analysis of Surfaces Using Ion Scattering Spectroscopy (ISS), XPS and HAXPES***, **Paul Mack**,* Thermo Fisher Scientific, UK

Recently there has been renewed interest in probing deeper into surfaces using HAXPES in addition to the more surface sensitive (soft X-ray) XPS. On modern XPS systems, with high sensitivity, the total sampling depth may be somewhere between 10nm and 15nm but HAXPES enables the analyst to look deeper, without having to destructively sputter the surface with ions. For a complementary, more comprehensive analysis, XPS and HAXPES can be combined with Ion Scattering Spectroscopy (ISS). ISS is far more surface sensitive than XPS, typically being thought of as a technique to analyse the top monolayer of a sample for elemental information.

In this work, the combination of XPS, HAXPES and ISS on a single tool has been used to give a non-destructive depth differentiated analysis of a range of samples, including a perovskite and an industrially relevant material containing multiple transition metals. The combination of all three techniques provides insight into the depth distributions of elements and chemical states, from the top monolayer to beyond 20nm into the surface.

12:00pm **AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-13 Towards Measurement of Molecular Shapes Using OrbiSIMS***, **Gustavo F. Trindade**, J. Vorng, A. Eyres, I. Gilmore,* National Physical Laboratory, UK

An OrbiSIMS [1] instrument features a dual analyser configuration with a time-of-flight (ToF) mass spectrometer (MS) and an Orbitrap™ MS, which confer advantages of speed and high-performance mass spectrometry, respectively. The ability to combine the MS performance usually found in a state-of-the-art proteomics and metabolomics MS with 3D imaging at the microscale and from nanolayers of <10 nm of material has proved popular in a broad field of application from organic electronics to drug discovery. For secondary ions to be efficiently transferred to the Orbitrap analyser, the sample is biased by a target voltage V_T necessary to match the acceptance window of the Orbitrap. Furthermore, the ions kinetic energy from the SIMS collision process must be reduced. Therefore, in the OrbiSIMS, a transfer system with helium gas at a pressure P_{He} slows the ions and reduces their kinetic energy distribution through inelastic collisions with gas atoms. Usually, an Orbitrap is used with an ambient pressure ion source and so here an extra gas flow of nitrogen is introduced that leads to an increase of pressure P_{N2} to compensate.

We conducted a systematic assessment of V_T and P_{He} and P_{N2} on the transmitted secondary ion intensities [2] and revealed a complex behaviour, indicating the possibility for additional separation of ions based on their shape, stability, and kinetics of formation. We showed that the V_T for maximum transmission of secondary ions will not be the same for all molecules of the same material and that sometimes multiple maxima exist. Here, we present recent progress towards the understanding of these phenomena and how we are leveraging it to measure molecular shape by using reference trisaccharides raffinose, maltrosiose and melozitose [3].

[1] M. K. Passarelli *et al.*, “The 3D OrbiSIMS—label-free metabolic imaging with subcellular lateral resolution and high mass-resolving power,” *Nat. Methods*, no. november, p. nmeth.4504, 2017, doi: 10.1038/nmeth.4504.

[2] L. Matjacic *et al.*, “OrbiSIMS metrology part I: Optimisation of the target potential and collision cell pressure,” *Surf. Interface Anal.*, no. November 2021, pp. 1–10, 2021, doi: 10.1002/sia.7058.

[3] G.F. Trindade *et al.*, In preparation.

Plasma Science and Technology Division
Room A107-109 - Session PS2+MS-WeA

Plasma-Surface Modeling

Moderators: Emilie Despiau-Pujo, Univ. Grenoble Alpes, CNRS, LTM, **Jun-Chieh Wang**, Applied Materials

2:20pm **PS2+MS-WeA-1 Modeling and Simulation of Plasma-Surface Interactions in Nanofabrication***, **David Graves**,* Princeton University **INVITED**

Plasma-enhanced atomic layer deposition (ALD) and etching (ALE) in principle offer an unprecedented opportunity to control surface composition and structure. By modulating process time, frequency, energy, and chemistry, it is possible to vastly increase the range of conditions and surface modification effects at surfaces. ALE/ALD can simplify the process by separating, for example, a chemical surface modification step from addition of energy through rare gas ion bombardment. It might be possible to design novel etch and/or deposition precursor molecules to take advantage of ALE/ALD modulation-oriented approaches. However, process modulation introduces the complexity of having the surface state change in time during the exposure. To understand and control these processes, an atomic scale plasma-surface interaction simulation is essential. In this talk, I briefly review the use of molecular dynamics (MD) simulations in plasma-surface interactions and how they have been used to help understand conventional plasma etching and deposition. I then use our recent studies of PEALE to highlight both successes and limitations of the current state of the art when used for modulated atomic layer processes. The key issues of interatomic force fields for many new chemistries and materials; using MD to simulate an intrinsically multi-timescale process; and the need to couple well-diagnosed experiments with atomistic simulations are emphasized.

3:00pm **PS2+MS-WeA-3 Mechanisms of Phosphorus Halides Gas Boosting Cryogenic Dry Process Etch Rate: A Quantum Chemistry Investigation***, **Yu-Hao Tsai**, D. Zhang,* TEL Technology Center, America, LLC*; T. Orui, T. Yokoyama, R. Suda,* Tokyo Electron Miyagi Limited, Japan*; T. Hisamatsu,* TEL Technology Center, America, LLC*; Y. Kihara,* Tokyo Electron Miyagi Limited, Japan*; P. Biolsi,* TEL Technology Center, America, LLC

3D-NAND fabrication requires ultrafast etch rate (E/R) of the dielectric material stacks to deliver the high-aspect-ratio contact (HARC) etch with an economical fashion. In a sperate report submitted about the cryogenic dry etch process development, we introduce the results of the drastically higher E/R of Ox/SiN (ONON) than the room temperature ones. We also reveal the catalytic etching reaction which enables the fast-etch process. We then identify the E/R booster gases: phosphorus halide, which brings the E/R to a higher level. To advance the booster-process development, a fundamental understanding of how the performance enhancing gases work is unavoidably crucial. This paper focuses on the mechanisms of phosphorus halides booster making the ONON E/R faster than the non-boosted cryogenic etch processes. Using the density functional theory (DFT), we identify the major chemical reactions behind the E/R enhancement. Based on the findings, we highlight the major properties required for the booster gases to function. The experimental results verify the mechanisms built upon the DFT study. In addition, we discuss the impact from the halogen atoms of the molecules on the etch performance. The paper does not only provide the insight toward an even higher E/R but also shed a light on the synergy of combing the experiments and atomistic modeling for the advanced node manufacturing technology developments.

3:20pm **PS2+MS-WeA-4 Molecular Dynamics Simulations of Diamond Surface Processing via Low-Energy Hydrogen and Argon Ion Bombardment***, **Jack Draney**,* Princeton University*; J. Vella,* Princeton University Plasma Physics Lab*; A. Panagiotopoulos, D. Graves,* Princeton University

Nitrogen-vacancy (NV) centers in diamond are promising for multiple applications in quantum information processing and sensing [1,2]. NV centers can locally detect and measure physical quantities such as magnetic and electric fields. However, these devices are currently limited by surface defects that compromise charge stability and spin coherence [1,2]. In this work, we explore plasma-assisted atomic layer etching of diamond using classical molecular dynamics (MD) simulations. We performed MD simulations of low-energy hydrogen (<50 eV) and argon (<200 eV) ion bombardment of diamond surfaces. Argon ion bombardment can be used to locally smooth initially rough diamond surfaces via the formation of an amorphous C layer, the thickness of which increases with argon ion energy. Subsequent exposure with hydrogen ions (or fast neutrals) will selectively etch this amorphous C layer, leaving the underlying diamond layer intact if the H energy is maintained between ~2–5 eV. The simulations suggest that combining Ar^+ smoothing with selective H removal of amorphous C could be an effective strategy for diamond surface engineering, leading to more reliable and sensitive NV center devices.

[1] Sangtawesin, S., Dwyer, B. L., Srinivasan, S., Allred, J. J., Rodgers, L. V., De Greve, K., ... & De Leon, N. P. (2019). Origins of diamond surface noise probed by correlating single-spin measurements with surface spectroscopy. *Physical Review X*, *9*(3), 031052.

[2] Stacey, A., Dontschuk, N., Chou, J. P., Broadway, D. A., Schenk, A. K., Sear, M. J., ... & Hollenberg, L. C. (2019). Evidence for primal sp2 defects at the diamond surface: candidates for electron trapping and noise sources. *Advanced Materials Interfaces*, *6*(3), 1801449.

4:20pm **PS2+MS-WeA-7 Yesterday, Today, and Tomorrow for High-Aspect-Ratio Contact Etching: Unraveling the Mysteries of Plasma-Surface Interactions with Modeling and Simulations***, **Du Zhang**, Y. Tsai,* TEL Technology Center, America, LLC*; M. Iwata, M. Yokoi, K. Tanaka,* Tokyo Electron Miyagi Limited, Japan*; T. Hisamatsu,* TEL Technology Center, America, LLC*; Y. Kihara,* Tokyo Electron Miyagi Limited, Japan*; P. Biolsi,* TEL Technology Center, America, LLC **INVITED**

The ever-growing demand for big data storage and processing has driven advancements in both the design and process technologies of advanced memory devices. In particular, the fabrication of high-aspect-ratio contacts (HARC) is a key process step. Etch throughput and profile control are crucial for reducing manufacturing cost and ensuring device performance. To meet these challenges, multiscale mechanistic understandings are essential for driving process and design optimization.

