Plasma Science and Technology
Room Ballroom A - Session PS-ThP

Plasma Science and Technology Poster Session

PS-ThP-1 CO_2 as an Alternative Oxidant to N_2O in Plasma–Enhanced CVD Oxide Deposition, ***Lipeng Qian,*** Micron technology, Singapore

Silane–based oxide and oxynitride films are widely deposited using plasma–enhanced chemical vapor deposition (PECVD) with silane (SiH_4) as the silicon precursor and nitrous oxide (N_2O) as the oxidant. Due to the high global warming potential and limited abatement efficiency of N_2O, alternative oxidants are being evaluated. In this study, a PECVD process is developed in which carbon dioxide (CO_2) replaces N_2O as the oxidation gas.

A schematic comparison of the conventional N_2O–based process and the CO_2–based process is shown in Figure 1. The primary technical challenges associated with this transition arise from the intrinsically lower reactivity of CO_2 relative to N_2O, which results in reduced oxidation efficiency during plasma activation. The higher bond energy of CO_2 limits its dissociation and oxide–forming capability with SiH_4, necessitating extensive process tuning to achieve acceptable film formation.

Significant differences in film composition are observed between the two processes, leading to challenges in matching key optical properties, including refractive index (n) and extinction coefficient (k), as shown in Figure 2. In addition, the CO_2–based process exhibits a shifted and narrower process window, with substantially degraded defect performance relative to the N_2O baseline. Defect sensitivity is strongly process–region dependent and requires targeted optimization to achieve manufacturable performance.

Integration impacts are also observed, as the CO_2–based films demonstrate different wet and dry etch behaviors, requiring adjustments to downstream photo and etch processes to maintain compatibility. Despite these challenges, successful implementation of an N_2O–free PECVD process is achieved through systematic optimization and process innovation. Representative film performance is summarized in Table I, showing reduced surface roughness, slower wet etch rate, and reduced dry etch rate compared to the N_2O reference process.

This work demonstrates the technical feasibility of CO_2–based PECVD oxide deposition for semiconductor manufacturing, providing a viable pathway toward N_2O–free deposition processes while maintaining film property control and integration compatibility.

PS-ThP-2 Effect of Electrode Configuration on Plasma Discharge Characteristics and PVDF Film Properties Using Atmospheric Pressure Plasma Jets, ***Eun Young Jung,*** The Institute of Electronic Technolog, Kyungpook National University, Republic of Korea*; Heung-Sik Tae,* School of Electronic and Electrical Engineering, Kyungpook National University, Republic of Korea*; Choon-Sang Park,* Department of Electrical Engineering, Milligan University

The development trends of piezoelectric nanogenerators (PENGs) will be flexible light weight and wearable self-poweredelectronics for an industrial application. For this reason, polyvinylidene fluoride (PVDF) for piezoelectric polymer materials seem to be attractive candidates for flexible PENGs owing to mechanical flexibility and good properties of the piezoelectric and ferroelectricity [1,2]. Recently, these PVDF-basedpolymers are used to produce films using the various plasma techniques such as low-pressure and atmospheric pressure plasma (APP). In particular,the APP process is the appropriate method to deposit the polymer film on the point of view a simple and low cost process. ThisAPP process are effective method for polymer deposition under ambient air due to easy, simple process, and room temperature[3]. There are few research on the piezoelectric polymers using the APP process [1,4].However, there are some problems such as low deposition rate, loss of monomer precursor, and small deposition area of the APP processes. Thus, to resolve these problems, the structural improvement of plasma reactor is essential for enhancing the efficiency of deposition rate and deposition area.Accordingly,this study investigates the plasma discharge characteristics and structural properties of PVDF thin film deposited by using APP reactor in terms of two different electrode configurations (metal-mesh and planar-type). The characteristics of PVDF thin films investigated using field-emission scanning electron microscope (FE-SEM), Fourier transforms-infrared spectroscopy (FT-IR), X-ray diffraction (XRD), and LCR meter. Through new APP plasma reactor electrode configurations, the thickness of PVDF thin film was increased by using a planar-type electrode compared to that of a metal-mesh type electrode at room temperature using a mixed polymer solution composing of PVDF nano powder and dimethylformamide solution. FE-SEM results show that PVDF nanoparticles are clearly observed and uniformly coated. In the FT-IR spectra, two types of chemical bonds (α and β phases) were observed in the deposited PVDF thin film. Based on these experimental results, we may expect that a new APP plasma reactor will be a great attractive method in order to synthesis the PVDF thin film under atmospheric pressure.The APP with new APP plasma reactor, FE-SEM, FT-IR, XRD, LCR meter, and related mechanism of PVDF thin film are studied and will be discussed in detail.

PS-ThP-3 Time Stability of Hafnium Nitride Thin Films Deposited by Plasma-Enhanced Atomic Layer Deposition, ***Sandra Schujman,*** NY Creates*; Natalya Tokranova, Christophe Valleé,* University at Albany*; Vidya Kaushik,* NY Creates

Transition metal nitrides are sought for semiconductor device applications due to their low electrical resistivity and because they can be excellent diffusion barriers for copper and oxygen. Such films prepared by Atomic Layer Deposition (ALD) have the additional advantage of spatial conformability to structured surfaces and tight thickness control.

In particular, for the ALD deposition of hafnium nitride there have been a number of studies demonstrating tunable electrical properties by controlling the process chemistry (varying the precursor and co-reactant), using thermal ALD versus Plasma-Enhanced ALD, using different plasma compositions, and by varying the deposition parameters (substrate temperature, plasma pressure, plasma composition, etc.). Even though very low electrical resistivity values have been reported, it has also been observed that over time, the resistivity of the layers tends to increase.

In this work, we concentrated on the analysis of electrical resistivity stability as a function of time for HfN thin films deposited on Si or SiO_2 substrates. Various ionic compositions of the plasma, different external RF bias of the substrate, and ALD cycle parameters, were used in order to obtain low electrical resistivity. The layers were characterized by X-ray Photoelectron Spectroscopy, Grazing Incidence X-ray Diffractometry, X-ray Reflectrometry, and Atomic Force Microscopy, and four-point probe measurements were done to determine resistivity.

The samples were kept under regular atmospheric conditions and remeasured over time to understand composition and crystallinity variations and their effect on layer resistivity.

PS-ThP-4 Study on Cryogenic SiO_2 Etching Mechanisms in High Aspect Ratio Contacts Using CF_3I-Based Plasmas with C_4F_6 and WF_6 Passivation, ***Junyeob Lee,*** *Mingyu Kim,* Daejeon University, Republic of Korea*; Hyunjun Kim,* Daejeon university, Republic of Korea*; Woongsun Lim, Changhwan Kim, Sanghee Gwak, Sungin Kim,* Korea Advanced Nano Fab Center, Republic of Korea*; Jeongwoon Bae, Kyongnam Kim,* Daejeon University, Republic of Korea

As 3D NAND flash memory integration increases, securing High Aspect Ratio Contact (HARC) etching technology capable of penetrating multi-layer dielectric stacks of hundreds of layers has become essential. Conventional fluorocarbon (C_xF_y) processes are prone to defects such as etch-stop and bowing as aspect ratios increase. Recently, cryogenic etching has gained significant attention as a solution due to its ability to form precise sidewall passivation layers. In this study, a cryogenic SiO_2 etching process was investigated using a Capacitively Coupled Plasma (CCP) system with a base gas chemistry of CF_3I and $H_2/Ar/O_2$, while incorporating C_4F_6 and WF_6 as passivation gases to elucidate the cryogenic etching mechanism. An Amorphous Carbon Layer (ACL) was used as a hard mask, and the substrate temperature was varied from 20℃ to –90℃ to investigate the effects of temperature on passivation and etching mechanisms. In the gas chemistry, the H_2/O_2 flow rate ratio was selected as a key variable to analyze the effect of hydrogen radical concentration on ACL mask protection and sidewall stability. Furthermore, the etching process was performed under various conditions, including the individual and simultaneous injection of C_4F_6 and WF_6, to systematically investigate the effects of CFx polymers and tungsten-containing compounds on cryogenic etching.

Changes in the etch profile were evaluated through cross-sectional SEM analysis. Additionally, XPS analysis was conducted to examine the content and chemical bonding states of Iodine (I), Carbon (C), and Tungsten (W) within the formed passivation layers. Through these analyses, this study aims to verify and propose the correlation between the multi-layer passivation mechanism and etch profile formation.

PS-ThP-5 Impact of Secondary Electrons on Scaling Wafer Bias to High Power, ***James Prager***, *Josh Perry, Paul Melnik, Timothy Ziemba,* Eagle Harbor Technologies, Inc. (dba EHT Semi)*; Max Kellermann-Stunt, Mark J. Kushner,* University of Michigan

The semiconductor market demands high-aspect-ratio (HAR) features that can be produced at high etching rates. This requires a high ion current to the wafer surface to increase the etch rate. Simultaneously, the aspect ratio of these features is increasing towards 100:1. To achieve high aspect ratios, the ion angular distribution must be well controlled to reduce the sidewall damage to the feature. To accomplish this, tool manufacturers are requesting tailored waveforms wafer bias power systems that can operate at higher voltage. As the wafer bias voltage increases, the secondary electron effects also increase.In this work, we investigate the effect of secondary electrons on the power scaling of a tailored waveform wafer bias power system as the voltage increases. This experimental work was conducted with a capacitively coupled plasma, whose top-side electrode is driven by a 60 MHz radio frequency generator. The bottom-side electrode is driven by a high-voltage tailored waveform generator (Perseus) operating at 400 kHz. Plasma measurements made with a retarding field energy analyzer will be presented along with power system measurement. The experimental results will be compared with modeling results from the Hybrid Plasma Equipment Model. This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Fusion Energy Science under Award Number(s) DE-SC0024861.

PS-ThP-6 An RF Generator Without a Matching Network for Capacitively Coupled Plasma and Bias Applications, ***Timothy Ziemba***, *Josh Perry,* Eagle Harbor Technologies, Inc. (dba EHT Semi)*; Paul Melnik, Chris Bowman, Connor Liston, Stephanie Geeson, James Prager,* Eagle Harbor Technologies Inc. (dba EHT Semi)

Capacitively coupled plasma (CCP) sources are used throughout the semiconductor and thin film industries. CCPs are driven by a radio frequency (RF) generator with a fixed output impedance that must be impedance matched to the plasma. However, matching networks increase the cost, complexity, thermal management requirements, and response times of CCPs, which all scale with power of the RF generator. EHT Semi has developed a new RF generator that eliminates the need for a matching network while driving a capacitive load. This RF generator is being tested on a CCP for plasma generation and bias applications across a range of experimental parameters (power, neutral pressure, and gases). EHT will present the output and electrode waveforms of this new type of RF generator as well as plasma measurements.

PS-ThP-7 Modeling Atomic Wall-Catalyzed Recombination Kinetics and Weakly Bound Surface Species, ***Jonathan Tran***, *David Graves,* Princeton University

Radical surface recombination kinetics are important in plasma reactors, but mechanisms are still poorly understood. Improving the models for these processes is the main goal of this work. This requires a better understanding of weakly-bound species, but how to handle them in surface kinetics models remains an open question. Understanding the dynamics of non-chemisorbed species will also provide valuable insight into other important problems in plasma-surface reactions, for example, cryogenic etching.

In this work, we use molecular dynamics (MD) simulations to identify fundamental mechanisms of weakly-bound chlorine on chlorinated silicon surfaces. The reactive empirical bond-order (REBO) potential form is used. Insights from these simulations can be leveraged to develop reduced-order models (ROMs). The model parameters are then fit to MD results and combined with nudged elastic band (NEB) REBO calculations. Finally, the ROM results are compared to experimentally observed radical surface recombination kinetics. We identify plausible surface recombination mechanisms, propose models for how we may treat weakly-bound species in plasma surface systems, and suggest future experiments and computational studies that are necessary to clarify the role of weakly-bound species in these systems.

PS-ThP-8 Low Thermal Budget Dopant Activation via Spike Plasma Enhanced Annealing, ***Zhihao Ma***, University of Texas at Dallas*; Mahsa Shekarnoush, Yuanning Chen, Malcolm Bevan, Harvey Stiegler,* MicroSol Technologies Inc.*; Lawrence Overzet,* University of Texas at Dallas

The formation of highly activated ultra-shallow junctions remains a critical challenge for advanced semiconductor device scaling, where dopant activation must be achieved while suppressing thermal diffusion and preserving structural integrity. Conventional annealing approaches, including furnace annealing and rapid thermal annealing (RTA), typically require temperatures above 800 ℃, resulting in undesirable dopant redistribution, junction broadening, and degradation of thermally sensitive device structures and materials.

Plasma Enhanced Annealing (PEA) has demonstrated strong potential as low thermal budget annealing approach through localized and controllable energy delivery from plasma ions, which significantly reduce substrate temperatures (300-500 ℃) by adjusting ion kinetic energy, flux, dose, and species. In this work, a spike plasma enhanced annealing (spike-PEA, millisecond scale) process was investigated for phosphorus-, arsenic- and B-implanted silicon wafers and the post-process properties were systematically characterized by four-point probe measurement, Raman spectroscopy, and secondary ion mass spectrometry (SIMS). Compared with conventional thermal annealing (TA) and RTA under identical temperatures, spike-PEA demonstrated substantially enhanced dopant activation, producing significant reductions in sheet resistance across all implantation profiles, together with improved crystallinity. The effective activation fractions as high as 105% relative to 800 ℃ RTA reference were achieved at only 400 ℃ with minimal junction broadening.

The results demonstrate that spike-PEA enables efficient dopant activation through selective near-surface ion energy deposition while minimizing dopant diffusion. These findings establish spike-PEA as a promising low-temperature annealing strategy for next-generation semiconductor manufacturing and advanced ultra-shallow junction integration.

PS-ThP-9 Effect of Thin Dielectric Layer Boundary Conditions on Electronegative Plasmas in Capacitively Coupled Plasma Reactors, ***Jeong-hoon Son***, KWT Solution Inc., Republic of Korea

As semiconductor processes become increasingly precise, simulation-based plasma analysis is attracting growing interest due to the inherent limitations of direct experimental measurement. However, a persistent challenge remains the discrepancy between simulation predictions and experimental results, often arising from insufficient representation of actual experimental conditions in plasma simulations.