In this paper, we will discuss the fundamental etch mechanisms of plasma-surface interactions for HARC etching assisted by atomistic / plasma / profile modeling. We will review the underlying surface reaction mechanisms of the conventional fluorocarbon gas chemistry. We will also discuss the typical process challenges with etch rate and profile control, as well as various possible mitigation methods. Moreover, we will introduce how hydrogen admixture into the fluorocarbon chemistry can alter the behavior of dielectric etch rate and surface chemistry in a way that breaks conventional wisdom, especially at lower wafer temperatures. By unraveling and utilizing these underlying mechanisms derived from multi-scale simulations, we have been able to design new processes to achieve enhanced performance.

5:00pm **PS2+MS-WeA-9 Optimization of Model Parameters in Simulations of High Aspect Ratio Plasma Etching***, **Florian Krüger**,* University of Michigan, Ann Arbor*; D. Zhang, M. Park, A. Metz,* TEL Technology Center, America, LLC, USA*; M. Kushner,* University of Michigan, Ann Arbor

Computational investigations of feature evolution during plasma etching of micro- and nano-electronics devices are highly dependent on a robust reaction mechanism and precise knowledge of reaction probabilities and coefficients to accurately represent the physical behavior of these processes. The increased complexity of the structures and use of novel gas compositions coupled with the necessarily reduced reaction set used by numerical investigations of feature evolution makes it difficult to choose these critical parameters from first principles. This problem is exacerbated by the fact that many of the physical and chemical processes occurring during plasma etching are based on different fundamental principles - i.e., physical sputtering, chemical sputtering, chemisorption, physisorption, spontaneous etching – that have different functional forms.

The aim of this work was to accelerate the development of reaction mechanisms for feature profile evolution during plasma etching.This is accomplished by selecting a subset of reaction rates and angular dependencies and matching the predictions of feature profiles to experimental data using autonomous optimization methods. To that end a series of etches of high aspect ratio (HAR) SiO_2 features using a C_4F_6 / C_4F_8 / Ar /O_2 plasma was performed and relevant quantities such as etch depth, etch rate, aspect ratio as well as critical widths at several depths were determined using scanning electron microscopy.

The same process was reproduced using gas phase and profile scale simulation tools, HEPM (Hybrid Plasma Equipment Model) and MCFPM (Monte Carlo Feature Profile Model), respectively. Some of the input parameters used by the MCFPM were coupled to a multi variate 2-step optimizer that adjusted relevant input parameters in to achieve the best

match between simulation and experiments.Thus, the profile etch simulation effectively acts as an objective function on which the optimization is based. Due to the specific nature of the data and objective function with respect to spatial discretization, the 2-step approach – a combination of gradient descent and Nelder-Mead optimization - proved most effective.

The outcome and development this optimization process will be discussed.The resulting reaction mechanism was used to simulate features using similar but quantitatively different processing conditions to demonstrate how broadly the mechanism can be applied.

____

* Work supported by Tokyo Electron, Samsung Electronics and the National Science Foundation.

5:20pm **PS2+MS-WeA-10 Prediction of Surface Morphology and Composition Evolution during Atomic Layer Deposition via Combined Ab-Initio and Monte Carlo Approach***, **Ting-Ya Wang**, G. Hwang,* University of Texas at Austin

Atomic layer deposition (ALD) has been proposed as a method for achieving greater precision and control over film thickness, conformality, and impurity levels as compared to traditional chemical vapor deposition. It uses alternating cycles of two half-cycle reactions to achieve sequential and self-limiting deposition. However, finding the optimal conditions for the desired film properties and surface states for a certain material has largely relied on a trial-and-error approach. To expedite the search process, understanding the underlying mechanisms that influence surface chemistry and structure is crucial. However, currently available experimental methods may be limited in their ability to non-invasively observe surfaces at the atomic level or hindered by overlapping signals.

Theoretical methods have their own set of limitations. First-principles calculations, such as density functional theory (DFT), can be used to study the electronic structure of atoms and have been applied extensively to study surface reaction pathways. However, they are generally limited to a few hundred atoms and do not consider temperature and pressure effects. Ab-initio molecular dynamics (AIMD) simulations allow for studying dynamic processes, but they are similarly limited by both length and time scales. Monte Carlo (MC) simulations provide a way to study the thermodynamic properties of larger systems, and kinetic MC (KMC) allows for real-time simulation of system evolution. However, without a description of potential for each atom, both MC methods rely on predetermined lists of allowed events, which limit their accuracy and applicability.

Combining MC with DFT can potentially enhance the accuracy and applicability of simulations. However, in order to make these methods more reliable in describing various systems and include unknown reaction mechanisms, streamlining the integration of these two methods and the auto-generation of required information for MC simulations is important. In our work, we have applied this approach to investigate the evolution of surface structure and film morphology during plasma-enhanced ALD. Film morphology is a critical factor affecting film properties such as refractive index and wet etching rate, while surface structure determines the surface chemistry and thus affects deposition kinetics. We have examined the effects of plasma and different types of precursors on ALD processes and film properties, as well as the impact of process conditions, such as temperature and pressure.

5:40pm **PS2+MS-WeA-11 Modeling Reaction and Diffusion at a Plasma-Liquid Interface***, **Sean Peyres**,* University of Illinois at Urbana-Champaign*; N. Üner,* Middle East Technical University, Turkey*; N. Abuyazid, R. Sankaran,* University of Illinois at Urbana-Champaign

Low-temperature, atmospheric-pressure plasmas can promote reactions at a liquid surface for various applications including nanoparticle synthesis, water purification, treatment of skin wounds, and chemical production. At the core of these processes, plasma-produced species, such as electrons and hydroxyl radicals, cross the gas-liquid boundary and rapidly react with solution-phase species, including the solvent, within a few nanometers to micrometers distance of the interface. A key consequence of the highly localized reactions is that the reaction rates are limited by mass transport of the solution species from the bulk liquid to the plasma-liquid interface. Previous experimental studies have observed such mass transport limitations, but a fundamental description of the mass transport has yet to be developed.

Here, we present a simple reaction-diffusion model for the reaction of plasma-produced species at a gas-liquid interface. The model consists of a set of nonlinear differential equations describing the reaction and diffusion of a single plasma species (referred to as a radical) and a single solution-phase species (referred to as a scavenger). The plasma-produced radical reacts both with the scavenger and itself in the solvent via recombination. To solve the equations analytically, simplifying assumptions were necessary. First, quasi-steady state was assumed, where the radical and scavenger concentrations quickly obtain a profile that can be solved for a given time. Then, various assumptions were made to solve the equations under limiting cases. Examples include negligible radical-scavenger reaction, uniform scavenger concentration, and fast reaction with the scavenger (compared to radical recombination). These results could be summarized by using dimensionless numbers that relate the competition between the radical-scavenger and radical recombination reactions along with the transport freedom of the scavenger.

Furthermore, we solved the full set of equations numerically and compared with the analytical solutions for the limiting cases. Finally, by adding a boundary condition for the diffusive layer, the bulk scavenger concentration could be calculated as a function of time and compared with previous experimental reports. We show that the model can be used to quantitatively predict and explain mass transport effects on reaction yields and selectivity.

6:00pm **PS2+MS-WeA-12 Integrated Modeling of Diamond Growth and the Surface Composition in CH_4/H_2 Plasma***, Y. Barsukov,* Princeton University Plasma Physics Lab*; A. Khrabry,* Princeton University*; **Igor Kaganovich**,* Princeton University Plasma Physics Lab

Microwave plasma generated in a mixture of CH4 highly diluted in H2 is typically used to grow diamonds. According to the broadly accepted mechanism, most of the surface of the growing diamond is unreactive because it is covered by hydrogen atoms. At a small fraction of the surface, hydrogen is removed by the so-called hydrogen-atom abstraction mechanism resulting in the formation of reactive sites (surface activation). Radical species produced in the CH4/H2 plasma are adsorbed on the reactive surface sites, changing the surface composition and promoting the diamond film growth. Atomic H radicals play a key role in the surface activation, allowing for the CH3 radicals to be adsorbed on the reactive sites which leads to the growth of diamond. Nevertheless, the main by-product of CH4 decomposition in the plasma is C2H2, but its role in the growth process is still debated. A complex kinetic model which links fluxes of gaseous reactants from the plasma to the surface composition is needed to identify the role of each reactant.

To consider complex plasma-surface chemistry we performed a 0D kinetic modeling, where 83 surface reactions between CH4, CH3, H, H2 and C2H2 gaseous species are considered. The rates of all 83 reactions were calculated under the same approach, namely, we used WB97XD DFT functional and transition state theory. The DFT functional was validated for gaseous reactions, for which rate constants were measured. The following processes were considered in the model: 1) surface activation/passivation by H, H2, CH3 and CH4, 2) adsorption/desorption of CH3 and C2H2 on the reactive surface sites, 3) hydrogen abstraction from the adsorbates, 4) incorporation of C atom from the adsorbate into the diamond network (sp3 phase), and 5) formation of sp2 phase from C2H2 adsorbate.

The model reproduces the experimental observation that the rate of diamond growth strongly depends on the substrate temperature and has a peak near 1200 K. Detailed analysis of the surface composition shows that the growth is suppressed at low temperature due to formation of sp2 phase. (The mechanism of sp2 phase formation is similar to the mechanism of soot growth). At temperatures higher than 1200 K, the growth is suppressed due to reverse reactions leading to separation of C atoms from the diamond network into the adsorbed state and their subsequent desorption. Thus, our 0D kinetic model allows to link fluxes of plasma reagents with the surface composition and growth rate. The model will be expanded with reactions leading to doping of diamond, which are critical for the synthesis of sensors and cubits.