One commonly overlooked condition is the dielectric coating applied to electrode surfaces in real equipment. In industrial plasma reactors, electrodes are routinely coated with materials such as Al_2O_3 or Y_2O_3 to prevent plasma-induced corrosion and contamination. These coatings modify the effective sheath voltage through surface charge accumulation, yet most simulation studies continue to model electrodes as bare conductors.

In this study, we analyze the effect of dielectric electrode coatings in a capacitively coupled plasma (CCP) reactor using the thin dielectric layer boundary condition provided by a commercial fluid simulation software. Particular attention is given to electronegative plasmas, in which the presence of negative ions (O^-) fundamentally alters the discharge structure. Simulations are performed at 250 mTorr and 13.56 MHz with an applied voltage of 100 V, while the Ar/O_2 gas composition is systematically varied to examine how the influence of the coating changes as the negative ion fraction increases relative to the electropositive baseline.

As the O_2 fraction increases, the negative ion density rises and the overall plasma density distribution undergoes a significant transition. At low O_2 fractions, the radial electron density profiles with and without coating show little difference. However, as the O_2 fraction increases, the coating boundary condition produces a pronounced change in the radial electron density distribution. These results indicate that in highly electronegative plasmas, accurate representation of electrode surface coatings is not a minor modeling detail, but a physically significant factor that substantially affects simulation fidelity.

Given the growing use of electronegative gases in plasma processing, proper treatment of surface coating effects will be an essential element for obtaining reliable simulation results.

PS-ThP-10 Implementation of a Surface Coverage Module in K-PLASMA(0D) and Validation Against a C4F8 Inductively Coupled Plasma Global Model, ***Yongil Lee***, KWT Solution, Republic of Korea*; Deuk-Chul Kwon,* Korea Institute of Fusion Energy, Republic of Korea*; Dong-Hun Yu,* KWT Solution, Republic of Korea

In spatially-averaged plasma simulations, surface reactions are often represented as interactions with a single, time-invariant wall state characterized by fixed sticking or recombination probabilities. This simplification cannot capture the evolving surface state during etching or deposition processes, where adsorbed species progressively modify the wall composition and thereby change the probability of each subsequent wall reaction. To address this limitation, the wall must be resolved into

multiple surface states whose fractional coverages are coupled with gas-phase kinetics. We report the implementation of a surface coverage module in K-PLASMA(0D), a 0D global plasma simulator currently under development and commercialization, and its validation against a reference C_4F_8 global model and inductively coupled plasma (ICP) measurements.

The new module couples gas-phase kinetics with a heterogeneous wall reaction set that distinguishes bare, fluorinated, and ion-activated sites of the fluorocarbon (fc) film. F atoms adsorb on the fc film and form a fractional surface coverage θ_F that blocks fc-radical deposition on bare sites and enables $CF_x + F(s) \rightarrow CF_{x+1}$ recombination (x = 0–3), including CF_4 formation. Ion-induced site activation and ion-enhanced etching releasing CF_2 are also incorporated. The reaction probabilities and the C_4F_8 gas-phase reaction set, comprising electron impact, ion recombination, autodetachment, neutral recombination, and associative detachment, follow the reference formulation.

Simulations were performed for a C_4F_8 ICP reactor at 200 sccm C_4F_8 / 10 sccm Ar, pressure of 9.7 mTorr, T_gas = 305 K, and source power of 500–2,000 W. Using the reference global model as a benchmark, K-PLASMA(0D) successfully reproduces the F, CF_2, and CF density trends and the surface coverage evolution, with θ_F reaching ~0.19 at 2,000 W[1]. The agreement confirms that the surface coverage module, including F-blocking and surface recombination pathways, has been correctly implemented in K-PLASMA(0D).

In this work, only the fractional coverages of three surface states — bare site, F-adsorbed site (θ_F), and ion-activated site — were considered during polymer formation. As a next step, the surface reaction rates obtained here can be aggregated to derive the macroscopic polymer deposition rate, enabling the present module to be applied to PECVD process modeling. The framework will also be extended to other surface chemistries, in particular SiO_2 etching.

1 G. Kokkoris *et al*., J. Phys. D: Appl. Phys. 41, 195211 (2008)

PS-ThP-11 Positive Pulse Biasing for Directional Electron Extraction in Capacitively Coupled Plasma*, Kyoung-Jae Chung,* ***Junbeom Park****, Daehyun Kim,* Seoul National University, Republic of Korea

In high aspect ratio (HAR) etching, ions are directionally accelerated through the sheath, whereas electrons cross the sheath mainly by thermal motion. This difference causes positive charge accumulation near the bottom of narrow structures, which can distort the etching profile. Our previous work demonstrated through simulations that positive pulse biasing can extract directional electrons from capacitively coupled plasma (CCP) and transport them into HAR structures. In particular, the simulations showed that a shorter pulse rise time produces more directional electrons by enhancing the transient electron extraction process. However, experimental validation is needed to determine whether this pulse-induced electron extraction can be realized in an actual CCP system. In this work, positive pulse biasing is applied to a CCP system to observe directional electron extraction and to experimentally examine the correlation between pulse parameters and electron extraction behavior suggested by the simulations. The influence of plasma density on the extraction process is also analyzed, and the results provide guidance for the development of pulse bias waveforms that mitigate charge accumulation and improve profile control in advanced plasma processing.

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PS-ThP-12 Plasma Impedance Monitoring of SiNx Etching Processes with Different Grounding Conditions*, hyun kyu Choi, Heeyeop Chae,* Sungkyunkwan University (SKKU), Republic of Korea

Plasma impedance variations at the RF grounding interface were monitored to assess the system status in this work. The experiment was conducted in a 300 mm ICP chamber using Ar/CF_4 plasma at 30 mTorr. A 13.56 MHz source power and a 2 MHz bias power were applied to the inductive coil on a quartz window and to the electrostatic chuck, respectively. The grounding conditions were controlled by mechanically tightening the inner liner bolts using a torque driver. The bolt torque was adjusted from 1 to 15 torque levels, and the 15 torque condition was served as the reference for comparison. A VI probe captured the electrical variations of the plasma response to grounding status. The electrical resistance at 15 torque exhibited a standard deviation of 29.04% compared to the 1 torque condition, and the reactance showed a standard deviation of 21.06% under the same conditions. Theoretical analysis using the CMY models (Int. J. Heat Mass Transfer, 1969) and Greenwood models (Proc. R. Soc. Lond. A, 1966) was performed to predict the interface mechanics. These models show that increased torque expands the effective contact area and enhances the surface conductance.In addition, SiN etching experiments were performed under different torque conditions. The etch rate at 1 torque was 2.495% lower than the value at 15 torque. These results indicate that the bolt contact status alters the grounding stability of the chamber.

PS-ThP-13 Particle-in-Cell Simulation of the Synchronous Effect in Pulsed Dual-Frequency Capacitively Coupled Plasma*, Jun Hee Mun,* KWTSolution, Republic of Korea

This study investigates the synchronization effects between high-frequency (HF) and pulsed low-frequency (LF) voltages in a dual-frequency capacitively coupled plasma (DF-CCP) system, which is widely utilized in semiconductor processing and advanced plasma-based manufacturing. Dual-frequency operation enables independent control of plasma density and ion energy; however, the introduction of pulsed LF biasing introduces temporal complexity whose underlying mechanisms remain poorly understood. In particular, pulsed LF excitation has been proposed as an effective approach to tailor ion energy distributions for high-aspect-ratio etching, but the role of its phase relationship with HF excitation in determining plasma characteristics remains largely unexplored.