CHIPS Act Mini-Symposium
Room C120-122 - Session CPS+MS-ThM

Chips and Science Act Implementation for Microelectronics (Including Workforce)

Moderators: Alain Diebold, SUNY Polytechnic Institute, **Tina Kaarsberg**, U.S. Department of Energy, Advanced Manufacturing Office

8:00am **CPS+MS-ThM-1 The Goals for the CHIPS and Science Act of 2022***, D. Lavan, **Jay Lewis**,* National Institute for Science and Technology (NIST) **INVITED**

The goals for the CHIPS and Science Act of 2022 are to strengthen American manufacturing, supply chains, and national security, and invest in research and development, science and technology, and the workforce of the future to keep the United States the leader in the industries of tomorrow, including nanotechnology, clean energy, quantum computing, and artificial intelligence. An update on progress implementing the CHIPS and Science act will be provided, focusing on R&D Programs including the NSTC, the NAPMP, Manufacturing USA and the Metrology Program.

8:40am **CPS+MS-ThM-3 U.S. CHIPS Act and Semiconductor R&D Centers: Accelerating American Innovation***, **David Anderson**,* NY CREATES **INVITED**

This presentation by David Anderson, President of the New York Center for Research, Economic Advancement, Technology, Engineering, and Science (NY CREATES), details the latest updates on the U.S. CHIPS and Science Act and discusses semiconductor R&D centers as key drivers for stimulating innovation, enhancing domestic chip manufacturing capabilities, and bolstering the United States' position in the global semiconductor industry. Through an analysis of the CHIPS Act's key components and the vision put forth by the Federal government, Mr. Anderson will highlight its unprecedented opportunities for accelerating semiconductor R&D and cultivating a robust ecosystem within the U.S. Additionally, this presentation showcases the pivotal role of semiconductor R&D centers in harnessing collaborative research efforts, fostering public-private partnerships, and nurturing talent. Drawing upon his decades of experience in the industry, Anderson demonstrates the positive impact of semiconductor R&D centers on industry growth, job creation, and national security. Attendees will gain insights into the innovative research initiatives, cross-sector collaborations, and technology roadmaps that these centers facilitate, and how the CHIPS Act will help to propel the U.S. to the forefront of the semiconductor industry.

9:20am **CPS+MS-ThM-5 A View on the 1000x Performance Efficiency Goal***, **Steve Pawlowski**,* Intel **INVITED**

Over the last two decades, large HPC machine efforts have become a procurement exercise. A large set of applications have been unable to leverage the additional computational power of newly-procured machines without significant additional software development. The machine architectures need to evolve: new systems architectures and innovations require a deep understanding of application uses cases and their needs. Memory and storage, as foundational elements, will be at the center of future innovative systems, driving both greater performance and increased energy efficiency. We have a performance efficiency goal of achieving 1000x over the next 20 years. This talk posits that $\geq$100x of the 1000x gain can be realized through repartitioning/packaging changes. The <10x that remains can come from re-architecting the system based on a detailed understanding of the targeted applications.

11:00am **CPS+MS-ThM-10 Re-Shoring and Re-Energizing Microelectronics: the Workforce Challenge***, M. Lundstrom, **Vijay Raghunathan**,* Purdue University **INVITED**

The CHIPS and Science Act is a bold initiative designed to re-shore semiconductor manufacturing, secure our supply chain, re-gain the lead in leading-edge chip technology, bolster our leading positions in design and semiconductor manufacturing equipment, and accelerate the pace of innovation. Accomplishing these ambitious objectives will require the kinds of mission-driven, deep university-industry-government partnerships that we have not seen since the Manhattan Project and Space Race. The semiconductor workforce is a key challenge – not just a larger workforce, but one educated to advance electronics in the new era we are entering. This talk will present the author's perspective on the magnitude of the challenge, the intimate connection between research, teaching, and innovation that must be maintained, the educational needs for new era electronics, how companies and universities should work together, and the role of international partnerships.

11:40am **CPS+MS-ThM-12 Saving Power with New Designs and Chiplets in the New Era of Advanced Packaging***, **Jan Vardaman**,* TechSearch International, Inc. **INVITED**

Energy saving through new designs and package architectures including chiplets are driving developments and options in high-performance computing. An increasing number of companies are turning to chiplets, not only to achieve the economic advantages lost with expensive monolithic scaling, but also to meet the power savings requirements for datacenters and other high-performance computing applications. Co-packaged optics holds promise and is under development by a number of companies. Design with chiplets is one approach under consideration.. A chiplet is not a package, but it is a new approach to system, package, and chip design. There are many package options that can be adopted and careful consideration is required to select the most appropriate options for the application. Options include the emerging 3DIC format with mircobumps or hybrid bonding, laminate substrate package, fan-out on substrate, and silicon interposer. Challenges include design, test, assembly, and thermal. This presentation focuses on the move to energy savings and design and package methods being introduced to achieve power and performance goals.

Plasma Science and Technology Division
Room A106 - Session PS1+MS-ThM

AI/ML in Plasma Applications

Moderators: Robert Bruce, IBM Research, T. J. Watson Research Center, **Yu-Hao Tsai**, TEL Technology Center, America, LLC

8:00am **PS1+MS-ThM-1 Approaches to Accelerate Etch Process Optimization by Using Virtual Experiment***, **Tetsuya Nishizuka**, R. Igosawa, T. Yokoyama, K. Sako, H. Moki, M. Honda,* Tokyo Electron Miyagi, Ltd., Japan **INVITED**

High Aspect Ratio Contact (HARC) hole etching is one of the processes which require a lot of efforts to optimize etch condition. As the aspect ratio increases, some issues such as "distortion" and "twisting" which are hole circularity degradation and deviation from vertical etch respectively, have been critical. Since they cause asymmetric profile along hole axis, not only vertical but also horizontal cross section is necessary to observe 3D profile image, it takes more time to conduct a series of experiments, and then it makes the optimization more difficult.

In this study, we created a model for a topography simulation which is based on Monte Carlo method, so that we can conduct "virtual experiment" on the simulator and expect to reduce the number of experiments by understanding etch mechanism. With respect to practicability for model building, we employed a procedure that representative ion and radical parameters which associate with etching behavior are carefully fitted to actual experimental results [1].

As the result, while this kind of asymmetric distortion profile is supposed to come from stochastic variation and charging in the hole [2], we found there is another systematic factor that is an interaction between re-deposition of sputtered etch material and initial mask profile by analyzing Amorphas Carbon Layer (ACL) etching precisely [3]. This model is consisted with the fact that the distortion deteriorates under low temperature condition. It was also applied to oxide-nitride (ON) layers etch and well reproduced twisting profile on the simulator.

Additionally, we attempted an automatic parameter fitting by using ML optimization for the purpose to minimize efforts in case of converting the model to the other applications than HARC.

[1] Ohmine et. al., Jpn. J. Appl. Phys. 50 (2011)

[2] Huang et. al., J. Vac. Sci. Technol. A 37 (2019)

[3] Igosawa et. al., Proceedings of international symposium on dry process 2022

8:40am **PS1+MS-ThM-3 Recipe Optimization for Plasma Etching with Machine Learning Model Trained by Initial Dataset Using D-Optimal Design***, **Ryo Morisaki**, T. Ohmori,* Hitachi, Ltd., Japan

The development of semiconductor fabrication processes is becoming more difficult due to a growing need for the miniaturization of semiconductor devices to the nano-scale level. Furthermore, growing demands for cutting-edge semiconductor devices of superior performance necessitate the swift development of the fabrication processes.

Plasma etching is a pivotal technique for semiconductor processes. Machine learning (ML) methods have been applied to optimize the recipe for these processes, which is a control parameter set including items such as plasma generation power, wafer bias power, gas species for plasma generation, and the flow rate of gases[1][2]. Datasets for training the ML model consist of recipes and their corresponding etching profiles. Generally, the recipes are curated by expert process engineers to reduce the cost of the etching experiments. On the other hand, design of experiments (DoE) methods can be utilized to obtain the training datasets without expert knowledge. Therefore, DoE has the potential to increase of the number of engineers who can optimize recipes for difficult etching processes.

In this work, two distinct approaches for creating an initial dataset for the training are compared to evaluate the efficiency of recipe optimization using an ML model. In the first approach, the initial dataset is created on the basis of the plasma etching knowledge of expert engineers, as has been conventionally practiced, and in the second approach, it is created on the basis of elementary knowledge for etching tool operations and a DoE method with the D-optimal criterion is used[3]. In the latter approach, a preliminary range of values for the recipe parameters, in which plasma generation and etching can occur, is established on the basis of fundamental knowledge of plasma etching. Subsequently, D-optimization is conducted on the recipe parameters within the specified range to generate a high-quality and diverse initial dataset that can improve the ML model for optimizing the recipes and profiles. In contrast to the conventional DoE with orthogonal array, this DoE with the D-optimal criterion method has no limitation on the number of experiments, thus making it suitable for creating small initial datasets to reduce the cost of the etching experiments. We report detailed comparison results of the efficiency of the etching optimization using each approach.

[1]T. Ohmori et al., in Proc. Int. Symp. Dry Process, pp. 9–10 (2017).

[2]H. Nakada et al., in Proc. Int. Symp. Dry Process, pp. 53–54 (2019).

[3]J. Keifer, Journal of the Royal Statistical Society. Series B (Methodological), vol. 21, no. 2, pp. 272–319 (1959).

9:00am **PS1+MS-ThM-4 Digital Twin Model to Compensate for Variations in Plasma Etching Process***, T. Nakayama, T. Ohmori,* Hitachi, Ltd., Japan*; **Naoto Takano**,* Hitachi High-tech America, Inc.

The miniaturization of semiconductor devices based on Moore's Law has necessitated increasingly demanding precision in the mass production of devices. To achieve a target etching profile with nano-scale accuracy during the manufacturing process, plasma etching systems must be equipped with technologies to minimize variations of the etching. A set of parameters for the control function of the etching system is called a recipe, which is used as input data for the system. While the same recipe is used for all systems in mass production, the etching profiles are varied due to the drift of etching chamber conditions or differences in the conditions of the inner chamber parts replaced at the time of chamber maintenance. Etching rate (ER) data are often utilized to check the variations of chamber conditions and construct a compensation model, but a large ER dataset is required for the model, which is time consuming.

Therefore, we have been investigating a compensation method that requires only a small amount of data. In our method, first, a reference digital twin (DT) model utilizing neural networks is trained by sufficient data. A large amount of the training data consisting of recipes and ER can be prepared in advance by experiments using a reference chamber. Further, in addition to the experimental ER, simulation data of ion and radical fluxes correlating with ER (calculated by a plasma simulator) are used for the training data [1]. The simulation data can also be prepared in advance. Next, a small amount of ER data is obtained from a target chamber that has a different ER from that in the reference chamber. A target DT model is obtained by additionally training the reference DT using the small amount of ER data. Finally, a recipe that compensates for the ER difference is predicted using the target DT.

We prepared several hundred experimental ER data and calculated fluxes data using the reference chamber and the plasma simulator, respectively. Several tens of ER data were obtained as a small amount of data using a target chamber. Predicted recipes by the trained target DT model for ER compensation were experimentally verified in the target chamber. As a result, the ER difference used to check the variation of chamber conditions was decreased by our compensation method using DT models.

[1] T. Nakayama et al., Proc. Gaseous Electronics Conf., Sendai (2022).

9:20am **PS1+MS-ThM-5 Deep Learning-Enabled Plasma Equipment Design Optimization in Semiconductor Manufacturing***, S. Ahn, **Jinkyu Bae**, S. Yoo, S. Nam,* Samsung Electronics, Republic of Korea

In plasma reactors, a focus ring which surrounds the wafer plays an important role in improving uniform fluxes and energy across the wafer. To ensure the uniformity and consistent processes, sophisticated design for the focus ring is necessary. However, focus ring design is very challenging due to the complexity of the design space and the high-dimensional geometry of the focus ring. Furthermore, the multi-scale and multi-physics nature of low-temperature plasmas (LTPs) makes it difficult to develop accurate simulation models that can capture the dynamics of plasma discharges. Simulating LTPs is the need to consider multiple physical and chemical processes that occur simultaneously, such as ionization, recombination, excitation, and attachment. These processes can be highly nonlinear and require a large range of integrating time scales from picosecond to millisecond. In this study, we present a Deep Neural Network framework employing the DeepONet, which is pre-trained deep neural operators between each physical quantities on behalf of physical governing equations. The training data is generated using HPEM (The Hybrid Plasma Equipment Model) plasma simulation solver. The framework involves two network types. The first network reduces the dimensions of the focus ring geometries to a latent representation. We used a geometric attention mechanism in Variational-Auto-Encoder (VAE) allowing us to discover the latent geometric features of focus ring parts. The high-dimensional design space was effectively reduced by the neural network model. We proposed the concept of using this latent representation in combination with the pre-trained neural networks. We pre-trained deep neural operators that can predict independently physical quantity fields, given general inputs. It is an efficient way of incorporating the plasma physics without embedding the partial differential equations into the loss function of the neural network.The proposed framework is shown to be efficient and effective in optimizing the focus ring design for different objectives, and the effects of variations in the design are thoroughly investigated based on very few measurements using pre-trained deep neural operators. This paper aims to develop framework for predicting plasma dynamics and carrying out focus ring design in reactors.

9:40am **PS1+MS-ThM-6 Wafer Arcing Detect Algorithm Using LSTM Autoencoder in Hardmask Strip Equipment with CCP Source***, **Heewoong Shin**,* PSK, Republic of Korea

“Wafer arc” is one of the phenomenon that occur in semiconductor manufacturing equipment that utilizes plasma, rather than being limited to arc discharge in plasma science. In this study, we discuss the possibility of successfully classifying normal manufacturing process of semiconductor equipment using CCP and the abnormal data by using deep learning methodology. In general, since wafer arcs data have an obvious characteristics that engineers can easily notice, it is thought that they can also easily be detected by general SPC methodology. But in some cases, there are pattern anomalies that cannot be detected by SPC, or there are problems such as requiring the subjectivity of engineers for determining the data is normal or not because it is hard to find common in each abnormal data. Because wafer arcs might cause serious malfunctions in most equipment and are a major cause of yield reduction, so a function that can diagnose abnormalities in advance is required. However, wafer arcs are generally known to be difficult to reproduce to make abnormal

data, and there are problems such as requiring high-resolution optical equipment to detect the arc phenomenon which also costs additional charge. In this study, we used specific parameters in lotlog of CCP equipment as an input of DL model. By training with LSTM-autoencoder, it shows the possibility of classifying normal and abnormal data successfully through simple learning. When the result of this research can be applied in mass-production, it is highly expected that it will effectively detect and predict wafer arcs and other anomaly related to electrical/plasma parameters, and will greatly benefit the yield of semiconductor equipment.

Manufacturing Science and Technology Group
Room C120-122 - Session MS+AP+AS+TF-ThA

Machine Learning for Microelectronics Manufacturing Process Control

Moderator: Tina Kaarsberg, U.S. Department of Energy, Advanced Manufacturing Office

2:20pm **MS+AP+AS+TF-ThA-1 Human-Machine Collaboration for Improving Semiconductor Process Development***, **Keren Kanarik**,* LAM Research **INVITED**

Although chips have been designed by computers for decades, the processes used to manufacture those chips are mostly developed manually – a costly endeavor using highly trained process engineers searching for a combination of tool parameters that produces an acceptable result on the silicon wafer. To assess whether AI could be beneficial in accelerating process engineering innovation and reducing costs, humans and machine algorithms were benchmarked on a virtual high aspect ratio plasma etch process [Kanarik, et al. Nature 616, 707–711 (2023)]. This talk will review results and take a behind-the-scenes look at the study, which showed a "human first, computer last" approach could reach process engineering targets dramatically faster and at half the cost compared to today's approach. While human expertise and domain knowledge are essential for the foreseeable future, the results point us to a path to foundationally change the way processes are developed for manufacturing chips.

3:00pm **MS+AP+AS+TF-ThA-3 Machine Learning-based Atomic Layer Deposition***, **Kanad Basu**,* University of Texas at Dallas **INVITED**

Atomic Layer Deposition (ALD) is dependent on a host of process parameters. These independent parameters can be set to a particular value to create customized recipes for growing films. Although they are considered to significantly influence the ALD process, existing research does not provide a methodology to quantify the impact of these parameters on growth rate and final thickness of a film. Moreover, process parameter-based thickness estimation is a resource- and time-intensive approach, requiring numerous experiments. To address these challenges, we propose a machine learning (ML)-aware strategy that generates "feature importance maps" to determine the most critical process parameters. In our study, we utilize a Veeco® Fiji Gen2 ALD system to grow a CeO2 film. Specifically, our study is associated with 78 process parameters, which include chuck temperatures, chamber temperatures, line temperatures, precursor temperatures, gas flow rates, among others. Our approach utilizes a random forest classifier, which is identifies the top-10 features (parameters) that affect ALD processes. The proposed approach furnishes promising results of up to 99% thickness prediction accuracy using the deduced top-10 features. These results are subsequently validated using in-situ spectroscopic ellipsometry, thereby advocating its effectiveness in generating the feature importance maps. We posit that only these ten features can be utilized to monitor and control ALD processes. Furthermore, in this analysis, we demonstrate the robustness of our solution, which is independent of the type of ALD process considered - standard ALD process or temperature-dependent Temperature-Time-Thickness (TTT) ALD processes. Moreover, by monitoring just ten of the 78 process parameters, the proposed approach has implications of reduced data dimensionality (up to 87.2% reduction in feature space).

3:40pm **MS+AP+AS+TF-ThA-5 Rapid Optimization of Gap-Fill Recipes Using Machine Learning***, **Sebastian Naranjo**, L. Medina de Oliveira, M. Chopra,* Sandbox Semiconductor

Creating and optimizing deposition recipes for nanostructured devices is costly and time-consuming. A major source of defects and device performance degradation is the formation of interior voids. These voids can have a number of causes, including non-uniform deposition rates along the substrate surface due to imperfect seeding and/or mass transport and reaction kinetics factors, as well as critical dimension variations in the initial profile due to imperfections in preceding processing steps. For example, during electroplating, the substrate surface is seeded before material deposition is set to fill the gap. Non-conformal seedings can cause the deposited material to accumulate at different rates and lead to localized voids. Void defects can also occur in highly conformal processes such as atomic layer deposition or chemical vapor deposition due to critical dimension variations such as bowing or tapering in the pre-deposition profile. Current methods for optimizing process performance rely largely on trial and error. Here we present a cost-effective and systematic computational approach to optimize recipe conditions using Sandbox Studio AI, which employs a combination of feature scale modeling and machine learning to rapidly predict process outcomes for a given electroplating system using a minimal number of experiments. In this approach, we first use critical dimension information about the fill height and void defects from a set of experiments to calibrate a feature scale model. We then use the calibrated model to predict critical dimension outcomes for thousands of possible process parameter combinations. These predictions are used to maximize process window stability and provide recipe recommendations that minimize the formation of voids even in the presence of seeding or initial profile imperfections. The showcased approach demonstrates how computational modeling can be used to accelerate learning cycles, improve process quality, and reduce development costs.