In this work, a two-dimensional particle-in-cell (PIC) simulation is performed to systematically analyze these synchronization effects. A 20 MHz sinusoidal HF voltage and a 400 kHz pulsed LF voltage are applied, with the LF duty cycle fixed at 50%. Two representative control strategies are considered: (1) varying the HF duty cycle from 50% to 100% to modulate the overall temporal overlap, and (2) maintaining a 50% HF duty cycle while introducing a controlled phase delay in the HF waveform within the LF pulse-on period. These approaches allow precise adjustment of the overlap ratio between HF excitation and the LF active phase, providing a consistent framework to isolate synchronization-driven phenomena.

The simulation results demonstrate that the degree of temporal overlap strongly affects the spatiotemporal evolution of plasma potential, sheath dynamics, and electron heating mechanisms. In particular, changes in overlap modify the phase-resolved electron power absorption and lead to distinct electron density distributions and potential structures. As a result, ion acceleration dynamics within the sheath are also altered, indicating that ion energy control is closely linked to waveform synchronization rather than solely to individual frequency components.

These findings highlight that synchronization between HF and pulsed LF voltages is a key operational parameter in DF-CCP operation. The results provide practical insight into waveform engineering strategies for precise control of plasma characteristics, provide pathways toward optimizing etching performance in next-generation semiconductor fabrication processes.

PS-ThP-14 3D PIC-MCC Simulation for Plasma Nonuniformity in off-centered DC Magnetron Sputtering*, Yu Gyeong Suh, Hae June Lee,* Pusan National University, Republic of Korea

DC magnetron sputtering (DCMS) remains a cornerstone of thin film deposition and is widely used for metal gap fill in semiconductor packaging processes. However, plasma nonuniformity arising from the closed E×B drift loop continues to limit target utilization and film uniformity. Nowadays, intentionally asymmetric magnet topologies offer an underexplored route to control plasma spatial structure and ion bombardment. This study utilizes a self-consistent 3D particle-in-cell with Monte Carlo collision (PIC-MCC) simulation to investigate a DCMS discharge driven by a non-circular off-centered magnet. Using an in-house-developed code, an Ar discharge at 5 mTorr with a planar Cu target has been investigated using a fully kinetic analysis under a realistic, azimuthally nonuniform magnetic field. We quantify how this non-circular topology reshapes the spatial distribution of electron and ion densities through the competition among E×B, ∇B, and diamagnetic drifts. Preliminary calculations confirm that the off-centered topology breaks the azimuthal symmetry of the trap region, inducing localized weakening of the curvature-driven gradients along the racetrack. These features drive azimuthally varying ion flux and measurable shifts in the IEAD high-energy tail. This work establishes a 3D kinetic framework for magnet design optimization, providing a physics-based basis for tuning film growth conditions in large-area, high-performance coatings.

PS-ThP-15 Two-Dimensional Particle-in-Cell Simulation of Electronegative Plasmas in Chlorine Capacitively Coupled RF Discharges*, Dongmin Lee, Hae June Lee,* Pusan National University, Republic of Korea

Capacitively coupled plasmas used in the etching process of advanced semiconductor fabrication include negative ions and reactive radicals. Unlike electropositive discharges, electronegative plasmas contain a large

amount of negative ions, depleted electron densities, and enhanced bulk electric fields. It has been reported that these features modify sheath dynamics, electron power absorption, radical generation, and charged-particle motion. However, ion dynamics near the bulk–sheath boundary remain insufficiently understood under RF-driven etching conditions. In this work, frequency-dependent charged-particle dynamics in chlorine capacitively coupled plasmas are investigated using a two-dimensional particle-in-cell Monte Carlo collision (PIC MCC) simulation. Chlorine is selected as a representative electronegative etching gas, where dissociative attachment and negative-ion confinement can lead to an ion-dominated bulk plasma. By changing the RF driving frequency, different degrees of electronegativity are obtained, enabling comparison of charged-particle motion. At lower driving frequencies, the discharge becomes highly electronegative. The bulk electron density is low because negative ions are confined in the plasma bulk, while positive ions are accelerated toward the electrodes through the RF sheath. This separation produces a localized space-charge density peak near the bulk–sheath boundary, thereby enhancing the local electric field. The resulting field perturbs the relative motion of positive and negative ions, generating a low-frequency ion-scale response that extends from the sheath edge into the plasma bulk. This ion motion is coupled to the electron power absorption, suggesting that the bulk–sheath boundary acts as an active region for energy exchange and charged-particle dynamics. As the driving frequency increases, the plasma becomes less electronegative, the localized space-charge peak weakens, and the ion-scale response near the sheath edge decreases. These results suggest that the localized electric field structure is governed by the balance among negative-ion confinement, ion inertia, and RF sheath motion. The results provide a kinetic interpretation of ion dynamics in electronegative chlorine CCPs and clarify how RF frequency can influence electronegativity and sheath-edge field formation. Understanding these mechanisms is important for high-aspect-ratio and profile-sensitive etching because the spatial distribution of ions, radicals, and energy deposition affects etch rate, selectivity, sidewall control, and process uniformity.

PS-ThP-16 Electrified C–N Coupling in Ethylene Glycol Using Nitrogen DC Plasma-Liquid Interactions, ***José Balena***, *Mikhail Vasilev,* University of Notre Dame*; R. Mohan Sankaran,* University of Illinois Urbana-Champaign*; Caue Ribeiro,* Embrapa Instrumentation, Brazil*; David Go,* University of Notre Dame

Direct-current (DC) plasma–liquid interactions have emerged as a promising strategy for electrified chemical transformations under mild conditions. Plasma systems are particularly attractive for nitrogen activation because cleavage of the N≡N bond is thermodynamically and kinetically challenging using conventional methods. Industrial nitrogen fixation still relies mainly on the energy-intensive Haber–Bosch process, and electrochemical and photocatalytic N-transformation often need highly active substrates, while suffering from low efficiencies and limited N_2 solubility in liquids. In this work, a nitrogen plasma generated directly over liquid ethylene glycol (EG) was employed to promote nitrogen incorporation into organic molecules. EG was selected as both solvent and carbon source due to its low cost, low volatility, biodegradability, and availability from biomass valorization, plastic recycling, and CO_2-derived routes. Reaction products were investigated by GC–MS using direct injection and silylation derivatization methods. The major nitrogen-containing product identified after derivatization was (2-hydroxyethyl) carbamate providing evidence for incorporation of nitrogen in the organic substrate. Total nitrogen analysis indicated a nitrogen fixation rate of approximately 370 μmol h^{-1} in EG. This rate was not significantly affected by either the reaction volume or reaction time, provided that the electrolyte concentration and gas flow rate were maintained constant at 0.17 M $NaClO_4$ and 50 sccm N_2, respectively. Control experiments using hydroxylamine (NH_2OH) and ammonium hydroxide (NH_4OH) under argon plasma yielded the same compound, suggesting NH_2• radicals as key intermediates. Comprehensive analysis of the samples revealed a broader distribution of nitrogen-containing compounds. GC-MS detected traces of amino acids after derivatization, while direct injection identified cyclic nitrogen compounds such as piperidinoacetonitrile. Ongoing studies are being performed to further elucidate reaction pathways and reactive intermediates. These findings demonstrate the potential of plasma-liquid systems for sustainable nitrogen fixation and electrified synthesis of value-added nitrogen-containing chemicals from abundant feedstocks.