Manufacturing Science and Technology Group
Room Oregon Ballroom 203-204 - Session MS-ThP

Manufacturing Science and Technology Poster Session

MS-ThP-1 Autonomous Synthesis in the MBE Using Real-Time Artificial Intelligence, ***Tiffany Kaspar**, L. Wang, J. Christudasjustus, M. Sassi, B. Helfrecht, J. Pope, A. Harilal, S. Akers, S. Spurgeon,* Pacific Northwest National Laboratory

Materials are the key components of nearly all advanced technologies, including quantum information systems, microelectronics, catalysis, and energy conversion and storage. Modern synthesis methods enable the fabrication of an ever-expanding array of novel, non-equilibrium, and/or metastable materials and composites that may possess unique and desirable functionality. Thin film deposition by molecular beam epitaxy (MBE) can produce atomically precise (or nearly so) materials with a wide range of functional electronic, magnetic, ferroelectric/multiferroic, optical, and/or ion-conducting properties. The current state of the art in precision design of functional materials is to manually explore the “growth phase space” of the deposition techniqueto optimize the film properties of interest. Limitations of time and resources often result in incomplete exploration of the growth phase space and resulting properties. Faced with this lack of complete information, materials design and synthesis decisions are made based in part on intuition and luck, slowing both materials optimization and materials discovery.This current synthesis paradigm can be disrupted by employing artificial intelligence (AI)-accelerated analysis of *in situ* and *ex situ* data streams that will enable targeted synthesis of novel materials with desired structure, chemical stability, and functional properties.Here we present a preliminary implementation of such an AI-controlled MBE.We are integrating the control of key synthesis parameters (temperatures, gas flow rates, shutters) with AI-guided computer control.Guidance will be based on near-real-time analysis of reflection high energy electron diffraction (RHEED) patterns using sparse data analytics, with low-latency feedback to the control software.As an initial demonstration, we will control the morphology and phase purity of epitaxial anatase TiO_2 thin films.

MS-ThP-2 Machine Learning Based Virtual Metrology for Effective Process Control in High Product Mix Manufacturing, ***Hyung Joo Lee**, S. Choi,* Siemens EDA, Republic of Korea*; N. Greeneltch, S. Jayaram,* Siemens EDA

1. Introduction

The semiconductor foundry industry faces challenges with high product mix manufacturing, requiring increased flexibility in managing diverse customer demands. Coordinating multiple chambers and process steps with different designs and technology nodes is complex, resulting in reduced yields and increased costs.

2. CVD Process Challenges

The CVD process in semiconductor manufacturing experiences thickness variations due to device layout design and chamber condition drift. Lack of control across layouts affects transistor parameters and yield. Managing chamber-by-chamber variations is crucial for high-volume manufacturing, but current solutions hinder fab line management and throughput.

3. VM Approach and Modeling

Virtual metrology (VM) addresses the trade-off between metrology activities and cost by utilizing data from the process chamber (FDC) to predict metrology results. Design features are extracted and used for prediction across layouts and technologies, benefiting new layouts and production stages. Siemens' Calibre® software is employed for feature extraction, and ML methodologies construct the VM model. Results demonstrate the superiority of the VM model with design features and FDC.

4. APC System and Results

An APC system using the VM model for R2R control is proposed. It incorporates design features, FDC, and measurements to achieve the desired thickness target. The system triggers updates to the VM model based on prediction errors. The APC system significantly improves process capability and reduces film thickness variations. Control simulation confirms the effectiveness of the APC system in a high-mix product foundry fab setting.

5. Summary

The semiconductor foundry industry faces challenges in high product mix manufacturing. The CVD process experiences thickness variations from design features and chamber conditions, impacting yield. A VM approach, incorporating design features and FDC, improves process control. An APC system based on the VM model further enhances thickness control, demonstrating significant improvements in process capability and thickness variation reduction.

MS-ThP-3 Experimental 3D Maintenance Work Measurement and Analysis for Maintenance Improvement and Enhancement of Productivity of Semiconductor Manufacturing Equipment, ***Takashi Numata**, Y. Ogi, K. Mitani, R. Kawamata, N. Ikeda, T. Ege,* Hitachi, Ltd., Japan*; Y. Kadomoto, R. Ishibashi, Y. Shengnan, Y. Sakka, Y. Nakamura, K. Sato,* Hitachi High-Tech Corporation, Japan

Recently, high machine availability of semiconductor manufacturing equipment has become more important, and shortage of field service engineers has become serious. Therefore, maintenance improvement which enable to increase the capacity with inexperienced field engineers and realize productivity improvement of semiconductor manufacturing equipment has been needed.

Based on these circumstances, we have proposed maintenance work measurement and analysis technologies for maintenance improvement of semiconductor manufacturing equipment. Our targets are to reduce durations of and maintenance work, and a rate of reclean (failure of maintenance) especially focusing on periodical maintenance. Maintenance work measurement and analysis have a potential to enable us to extract work differences between skilled and unskilled maintenance workers, extract complex and difficult characteristics of maintenance work, and support and/or reduce such complex and difficult maintenance work.

In this study, we developed a measurement system with 3D sensors and motion sensors, experimentally measured maintenance work of semiconductor manufacturing equipment such as parts assembly and wiping by using the developed system, and extracted indicators of personal differences among workers. We extracted various indicators including task time, working posture, amount of head motion, change of eyesight, amount of hand motion. As a result, we demonstrated representative differences of extracted indicators between an experienced maintenance worker and an inexperienced maintenance worker.

From the result, it was suggested that application of maintenance work measurement and analysis system with results of maintenance enable us to extract important factors to cause reclean, and standardize maintenance work based on skilled workers’ movements and/or successful works. Then effective countermeasures for support and/or reduction of difficult task will be applied based on the results of maintenance work analysis.

Applied Surface Science Division
Room B117-119 - Session AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM

Industrial Applications

Moderators: Marko Sturm, University of Twente, Netherlands, **Alan Spool**, Western Digital Corporation, **Yundong Zhou**, National Physical Laboratory, UK

8:20am **AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-1 Correlative Analysis Using Time-of-flight Secondary Ion Mass Spectrometry for Beam Sensitive Samples*, Jean-Paul Barnes,* *C. Guyot, P. Hirchenhahn, A. De Carvalho, N. Gauthier, T. Maindron, B. Gilquin, D. Ratel, C. Gaude, O. Renault,* Univ. Grenoble Alpes, CEA, Leti, France*; A. Galtayries,* Chimie ParisTech, PSL University, CNRS, Institut de Recherche de Chimie Paris, France*; G. Fisher,* Physical Electronics USA*; C. Seydoux, P. Jouneau,* Univ. Grenoble Alpes, CEA, IRIG-MEM, France **INVITED**

Time-of-flight Secondary Ion Mass Spectrometry (TOF-SIMS) is now widely used for materials analysis in domains such as semiconductor and energy applications. These challenging applications also provide access to well-controlled, custom made samples that have allowed the limits of TOF-SIMS analysis to be identified and helped in the development of correlative analysis approaches. Recent examples include combining AFM measurements with TOF-SIMS depth profiling to correct for sputter rate differences [1] or to measure mechanical or electrical properties and performing X-ray tomography prior to FIB-TOF-SIMS analysis to allow morphological and compositional data from the same volume to be visualized [2]. Currently we are working on two aspects. Firstly improving the quantification and chemical sensitivity of the technique by combining TOF-SIMS with photoemission techniques (XPS or XPEEM), and secondly trying to improve the lateral resolution by correlation with SEM and AFM measurements. Recent examples will be shown for the analysis of beam sensitive organic samples such as OLED devices, brain tissue samples after medical device implantation [3] and symbiotic microorganisms [4]. As well as the correlative aspects between techniques, we will show how tandem mass spectrometry can help in analyzing complex organic samples. In all cases the importance of sample preparation is paramount, especially for biological samples. For example, for the correlation between TOF-SIMS and XPS on OLED samples, a wedge crater protocol has been developed to allow analysis on exactly the same area of the sample whilst minimizing beam damage to the sample. Wedge crater preparation and transfer between instruments is performed under a protected environment (vacuum or inert gas) to avoid unwanted surface modifications.

Part of this work, carried out on the Platform for Nanocharacterisation (PFNC), was supported by the “Recherches Technologiques de Base” and the “CARNOT” program of the French National Research Agency (ANR).

[1] M. A. Moreno *et al. JVST B,* vol. 36, MAY 2018.

[2] A. Priebe *et al. ULTRAMICROSCOPY,* vol. 173, pp. 10-13, FEB 2017.

[3] A. G. De Carvalho *et al. Biointerphases,* vol. 15, 2020.

[4] C. Uwizeye *et al. PNAS.* **Vol 118**, e2025252118, 2021.

9:00am **AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-3 Secondary Ion Mass Spectroscopy of Battery Surface and Interface Chemistry – Metrology and Applications***, Yundong Zhou,* *S. Marchesini, X. Yao, Y. Zhao, I. Gilmore,* National Physical Laboratory, UK

Batteries are very important to achieve carbon net zero. Understanding battery materials change, electrode surfaces, solid electrolyte interphase (SEI) evolution and novel solid-state electrolyte structures is very helpful for developing better batteries. Surface chemical analysis techniques such as X-ray photoelectron spectroscopy (XPS) and Raman spectroscopy are often used but they have their limitations. XPS analysis cannot always resolve overlapping binding energies for some key SEI elements. The SEI often has poor Raman signal intensity. These are all hurdles for battery applications.