PS-ThP-17 Effect of H_2O Additive Gas on Sio_2 and Si_3N_4 Films in C_4F_8 Self-Bias Plasma, *Heeyeop Chae,* ***Haegeon Jung***, Sungkyunkwan University (SKKU), Republic of Korea

Fluorocarbon (FC) layer formation affects surface reactions and profile evolution in low-temperature plasma processing. This study investigates the effect of H_2O addition on FC layer formation on SiO_2 and Si_3N_4 films in C_4F_8 self-bias plasma. An inductively coupled plasma chamber generates C_4F_8/Ar plasma without external RF bias. Substrate temperature ranges from 20 °C to −60 °C. FC layer thickness is evaluated by ellipsometry and VSEM, and surface bonding structure is analyzed by XPS. Low substrate temperature increases FC layer thickness on both SiO_2 and Si_3N_4 films due to enhanced polymer accumulation and reduced desorption. SiO_2 surfaces exhibit thicker FC layer formation than Si_3N_4 under identical plasma conditions. XPS analysis confirms increased C–C and C–CF bonding fractions at low temperature, indicating stabilization of carbon-rich FC structures. H_2O addition further increases FC layer thickness in C_4F_8 plasma, particularly on Si_3N_4 surfaces, while O_2 addition suppresses carbon accumulation through oxidation-related reactions. These results indicate that H_2O addition modifies FC surface chemistry and temperature-dependent polymer stabilization behavior in C_4F_8 self-bias plasma. The study suggests material-dependent FC layer formation behavior in low-temperature fluorocarbon plasma processing.

PS-ThP-18 Aqueous Electron Yields for Non-thermal Plasma in Contact with a Water Cathode: Effects of Plasma Gas Composition, ***Mikhail Vasilev***, *David Bartels, David Go,* University of Notre Dame

Nonthermal plasmas in contact with liquids present a unique plasma–surface interaction challenge: the liquid surface acts as the cathode and must supply electrons to sustain the discharge and maintain charge balance. Despite this fundamental role, the mechanism of secondary electron emission from the liquid cathode remains poorly understood. Proposed mechanisms include photoionization, field emission, and ion-induced emission. One candidate process involves plasma-generated reactive species producing free conduction-band electrons in the liquid, with a small fraction escaping into the plasma while the majority thermalize and solvate to form aqueous (solvated) electrons[1]. The probability of electron emission from the liquid surface is extremely low, with only ~10^{-6} of conduction-band electrons estimated to escape into the plasma, making direct measurement difficult and mechanistic assignment challenging.

Water has an ionization energy of ~10 eV, yet the average kinetic energy of ions impinging on the liquid surface through the plasma sheath is estimated at only ~1 eV for argon systems. This energy gap argues against simple ion-induced ionization of water and suggests that alternative interfacial processes, such as proton-transfer pathways or metastable-driven reactions, contribute to electron generation. Prior work using argon plasma–liquid systems and chloroacetate reduction as a liquid-phase electron dose probe has estimated apparent electron yields on the order of unity. In this work, we quantify how different gas ions affect electron generation at the plasma–liquid interface using in situ chloride ion measurements produced by the reaction of aqueous electrons with chloroacetate. By varying plasma gas composition (H_2, He, Ar, Kr, Xe), this work investigates how ion mass, metastable energy, and chemical reactivity govern electron generation pathways at plasma–liquid interfaces, with implications for secondary electron emission modeling in plasma–liquid systems.

PS-ThP-19 Plasma Monitoring for Chamber Conditioning Steady-State Detection Using He-Normalized SiF Saturation in Inductively Coupled Plasma, ***Suyoung Ko***, *Heeyeop Chae,* Sungkyunkwan University (SKKU), Republic of Korea

The He-normalized SiF Saturation Index (SSI) was developed as a real-time chamber wall condition indicator. SSI monitored chamber wall stabilization during post-preventive maintenance (PM) chamber conditioning in inductively coupled plasma etchers with Y_2O_3-coated walls. Optical emission spectroscopy (OES) monitored full-spectrum emission in situ during plasma cleaning cycles on a 300 mm ICP etcher with Y_2O_3-coated walls across three PM events. Partial least squares variable importance in projection (PLS-VIP) analysis identified SiF (440.1 nm) as the wall-state-sensitive emission line. SSI was defined as the cycle-averaged I(SiF)/I(He) ratio, using He (706.5 nm) as the normalization reference. Blanket oxide etch rate was measured to validate SSI. He normalization reduced the CV of SiF emission from 17.6% to 3.8%. This reduction isolated the wall-state-dependent SiF signal from plasma source fluctuations, enabling SSI to track chamber wall condition independently. SSI converged to a ±2% stability band at the 7th conditioning wafer across three PM events, indicating faster chamber stabilization than the conventional fixed 24-wafer chamber conditioning protocol. SSI correlated with blanket oxide etch rate at $r = 0.965$ ($p < 0.001$), confirming SSI as a process-relevant chamber wall condition indicator. SSI identified the chamber stabilization point in real time, replacing the conventional fixed-count chamber conditioning

protocol. This work demonstrated that SSI is a practical in-situ wall condition indicator applicable to production ICP etchers.

PS-ThP-20 Time-Resolved Langmuir Probe Measurements of Pulsed RF Argon Plasmas, ***Collin Clay***, *Kylan Herring, David Ruzic,* University of Illinois

Pulsed RF plasmas are a powerful tool for etching and other plasma processes. The pulsing of the RF plasma provides a number of variables to control the plasma treatment process such as pulse repetition rate and duty cycle. While computational models have provided insight into the fundamental physics of pulsed RF plasmas, there is still a significant lack of experimental validation of these models. In this we work, we present progress on measuring the time-resolved evolution of the electron energy distribution function (EEDF) in a pulsed RF argon plasma. The energy distribution of electrons in pulsed plasmas is unique because the electrons are constantly adjusting to the on- and off-states of the RF plasma. Models have predicted that the electrons at the beginning of a pulse have a low density with a high electron temperature, and over time, the density increases while the temperature decreases. This work uses time-resolved Langmuir probe measurements with a sub-nanosecond temporal resolution to experimentally determine the evolution of the EEDF in a pulsed plasma system. We present initial work measuring the IV traces of argon plasmas under pulsed RF ignition conditions at pressures from 30 – 100 mTorr. We explore the impact of pressure and pulse parameters on the EEDF. We will also discuss how the time-evolution of the EEDF can impact the application of pulsed RF plasmas for industrial processes.

PS-ThP-21 Optical Emission Diagnostics of Electron Temperature and Density in Argon ICP Assisted by Collisional-Radiative Modeling, ***JiHyun Park***, Samsung Electronics Co., Republic of Korea

Optical emission spectroscopy (OES) is a useful non-invasive diagnostic technique for low-temperature plasmas, but measured emission intensities are governed by coupled collisional and radiative processes. Consequently, direct estimation of electron temperature (Te) and electron density (Ne) from emission intensities alone requires a collisional-radiative (CR) model. In this study, Te and Ne in argon inductively coupled plasma (Ar ICP) were estimated using OES combined with a CR model.

Ar I emission spectra were measured in a cylindrical quartz-tube ICP reactor operated at 13.56 MHz. RF power was varied from 30 to 50 W and gas pressure from 200 to 400 mTorr, giving nine operating conditions. For each condition, five repeated OES measurements were performed to evaluate repeatability. The spectra were corrected by wavelength-dependent and spectral-response calibration, and Ar I emission lines selected from the 696–978 nm range were used for analysis.

The CR model included the Ar ground state, four 4s metastable/resonance states, and ten 4p excited states. Electron-impact excitation and de-excitation, ionization, collisional quenching, diffusion loss to the wall, radiative transitions, and radiation trapping were considered. The diagnostic procedure was performed sequentially. First, Te was determined by minimizing the root-mean-square error between measured and CR-model-predicted line-intensity ratios. The 763.51 nm line was used as the reference, and five lines at 750.39, 772.38, 801.48, 826.45, and 912.30 nm were used to construct the ratio vector. Next, Ne was estimated by scaling the CR model intensity to match the experimental intensity at the determined Te. The Ar I 811.53 nm intensity at 300 mTorr and 40 W was used as the normalization reference.

The estimated Te ranged from 1.604 to 1.814 eV, while Ne ranged from 2.84 × 10^{12} to 8.07 × 10^{12} cm^{-3}. Te decreased with increasing pressure and showed a slight decrease with increasing RF power, whereas Ne increased with both pressure and RF power. The relative standard deviation was 0.14–0.96% for Te and 2.14–7.27% for Ne, indicating good repeatability. Comparison with a 0D global model showed that Te agreed within ±5%, while Ne showed larger quantitative deviations but reproduced the trends with operating conditions.

These results demonstrate that the sequential CR-OES approach provides physically consistent, non-invasive estimates of Te and Ne in Ar ICP, and is applicable to conditions where probe insertion is impractical or may perturb the plasma.

PS-ThP-22 ReaxFF Development by Latent Space Exploration for Plasma Etch Modeling, ***George Arsnow***, *David Graves,* Princeton University

Extension of molecular dynamics (MD) etching simulations to industrially relevant plasma etching systems including silicon (Si), fluorine (F), chlorine (Cl), sulfur (S), and oxygen (O) necessitates the development of new interatomic potentials with suitable accuracy, transferability, and computational cost. These criteria can be balanced by the ReaxFF potential, which has sufficient flexibility and physicality to handle the highly non-equilibrium atomic environments replete in plasma etching simulations. Growing use of data-intensive machine learning interatomic potentials has spurred the creation of systematic and user-agnostic protocols for training set generation [1]; such active learning algorithms can also be harnessed to produce data sets for ReaxFF parameterization.

We demonstrate an active learning algorithm to sample an atomic configuration set's latent space, which comprises the first few principal components of the set's atomic descriptors. Latent space exploration enables efficient interpolation between user-defined boundary configurations, allowing the user to institute limits on the resulting potential's transferability [2]. We use this latent space exploration–based active learning algorithm to parameterize ReaxFF potentials for elemental subsets of the Si/F/Cl/S/O system. Parameterization is performed with version 2 of the JAX-ReaxFF global optimization software [3]. Validation entails comparison of ReaxFF-predicted energies and forces on a test data set to those calculated by density functional theory (DFT) and comparison of experimental etch rates and etch product selectivities to those manifested in MD etching simulations.

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PS-ThP-23 Enhanced Catalytic Performance in Plasma-Assisted Dry Methane Reforming via Ferroelectric Perovskites, ***Shanza Baig***, University of Oklahoma

Non-Thermal Plasma technology holds significant potential for activating CH_4 and CO_2 molecules, enabling their conversion into H_2 and other valuable chemicals under mild conditions. However, conventional thermal catalysts which are primarily heat responsive often lack compatibility with non-thermal plasma environment, where reaction mechanisms and dominant species differ considerably. Moreover, as CO_2 has a higher bond dissociation energy than CH_4, there is a necessity to design a catalyst that can enhance CO_2 dissociation kinetics to improve overall DRM efficiency. This study integrates ferroelectric materials into plasma catalytic systems enhancing energy transfer to reactant molecules, increasing electron density in discharge regions, and elevating average electron energy – key factors critical to increasing the conversion rates of both CH_4 and CO_2 in plasma-assisted DRM. Perovskite oxides synthesized via the Pechini method were categorized into three classes: titanates ($BaTiO_3$, $CaTiO_3$, $SrTiO_3$), zirconates ($BaZrO_3$, $CaZrO_3$, $SrZrO_3$), and niobates ($KNbO_3$, $NaNbO_3$, $KNaNbO_3$), each exhibiting distinct curie temperatures and ferroelectric properties. Niobate-based ferroelectric catalysts, particularly $KNbO_3$ and $NaNbO_3$, demonstrated the highest CH_4 conversions of 71.7% and 71.9%, CO_2 conversions of 62.4% and 60.5%, H_2 yield of 33.6% and 33.3%, and CO yield of 33.5% and 32.9%, respectively. $KNbO_3$ resides in its orthorhombic ferroelectric phase at 800 V and 5 kHz enabling sustained polarization and enhanced surface charge effects. To further enhance performance and stability of traditional supports, ferroelectric $KNbO_3$ was incorporated into Al_2O_3 and SiO_2 using a co-precipitation method. This integration further improved CH_4 and CO_2 conversions to 75.5% and 54.6% with Al_2O_3, and 81.7% and 64.6% with SiO_2. To study the effect of loading active metal, nickel was introduced via incipient wetness impregnation. However, its addition to ferroelectric catalysts such as $KNbO_3$-Al_2O_3 and $KNbO_3$-SiO_2 led to reduced CH_4 and CO_2 conversions and a shift in product selectivity towards CO, highlighting the pivotal role of spontaneous polarization in directing plasma induced reaction pathways. In contrast, paraelectric perovskites exhibited poor catalytic performance due to their inability to maintain polarization under plasma conditions either due to inherently non-ferroelectric structures or low curie temperatures. Overall, among all tested catalysts, ferroelectric $KNbO_3$ based catalysts demonstrated superior control over electric field interactions at the catalyst surface, promoting localized micro-discharges, enhancing CO_2 dissociation, and reducing energy losses.

PS-ThP-24 Plasma-Enhanced CO_2 Dissociation for Chemical Synthesis: Modeling and Experimental Verification, ***Andrew Herschberg***, *Nathan Bartlett, Jameson Crouse, Emily Greene, Jaime Robertson, David Ruzic,* University of Illinois at Urbana-Champaign

The conversion of carbon dioxide into carbon monoxide using non-equilibrium plasmas is of growing interest for carbon utilization, syngas generation, and plasma-assisted chemical synthesis. Radio frequency inductively coupled plasmas are attractive for this application due to stable operation, high plasma density, and efficient power coupling. In this work, a combined modeling and experimental study of CO2 dissociation in an intermediate-pressure RF ICP reactor is presented. A physics-based numerical model is being developed to simulate electromagnetic power deposition, plasma transport, and reaction pathways relevant to CO2 conversion. Parametric studies examine the influence of applied power, pressure, residence time, and feed composition on predicted dissociation behavior and energy utilization.

Experimental validation is being conducted using an RF ICP reactor operated under comparable conditions. A combination of mass spectrometry and remote OES actinometry methods are used to measure species concentrations in the reactor effluent. Comparison of experimental measurements with model predictions will be used to refine the simulation framework and identify operating conditions for efficient plasma-assisted CO2 conversion. This work supports the development of scalable plasma reactors for chemical synthesis and carbon utilization applications.