Secondary ion mass spectrometry has great potential to study interfacial chemistry in batteries owing to high sensitivity and high-resolution imaging in 2D and 3D.In this study, we use an OrbiSIMS instrument which is equipped with two complementary mass spectrometers (MS). A time-of-flight (ToF) MS has the capability for 2D and 3D imaging using a Bi_3^+ liquid metal ion gun with a spatial resolution of up to 200 nm but with modest mass resolving power. The Orbitrap MS offers high mass resolution and mass accuracy (> 240,000 at m/z 200 and < 2 ppm, respectively). The instrument is equipped with low energy Cs and O_2 sputter beams for high resolution depth profiling of inorganic materials. It also has a Leica docking station enabling samples to be transferred using a vacuum sample transfer chamber from an argon glove box without atmospheric exposure. To improve the quality of measurements on battery materials, we have used ion implanted materials to determine relative sensitivity factors for relevant elements. We have also conducted a systematic study to optimise the OrbiSIMS depth profiling capability. These findings along with recommendations to reduce effects of signal saturation will be discussed and examples of the application to batteries will be provided. We will provide examples of the application of ToF MS and Orbitrap MS. (1,2)

1. X. Yao et al., Energy Environ. Sci., 2023, DOI: 10.1039/D2EE04006A.
2. S. Marchesini et al., ACS Appl. Mater. Interfaces, 14(2022)52779-52793.

9:20am **AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-4 Characterizing Ion Distribution at the Solid-Electrolyte Interface in Solid-State Lithium Ion Batteries with ToF-SIMS***, Teodora Zagorac,* University of Illinois - Chicago*; M. Counihan, J. Lee, Y. Zhang,* Argonne National Laboratory, USA*; L. Hanley,* University of Illinois - Chicago*; S. Tepavcevic,* Argonne National Laboratory, USA

Interest in solid state lithium-ion batteries as the next generation of energy storage devices has led to intense study of the chemistry, structure, and manufacturing processes for polymer electrolytes. Lithium bis(trifluoromethanesulfonyl) imide (LiTFSI) salt is often used to introduce Li ions into the solid-state electrolyte. Lithium bis(fluorosulfonyl)imide salt (LiFSI) and lithium nitrate ($LiNO_3$) are less expensive salts with the potential to improve performance characteristics over pure LiTFSI in certain electrolyte formulations. The differences in distribution and reactivity of these different salts are still unknown but are critical to battery performance. Time-of-flight secondary ion mass spectrometry (ToF-SIMS) imaging and depth profiling was performed to compare the distributions of Li^+ cations and $TFSI^-$, FSI^-, and NO_3^- anions across the solid-electrolyte interface (SEI) formed between the polymer electrolyte and thin lithium metal electrode. Experiments were performed on ~600 nm salt-rich poly(ethylene oxide) electrolytes with ~10 nm overlayers of vapor-deposited Li metal. Samples were probed with 30 keV Bi_3^+ from a liquid metal ion gun while depth profiling with 10 keV Ar_{1400} gas cluster ion beam to collect both positive and negative ion mass spectra. Ion distributions from the three salts and their 3D images will be presented and discussed in terms of the relative composition of their SEI layers. Chemical differences from ToF-SIMS analysis help explain the differences in electrochemical SEI formation and half cell cycling: LiTFSI and LiFSI are similar, but $LiNO_3$ presents much different electrochemical properties.

9:40am **AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-5 A Perspective on X-ray Photoelectron Spectroscopy (XPS) Peak Fitting, and Reporting of XPS Data Acquisition and Peak Fitting Parameters in the Literature***, Matthew Linford,* *G. Major, J. Pinder,* Brigham Young University

We recently reported that a rather large fraction (ca. 40 %) of the XPS peak fitting in the literature is at best suspect. In a recent Perspective article (doi: 10.1116/6.0002437) we argue that the various stake holders of the problem can act together to improve the current situation. This Perspective begins with representative examples of poor XPS peak fitting. The purpose of showing these examples is to demonstrate to the reader that we are not quibbling or arguing over subtle interpretations of the data. Increasingly, we see errors that might be classified as egregious. We argue that science is in a state of ‘pre-crisis’ more than in a state of ‘crisis’. We suggest that if too much incorrect data analysis enters the literature it may cease to be self-correcting. We note the very large number of surface and material characterization techniques available today and how this presents a challenge for scientists. Consequently, it is likely that many manuscripts are incompletely reviewed today. Graduate students and post-docs at research institutions are often given minimal training on acquiring and analyzing XPS data. High fees for instruments can limit access to them and student training. Prisoner’s dilemmas may help explain situations in science that lead to suboptimal outcomes for the community. Authors are primarily responsible for the quality of the research in their papers, not reviewers or editors. We question the wisdom of placing the names of reviewers and editors on papers. In some cases, staff scientists are not adequately recognized for their intellectual contributions to projects. Selective reviewing may allow more reviews to be performed without overtaxing the community. Reviewing at some open access journals may be inadequate.

Collaboration needs to be encouraged to a greater extent at some institutions.

10:00am **AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-6 Unsupervised and Supervised Machine Learning Applied to ToF-SIMS of an Organic Matter-Rich Mudstone with Molecular Biomarker**, *M. Pasterski,* University of Illinois Chicago*; M. Lorenz,* Oak Ridge Natinal Laboratory*; A. Ievlev,* Oak Ridge National Laboratory*; R. Wickramasinghe,* ***Luke Hanley****, F. Kenig,* University of Illinois Chicago

Time-of-flight secondary ion mass spectrometry (ToF-SIMS) imaging has been used to detect organic compounds including molecular biosignatures (biomarkers) in geologic samples (R.C. Wickramasinghe, *et al.,* Anal. Chem., 2021, 93, 15949). The spatial distribution of these biomarkers can help determine when and how these organics were incorporated into the host rock. ToF-SIMS imaging can rapidly collect a large amount of data, but molecular and fragment ions of different species are mixed together in complex mass spectra that are difficult to interpret. Here, we apply unsupervised and supervised machine learning (ML) to help interpret the mass spectra obtained by ToF-SIMS of an organic-carbon-rich mudstone from the Middle Jurassic of England (UK). It was previously shown that the presence of sterane molecular biomarkers in this sample can be detected via ToF-SIMS (M.J. Pasterski, *et al.*, Astrobiol., in press). We use unsupervised ML on field emission scanning electron microscopy – electron dispersive spectroscopy (SEM-EDS) measurements to define compositional categories based on differences in elemental abundances. We then test the ability of four ML algorithms - k-nearest neighbors (KNN), recursive partitioning and regressive trees (RPART), eXtreme gradient boost (XGBoost), and random forest (RF) - to classify the ToF-SIMS spectra using the categories assigned via SEM-EDS, using organic and inorganic labels, as well as using presence or absence of detectable steranes. KNN provided the highest predictive accuracy and balanced accuracy. The feature importance, or the specific features of the ToF-SIMS data used by the KNN model to make classifications could not be determined, preventing post-hoc model interpretation. However, the feature importance extracted from the other three models was useful for interpreting spectra. We determined that some of the organic ions used to classify biomarker containing spectra may be fragment ions derived from kerogen.

10:40am **AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-8 Probing Thin Film Interfaces at the Nanoscale by Low Energy Ion Scattering**, ***Marko Sturm****, A. Chandrasekaran, A. Valpreda, A. Zameshin, R. Van de Kruijs, A. Yakshin, F. Bijkerk, M. Ackermann,* University of Twente, Netherlands **INVITED**

The growth of thin films with nanometer range thickness is of great importance for application topics as nanoelectronics, oxidation protection of thin films and optical coatings for X-ray applications. The performance of these coatings often critically depends on the sharpness of the interfaces between different layers. In this talk I will outline how we use Low-energy ion scattering (LEIS) to study interface formation between layers of different transition metals (TMs) and between TMs and Si.

LEIS with noble gas ions as projectiles yields surface peaks that indicate the composition of the outermost atomic layer of a sample. This makes the technique excellently suited to study whether deposition of a thin films leads to a closed layer. However, deposition of an overlayer on top of an underlayer may result in surface segregation of underlayer atoms (driven by surface energy differences or stress), such that the surface composition is not directly representative for the in-depth concentration profile. We analyzed the evolution of surface coverage versus deposited thickness for a large set of TM/TM film combinations, deposited by magnetron sputtering in a system that allows LEIS analysis without vacuum break after deposition. By applying a model that takes into account surface segregation, the interface profiles were derived from these layer growth profiles, which we call deposition depth profile. In addition, we demonstrated that the sharpness of interfaces in TM/TM film systems can be predicted by a phenomenological model with the crystal structure and surface energy of the materials as input parameter. This model in principle predicts the sharpness of the interface in any TM/TM thin film combination! [1]

Apart from surface peaks, LEIS spectra typically also contain so-called tails, caused by projectiles that, after sub-surface scattering, are reionized when leaving the sample. It was demonstrated before that LEIS tails can be used to determine thickness of various thin film systems, when the stopping power of the projectiles is known. Here, we show that LEIS tails can also be used to determine the sharpness of interfaces of few nm Si-on-W and Si-on-Mo films, by comparing LEIS measurements with Monte Carlo simulations with the TRBS code, which takes into account multiple scattering and stopping in the target. This approach allows interface characterization from a single sample, without the need to make a deposition depth profile.

References:

[1] A. Chandrasekaran, R.W.E. van de Kruijs, J.M. Sturm, A.A. Zameshin and F. Bijkerk, ACS Applied Materials & Interfaces **11**, 46311 (2019)

11:20am **AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-10 The Effect of Instrument Settings, Sample Distance, and Tilt on TofsimsSecondary Ion Intensities**, ***Alan Spool****, L. Finney,* Western Digital

Experiments were performed to explore the effects of various instrument settings and sample placements on secondary ion intensities to better understand what factors have the greatest effect on repeatability and replicability in TOF-SIMS. A batch of magnetic recording disks used in hard disk drive manufacture, natively flat and homogeneous, were used as test samples for the purpose. As expected, by far the largest variable altering raw intensities was the LMIG tip stability. LMIG tips can have stable emission currents while still producing variable pulsed LMIG beam currents with resultant variable secondary ion counts. This variability sometimes is seen in slow current drift, but is sometimes so rapid that measurements taken directly before each measurement are not close enough in time to properly scale the measurement results. In these cases, normalization is the only solution. Secondary ion intensities were remarkably insensitive to small variations in sample height (position relative to the extractor). Far more interesting were the changes to the secondary ion intensities that resulted from tilting the sample. These effects varied amongst the secondary ions detected such that normalization did not remove them. Secondary ion emission as a function of emission angle has long been understood to be like a cosine function and to vary somewhat from ion to ion. These different angular profiles explain the differences seen in ion detection as a function of tilt. Some of these differences proved to be asymmetrical, varying depending on whether the sample was tilted toward or away from the primary ion source, an indication that in some situations some residual momentum from the initial primary ion impact onto the surface is carried into the secondary ion emission. These results have implications for attempts to do quantitative analysis on any sample that is not completely flat.

11:40am **AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-11 Evaluation of Unaltered and Irradiated Nuclear Graphite Surfaces through Integrated Traditional XPS and HAXPES Techniques**, ***Jonathan Counsell****, L. Soomary, K. Zahra,* Kratos Analytical Limited, UK*; B. Spencer, A. Theodosiou,* University of Manchester, UK

Graphite-moderated reactors have been operational worldwide for several decades. There exists a substantial body of research in this domain, with particular emphasis on investigating the impact of irradiation damage on the graphite matrix. In order to satisfy the design and regulatory requisites of these advanced reactors, it becomes imperative to gain a deeper comprehension of the retention and transportation mechanisms of fission products within graphite.

This study outlines a technique for the precise assessment of the surface chemistry of highly-oriented pyrolytic graphite (HOPG), serving as a representative model akin to the current graphite grades utilized in the nuclear sector. We delve into the process of surface etching aimed at eliminating surface adsorbates and contaminants. This process involves the utilization of both monatomic and cluster ions, the former inadvertently causing undesirable damage to the graphite structure. Such damage is evidenced by a significant reduction in the sp2 component of C 1s. We introduce the use of UPS analysis as a straightforward means of determining the presence of sp2 characteristics in the uppermost atomic layers.

Moreover, we examine the consequences of high-energy ion implantation (Cs^+) and the ensuing damage to the HOPG surface. This examination is carried out using XPS (1486eV) and HAXPES (2984eV), thereby showcasing the capability to characterize the resulting surface damage and the associated alterations within the probed depths.

Manufacturing Science and Technology Group
Room C120-122 - Session MS-FrM

Microelectronics R&D for Life-Cycle Energy Efficiency

Moderators: Nicholas Johnson, Energetics, **Tina Kaarsberg**, U.S. Department of Energy, Advanced Manufacturing Office

8:20am **MS-FrM-1 Energy Efficient Scaling in Microelectronics: Enabling a New Era in Computing for a Sustainable Future*, Sadasivan Shankar,*** SLAC National Accelerator Laboratory **INVITED**

The geometrical scaling of integrated circuit technology (known by the moniker as Moore's law) has led to many of the computing-based innovations over the last half century. Given the slowing down of scaling, it is important that the energy efficiency of computing should increase to offset the increasing number of digital devices and growing ubiquity of computing in all aspects of the world economy. To understand energy limits for information processing, we explore energy associated with both human-made and natural systems.

Based on lessons from the nature and fundamental analysis, we propose a new paradigm is to double the energy efficiency of computation in every succeeding generation in addition to the ongoing technological scaling. Using examples of synapses from a mammalian brain and quantum information, we estimate the headroom available for energy reduction to be of the order of 1000X to a million or more depending on the metrics. This can be enabled by trade-offs of the performance at the single switch level, with that at the system level including communication and storage, and with the total compute operations needed at the application level.

The opportunities for this new trajectory in computing resides in combinations of architectures, materials, devices, and algorithms/software and application-specific information processing. This energy-based design and scaling in turn could lead to exponential use of computing in even more innovative ways from Artificial Intelligence-driven applications, driverless cars, and smart grids due to the resulting Rebound Effect.As computing is the foundation of new sustainable economy, the intent of this new era is to leverage innovations in science and technology to form a green framework for the planet.

9:00am **MS-FrM-3 Improving Asic Energy Efficiency from Systems to Silicon*, Godwin Maben,*** Synopsys, Inc **INVITED**

Improving Energy efficiency while designing an electronic product, includes considering power as one of the constraints from the beginning of chip design, Macro Architecture selection, power performance trade-offs, appropriate workload selection, defining a power efficient architecture from Hardware perspective and designing an efficient Firmware, System's software , Application Software....etc.

In this presentation, we will look into every aspect of design cycle, in developing a complete platform, which is energy efficient from Systems to Silicon and How EDA tools have emerged as one of the key component in addressing Energy Efficiency, in addition to traditional Performance.

9:40am **MS-FrM-5 Atomic Precision Advanced Manufacturing for Tunnel Field Effect Transistors*, Shashank Misra,*** Sandia National Laboratories **INVITED**

The energy efficiency of microsystems improved by more than 1000x every 20 years under Dennard scaling, where shrinking the linear dimension of a transistor while maintaining a constant electric field scaled the frequency and the voltage of operation. Satisfying the continued demand for computing, when scaling is projecting a single doubling of energy efficiency over the next 15 years, will require innovation across algorithms, architectures, and devices. Sandia has established programs pursuing the basic research underlying probabilistic neuromorphic computing, reconfigurable architectures, energy-efficient AI at the edge, and material manipulation for fine-grained integration of sensing and computation. In this talk, I will focus on a specific transistor that circumvents the physical limitation that ended Dennard scaling, and lowers the operating voltage of a circuit.

Tunnel field effect transistors (TFETs) rely on band-to-band tunneling, and promise a 10x improvement in energy efficiency compared to metal oxide semiconductor transistors (MOSFETs), all while maintaining the same materials. They have not achieved this promise due to poor on:off current ratios, and smeared dopant profiles producing gradual turn-on currents. We have designed a TFET in a vertical geometry which uses atomic precision advanced manufacturing (APAM) to form the buried electrode and the intrinsic tunnel barrier. This design boosts current by scaling with the area of the device instead of a 1D edge and obviates limitations from the abruptness of the doping profile. However, APAM has traditionally only been used to fabricate qubits, and has little to do with microelectronics.

Here, we integrate APAM with conventional fabrication, providing a straightforward path both to advanced transistor devices that work in practical conditions, and to scaled manufacturing. We first demonstrate both the two halves of the vertical TFET device operating at room temperature. We show an APAM nanowire integrated with common back end of line processing, which reveals the APAM nanowire strongly confines carriers, leading to current densities that exceed that of copper. Next, we demonstrate the gated top half the TFET device, limiting processing to thermal budgets tolerated by APAM. The low-thermal budget MOS transistor is used to evaluate the quality of APAM material. Next, we demonstrate integration into a CMOS fabrication flow, complete with working hybrid APAM-CMOS circuits. Finally, we explore operational robustness by showing that CMOS features fail before APAM features in accelerated lifetime testing.

SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

10:40am **MS-FrM-8 Materials, Devices, and Packaging Opportunities Towards a Super Energy Efficient Future*, Paul Fischer,*** Intel Corp. **INVITED**

As highlighted in the SRC's decadal plan, the total energy consumption by microelectronics is doubling approximately every three years while the world's energy production is growing only linearly and at about 2% per year.Despite the efficiency gains from continued Moore's Law scaling, global hunger for compute is growing faster.At Intel we are committed to building a more Responsible, Inclusive, and Sustainable world Enabled by our collective actions and in 2020 laid out our RISE strategy and goals which include a 10x increase in product energy efficiency by 2030.

But what emerging technology options are in the research pipeline to enable product energy efficiency which could shape future opportunities consistent with the Department of Energy's Energy Efficiency Scaling over 2 decades (EES2) effort?Product energy consumption is ultimately the culmination of broad technology ingredients spanning applications, software, algorithms, architectures, circuits, materials, devices, and packaging.In this talk Dr. Fischer will discuss a subset of these ingredients best aligned with AVS conference themes: emerging materials, devices, and packaging technologies which could drastically alter the energy requirements of future microelectronic products.