PS-ThP-25 Effect of Steric Hindrance and Precursor Reactivity on Aluminum Oxide Area-Selective Atomic Layer Deposition, ***Sharmistha Bhattacharjee***, *Nicholas C. Strandwitz,* Lehigh University

Area-selective atomic layer deposition (AS-ALD) offers a promising route for bottom-up fabrication of advanced nanoscale devices by enabling deposition only on targeted surfaces while suppressing growth on undesired regions. However, maintaining selectivity during deposition remains a major challenge, particularly for highly reactive precursors that can penetrate blocking layers and nucleate on non-growth regions. In aluminum oxide AS-ALD, precursor properties such as molecular size, ligand structure, and reactivity play a critical role in determining interactions with self-assembled monolayer (SAM) blocking layers, surface defects, and precursor diffusion pathways. Small and highly reactive precursors such as trimethylaluminum (TMA) can readily infiltrate non-growth surfaces, leading to faster selectivity loss. Therefore, tailoring precursor chemistry is important for improving blocking efficiency and sustaining selective growth.

In this study, the influence of precursor molecular size and reactivity on Al_2O_3 AS-ALD was investigated using TMA, aluminum tri-sec-butoxide, and tri-i-butylaluminum with H_2O as the co-reactant. Dodecanethiol SAM deposited on copper substrates was employed as a blocking layer, and deposition behavior was examined over a temperature range of 100–160 °C. Film thickness and density were analyzed using spectroscopic ellipsometry and X-ray reflectivity, while blocking performance was evaluated through X-ray photoelectron spectroscopy measurements of Al atomic concentration. Compared with TMA, the larger precursors demonstrated substantially improved resistance to precursor infiltration and enhanced selectivity. Aluminum tri-sec-butoxide maintained 100% selectivity at low temperature, while tri-i-butylaluminum preserved selectivity above 90% after 100 ALD cycles of Al_2O_3. These findings highlight the importance of precursor design in AS-ALD and demonstrate that combining bulkier, lower-reactivity precursors with well-ordered SAM blocking layers provides an effective pathway for improving long-term selectivity performance.

PS-ThP-26 Evolution of Ion Energy Distribution Functions in High Aspect Ratio Features, ***David Kanfer***, North Carolina State University*; Krista Morris, Rex Anderson,* Micross*; Tanjina Akter,* North Carolina State University*; Chenyao Huang, Mark Kushner,* University of Michigan, Ann Arbor*; Steven Shannon,* North Carolina State University

The growing demand for High Aspect Ratio (HAR) features in micro and nanoscale devices motivates an understanding of the evolution of the ion energy distribution function (IEDF) as ions travel down a HAR feature. As the aspect ratio (AR) increases, features undergo bowing, tapering, and notching, deviating from the expected HAR geometry; these are largely attributed to AR dependent changes in the IEDF. By combining a retarding field energy analyzer (RFEA) with capillary plates (CPs) of varying ARs, the evolution of IEDFs as a function of depth into an HAR feature can be directly measured. This method has been previously demonstrated in inductively coupled plasmas. Industry often uses capacitively coupled plasmas (CCPs) to perform the HAR etch. A CP design has been developed with feature diameters from 20 um to 90 um, and thicknesses from 200 um to 450 um, yielding features with ARs ranging from 2-22. The CPs are fabricated on backlapped silicon wafers. Copper is sputtered onto the back of the wafer as an etch-stop. A mask with an array of holes is exposed onto the wafer. The subsequent etch step varies, with larger diameter holes requiring a longer etch. The copper is then removed. Finally, dry thermal oxidation is used on some samples, forming a thin layer of SiO2 throughout the feature. An argon / oxygen / nitrogen dual-frequency CCP is used to test the fabricated CPs. The CCP is powered by a 60 MHz high frequency to sustain sufficient density, and a 13.56 MHz low frequency for sheath control.

By varying the AR of the CP used, power ratio of the dual-frequencies, pressure, and gas, the IEDF through the HAR can be measured with the RFEA. Additionally, by comparing the SiO2 HAR features to the non-oxidized features, the effect of insulating sidewalls is determined. These results provide insight into how IEDFs evolve within HAR features in dual-frequency CCPs.

This work is supported by Department of Energy grant DE-SC0024545.

PS-ThP-27 Complex Transient Processes Observed During in-Plasma Nanocalorimetry, ***Carles Corbella***, National Institute of Standards and Technology (NIST)/ University of Maryland, College Park*; Caroline Adam, Holger Kersten,* Kiel University, Germany*; Feng Yi, Andrei Kolmakov,* National Institute of Standards and Technology (NIST)

Nanocalorimetry is a promising diagnostics tool to measure and analyze the energy fluxes from plasma discharges used for surface processing, such as film deposition, etching, and cleaning. Nanocalorimeter sensors consisting of silicon dies usually include a Pt thin film microstrip acting as a resistor, deposited on an ultrathin, free-standing SiN_x membrane. Recently, a two-timescale temperature profile upon plasma ignition has been observed: (1) initial fast sensor heating associated with the heat dissipation to the ultrathin SiN_x supporting membrane, followed by (2) slow heating of the silicon die in contact with the aluminum envelope. The reduced thermal mass of the membrane-supported Pt sensor enables a rapid temperature response down to the millisecond resolution. Nanocalorimeters' characteristic short response times, together with their sensitivity and selectivity, make such devices ideal for transient thermal processes' analysis during plasma processing. From plasma ignition to pulsed discharges, plasma-surface physics and chemistry are governed by transition processes where plasma parameters rapidly evolve. The energy fluxes during such non-stationary conditions can now be studied with nanocalorimetry sensors, whose thermal responses are validated using an array of independent plasma monitor techniques, such as electrical and optical probes. The time evolution of sensor temperature is correlated with RF discharge parameters (gas pressure, power, and residence time) and electrode materials (aluminum, copper, gold) to provide a unified description of the substrates' heating mechanisms. The roles played by the gas phase conditions and chemistry on the electrodes are discussed, as well as the separate contributions of gas, ions, electrons, and photons heat fluxes in the global heating of the nanocalorimeter.

PS-ThP-28 Three-Dimensional Kinetic Plasma Simulations for Predictive Modeling of ExB Plasma Processing Devices, ***Andrew Tasman Powis***, Princeton Plasma Physics Laboratory*; Jian Chen,* Sun Yat-sen University, China*; Igor Kaganovich,* Princeton Plasma Physics Laboratory

Three-dimensional kinetic plasma simulations are emerging as an essential tool for first-principles modeling of low-temperature plasmas used in materials processing. In many plasma sources, including partially magnetized discharges relevant to etching, deposition, surface functionalization, and ion-beam-assisted processing, device behavior is controlled by kinetic electron transport, self-consistent sheath formation, wave–particle interactions, and plasma–surface coupling. These effects are often reduced or parameterized in lower-dimensional models, but they can depend sensitively on the third spatial dimension, boundary conditions, and nonlinear instability dynamics. This talk highlights recent progress in high-performance 3D3V particle-in-cell simulations as a pathway toward predictive modeling of processing-relevant plasmas.