11:20am **MS-FrM-10 EES2 Update—A Pledger's Perspective*, Steve Pawlowski,*** Intel **INVITED**

Author Index

Bold page numbers indicate presenter

— A —

Abuyazid, N.: PS+MS-TuA-7, **2**; PS2+MS-WeA-11, 7
Ackermann, M.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-8, 14
Adams, D.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-6, **5**
Addamane, S.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-6, 5
Ahn, S.: PS1+MS-ThM-5, 9
Akers, S.: MS-ThP-1, 12
Anderson, D.: CPS+MS-ThM-3, **8**
Armstrong, G.: PS+MS-TuA-1, 1
Artyushkova, K.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-5, 4

— B —

Bae, J.: PS1+MS-ThM-5, **9**
Barnes, J.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-1, **13**
Barnum, A.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-5, 4
Barsukov, Y.: PS2+MS-WeA-12, 7
Basu, K.: MS+AP+AS+TF-ThA-3, **11**
Benayad, A.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-4, 4
Bera, K.: PS+MS-TuA-12, 3; PS+MS-TuA-3, **1**; PS+MS-TuA-8, 2
Bijkerk, F.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-8, 14
Biolsi, P.: PS2+MS-WeA-3, 6; PS2+MS-WeA-7, 6
Boyce, B.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-6, 5

— C —

Cary, J.: PS+MS-TuA-9, 2
Chandrasekaran, A.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-8, 14
Charvier, R.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-4, 4
Chen, J.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-5, 4
Choi, S.: MS-ThP-2, 12
Chopra, M.: MS+AP+AS+TF-ThA-5, 11
Christudasjustus, J.: MS-ThP-1, 12
Colburn, T.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-5, 4
Counihan, M.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-4, 13
Counsell, J.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-11, **14**
Custer, J.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-6, 5

— D —

Dauskardt, R.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-5, 4
De Carvalho, A.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-1, 13
DelRio, F.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-6, 5
Diebold, A.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-10, **5**
Dingreville, R.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-6, 5
Draney, J.: PS2+MS-WeA-4, **6**

— E —

Ege, T.: MS-ThP-3, 12
Eyres, A.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-13, 5

— F —

F. Trindade, G.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-13, **5**
Finney, L.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-10, 14
Fischer, P.: MS-FrM-8, **15**
Fisher, G.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-1, 13
Fowler, E.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-6, 5

— G —

Galtayries, A.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-1, 13
Ganta, S.: PS+MS-TuA-10, 2; PS+MS-TuA-3, 1; PS+MS-TuA-8, **2**
Gaude, C.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-1, 13
Gauthier, N.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-4, 4; AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-1, 13
Gilmore, I.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-13, 5; AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-3, 13
Gilquin, B.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-1, 13
Golding, M.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-5, 4
Graves, D.: PS2+MS-WeA-1, **6**; PS2+MS-WeA-4, 6
Greeneltch, N.: MS-ThP-2, 12
Guyot, C.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-1, 13

— H —

Hanley, L.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-4, 13; AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-6, **14**
Hara, K.: PS+MS-TuA-2, **1**
Harilal, A.: MS-ThP-1, 12
Helfrecht, B.: MS-ThP-1, 12
Hirchenhahn, P.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-1, 13
Hisamatsu, T.: PS2+MS-WeA-3, 6; PS2+MS-WeA-7, 6
Honda, M.: PS1+MS-ThM-1, 8
Hwang, G.: PS2+MS-WeA-10, 7

— I —

Ievlev, A.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-6, 14
Igosawa, R.: PS1+MS-ThM-1, 8
Ikeda, N.: MS-ThP-3, 12
Ishibashi, R.: MS-ThP-3, 12
Iwata, M.: PS2+MS-WeA-7, 6

— J —

Jain, M.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-6, 5
Jayaram, S.: MS-ThP-2, 12
Jenkins, T.: PS+MS-TuA-9, 2
Jernigan, G.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-1, **4**
Jouneau, P.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-1, 13

— K —

Kadomoto, Y.: MS-ThP-3, 12
Kaganovich, I.: PS+MS-TuA-12, 3; PS2+MS-WeA-12, **7**
Kalaswad, M.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-6, 5
Kanarik, K.: MS+AP+AS+TF-ThA-1, **11**
Kaspar, T.: MS-ThP-1, **12**
Kawamata, R.: MS-ThP-3, 12
Kenig, F.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-6, 14
Khrabrov, A.: PS+MS-TuA-12, 3
Khrabry, A.: PS2+MS-WeA-12, 7
Kihara, Y.: PS2+MS-WeA-3, 6; PS2+MS-WeA-7, 6
Kothari, R.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-6, 5
Krüger, F.: PS2+MS-WeA-9, **6**
Kruger, S.: PS+MS-TuA-9, 2
Kushner, M.: PS+MS-TuA-11, 2; PS2+MS-WeA-9, 6

— L —

Lanham, E.: PS+MS-TuA-9, 2
Lavan, D.: CPS+MS-ThM-1, 8
Leddy, J.: PS+MS-TuA-9, 2
Lee, H.: MS-ThP-2, **12**; PS+MS-TuA-11, 2
Lee, J.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-4, 13
Lemishko, K.: PS+MS-TuA-1, 1
Lewis, J.: CPS+MS-ThM-1, **8**
Linford, M.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-5, **13**
Litch, E.: PS+MS-TuA-11, **2**
Lorenz, M.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-6, 14
Lundstrom, M.: CPS+MS-ThM-10, 8

— M —

Maben, G.: MS-FrM-3, **15**
Mack, P.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-12, **5**
Main, D.: PS+MS-TuA-9, **2**
Maindron, T.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-1, 13

Author Index

Major, G.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-5, 13
Marchesini, S.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-3, 13
Marković, D.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-3, 4
Martinez, E.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-4, 4
Medina de Oliveira, L.: MS+AP+AS+TF-ThA-5, 11
Metz, A.: PS2+MS-WeA-9, 6
Misra, S.: MS-FrM-5, **15**
Mitani, K.: MS-ThP-3, 12
Mohr, S.: PS+MS-TuA-1, **1**
Moki, H.: PS1+MS-ThM-1, 8
Morisaki, R.: PS1+MS-ThM-3, **9**
— N —
Nakamura, Y.: MS-ThP-3, 12
Nakayama, T.: PS1+MS-ThM-4, 9
Nam, S.: PS+MS-TuA-11, 2; PS1+MS-ThM-5, 9
Naranjo, S.: MS+AP+AS+TF-ThA-5, **11**
Nishizuka, T.: PS1+MS-ThM-1, **8**
Numata, T.: MS-ThP-3, **12**
Nunney, T.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-3, **4**
— O —
Ogi, Y.: MS-ThP-3, 12
Ohmori, T.: PS1+MS-ThM-3, 9; PS1+MS-ThM-4, 9
Orui, T.: PS2+MS-WeA-3, 6
Owens, A.: PS+MS-TuA-1, 1
— P —
Panagiotopoulos, A.: PS2+MS-WeA-4, 6
Park, M.: PS2+MS-WeA-9, 6
Pasterski, M.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-6, 14
Pawlowski, S.: CPS+MS-ThM-5, **8**; MS-FrM-10, **15**
Peyres, S.: PS+MS-TuA-7, 2; PS2+MS-WeA-11, **7**
Pinder, J.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-5, 13
Pope, J.: MS-ThP-1, 12
— R —
Radetić, M.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-3, 4
Raghunathan, V.: CPS+MS-ThM-10, **8**
Ratel, D.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-1, 13
Rauf, S.: PS+MS-TuA-10, **2**; PS+MS-TuA-12, 3; PS+MS-TuA-3, 1; PS+MS-TuA-8, 2
Renault, O.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-4, **4**; AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-1, 13
Risner-Jamtgaard, J.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-5, **4**
Rodriguez, M.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-6, 5
— S —
Sakka, Y.: MS-ThP-3, 12
Sako, K.: PS1+MS-ThM-1, 8
Sankaran, R.: PS+MS-TuA-7, 2; PS2+MS-WeA-11, 7
Sassi, M.: MS-ThP-1, 12
Sato, K.: MS-ThP-3, 12
Seydoux, C.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-1, 13
Shankar, S.: MS-FrM-1, **15**
Shengnan, Y.: MS-ThP-3, 12
Shi, X.: PS+MS-TuA-10, 2
Shin, H.: PS1+MS-ThM-6, **9**
Sobczak, C.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-6, 5
Soomary, L.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-11, 14
Spencer, B.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-11, 14
Spool, A.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-10, **14**
Spurgeon, S.: MS-ThP-1, 12
Sturm, M.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-8, **14**
Suda, R.: PS2+MS-WeA-3, 6
Sydorenko, D.: PS+MS-TuA-12, 3
— T —
Takano, N.: PS1+MS-ThM-4, **9**
Tanaka, K.: PS2+MS-WeA-7, 6
Tennyson, J.: PS+MS-TuA-1, 1
Tepavcevic, S.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-4, 13
Theodosiou, A.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-11, 14
Tsai, Y.: PS2+MS-WeA-3, **6**; PS2+MS-WeA-7, 6
Tseng, H.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-3, 4
— U —
Uner, N.: PS+MS-TuA-7, 2
Üner, N.: PS2+MS-WeA-11, 7
— V —
Vailionis, A.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-5, 4
Valpreda, A.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-8, 14
Van de Kruijs, R.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-8, 14
Vardaman, J.: CPS+MS-ThM-12, **8**
Vella, J.: PS2+MS-WeA-4, 6
Verma, A.: PS+MS-TuA-12, **3**; PS+MS-TuA-3, 1; PS+MS-TuA-8, 2
Vorng, J.: AS+2D+CA+EL+EM+MS+NS+SE+SS+TF-WeM-13, 5
— W —
Wang, L.: MS-ThP-1, 12
Wang, T.: PS+MS-TuA-10, 2; PS2+MS-WeA-10, **7**
Wickramasinghe, R.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-6, 14
Wu, W.: PS+MS-TuA-1, 1
— Y —
Yakshin, A.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-8, 14
Yamashita, Y.: PS+MS-TuA-2, 1
Yao, X.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-3, 13
Yokoi, M.: PS2+MS-WeA-7, 6
Yokoyama, T.: PS1+MS-ThM-1, 8; PS2+MS-WeA-3, 6
Yoo, S.: PS1+MS-ThM-5, 9
— Z —
Zagorac, T.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-4, **13**
Zahra, K.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-11, 14
Zameshin, A.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-8, 14
Zhang, D.: PS2+MS-WeA-3, 6; PS2+MS-WeA-7, **6**; PS2+MS-WeA-9, 6
Zhang, Y.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-4, 13
Zhao, Y.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-3, 13
Zhou, Y.: AS+2D+CA+EM+MS+NS+SE+SS+TF-FrM-3, **13**