Two recent studies illustrate this point. In Hall-thruster-like crossed-field plasmas, 3D kinetic simulations show that radial boundary conditions can qualitatively alter density, temperature, electric-field structure, instability spectra, and cross-field electron transport [1]. In beam-generated partially magnetized plasmas, 3D PIC-MCC simulations reveal a transition from quasineutral lower-hybrid spiral arms to non-neutral diocotron-driven helical rotation, demonstrating that structures appearing spoke-like in

projection may be intrinsically three-dimensional [2]. Together, these studies show that fully 3D kinetic simulations are not merely computational refinements, but necessary tools for connecting fundamental plasma instabilities to transport, wall interaction, and ultimately process control in advanced plasma technologies.

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PS-ThP-29 PICLas: An Open-Source Kinetic Simulation Framework for Plasma Science and Technology, ***Paul Nizenkov***, *Asim Mirza, Stephen Copplestone, Julian Beyer,* boltzplatz - numerical plasma dynamics GmbH, Germany*; Marcel Pfeiffer,* Institute of Space Systems, University of Stuttgart, Germany

PICLas (https://github.com/piclas-framework/piclas, GPLv3) is an open-source, massively parallel kinetic simulation framework combining Particle-in-Cell (PIC), Monte Carlo Collisions (MCC), and Direct Simulation Monte Carlo (DSMC), Bhatnagar-Gross-Krook (BGK), and Fokker-Planck methods for rarefied gas and plasma dynamics. This poster demonstrates its versatility through three applications spanning plasma processing, beam physics, and radiation transport. First, reactive magnetron sputtering of titanium in an O_2/Ar atmosphere is simulated within an industrial coating chamber using DSMC. A reactive wall model (Tonneau et al. 2018, J. Phys. D 51, 195202) couples target surface coverage to incoming particle fluxes and sputter emission. Gas distribution, sputtered particle transport with configurable emission distributions, and deposition rates are analyzed under varying reactive gas inflow conditions, capturing the characteristic racetrack erosion pattern and the poisoning transition from metallic to compound target mode. A parametric racetrack model is introduced, enabling the simulation of rotating substrates by rotating the racetrack position accordingly, providing a computationally efficient approach for industrial coating geometries. Second, electron beam propagation in a PVD system is modelled with coupled PIC-MCC. Ionization of the background neutral gas, self-fields of charged species, and a superimposed magnetic field are included. The ionization-induced self-focusing of the beam is shown, and simulated beam widths are validated against burn-in diameter measurements within the beam generator. A species-specific time step bridges the different timescales of electrons and ions. Third, PICLas is bidirectionally coupled with a line-by-line radiation solver and a photon Monte Carlo transport method. The capabilities are demonstrated for an atmospheric entry plasma, a strongly non-equilibrium environment that shares key physical characteristics with high-power industrial plasma processes, enabling prediction of radiative transport properties and spectroscopic signatures in flow regimes inaccessible to continuum-based CFD. Together, these cases establish PICLas as a versatile kinetic simulation platform freely available to the plasma science and technology community.

PS-ThP-30 Time-Resolved Ion Energy Distribution Function Study of High Power Impulse Magnetron Sputtering with Positive Cathode Reversal using a Linear Magnetron for Cu and Ti, ***Collin Jeckell***, *Tag Choi, Matt Egly, Ricky Pickering, David Ruzic, Dren Qerimi,* University of Illinois at Urbana Champaign

High-Power Impulse Magnetron Sputtering (HiPIMS) is a physical vapor deposition (PVD) technique that, through short voltage pulses with high peak currents, is able to achieve higher density plasmas compared to traditional DC magnetron sputtering. This higher density leads to a significant increase in the ionization fraction, which leads to higher quality films by improving their adhesion, density, and roughness. A recent area of study has been how changing the polarity of the cathode affects the energies of the deposited ions. This work seeks to show how changing different parameters of the HiPIMS pulse with the positive cathodic reversal, and the position of the magnetron affects the time-resolved Ion Energy Distribution Function (IEDF). This data was collected using a Plasma Sampling Mass spectrometer (PSM) from Hiden Analytical Inc. For each experiment the IV trace was also collected allowing us to verify that the plasma is stable. By understanding how changing these parameters leads to changes in the IEDFS we can better design HiPIMS plasmas to obtain the desired film. For this both copper (Cu) and titanium (Ti) targets were studied changing 9 parameters to see how each of them affects the IEDF. Parameters such as main pulse length between 10 – 30 µs, peak current between 100 – 300 A, positive pulse length between 50 – 150 µs, with/without positive voltage of the cathode, angles of the PSM to target, etc. are varied. By testing all of these parameters we are able to see how they affect the behavior of the plasma. Secondarily by comparing the results between the two materials, we are able to observe if changing material properties has a large impact on the trends observed.

PS-ThP-31 Neural-Network Based Reconstruction for Limited-Line-of-Sight CT-OES Plasma Diagnostics, ***Jiseong Nam***, *Kyoung-Jae Chung, Sang Yoel Park,* Seoul National University, Republic of Korea

Computed-tomographic optical emission spectroscopy (CT-OES) is a non-invasive diagnostic technique for reconstructing the spatial distribution of local optical emissivity in plasmas from line-integrated emission signals. In practical plasma devices, however, the number and angular coverage of available lines of sight (LOS) are often limited by chamber geometry, viewport configuration, and optical-access constraints. Under such limited conditions, the reconstruction problem becomes highly ill-posed, and different non-axisymmetric emissivity distributions may produce similar projection signals. In this work, we propose a neural-network-based reconstruction model for CT-OES under limited-LOS conditions constrained by chamber structure and optical access. The model is designed to infer local emissivity distributions from sparse LOS signals while capturing non-axisymmetric and localized plasma emission structures. By learning physically plausible emissivity patterns from training data, the proposed model acts as an implicitly regularized inverse solver, enabling robust reconstruction from sparse LOS measurements with reduced dependence on manually tuned regularization parameters.

PS-ThP-32 Stannane Decomposition and Sticking Coefficients under Different Sample Conditions, ***Emily Greene***, *Jameson Crouse, Nathan Barlett, Eric Mushrush,* University of Illinois at Urbana-Champaign*; Niels Braaksma,* ASML*; David Ruzic,* University of Illinois at Urbana-Champaign

This is a placeholder abstract. I will update with the real abstract as soon as I receive sponsor approval. Thank you again for your patience and understanding!

PS-ThP-33 Plasma Torch Method for Silicon Carbide (SiC) Dopant Implantation, ***Victor Veltmeyer***, *Renato Beraldo, José Pissolato Filho, José Diniz, Marcos Puydinger dos Santos,* State University of Campinas, Brazil

Silicon Carbide (SiC) has been shown to be a capable semiconductor for power electronics applications, as it supports high forward currents whilst blocking high reverse voltages, while switching up to MHz frequencies. Those properties are enabled by an exceptionally durable crystalline lattice that allows it to withstand remarkably high temperatures, enabling it to sustain transient power regimes that would otherwise destroy standard silicon semiconductors.

This exceptional crystal lattice, however, also represents the main challenge in fabricating large SiC power electronics, as it is extremely difficult to dope (or alter in general) with standard fabrication techniques, whether it be thermal diffusion or ionic implantation. The former requires heating the substrate to temperatures as high as 2100 K for several minutes, while the latter requires 100-300 keV per µm of implant depth for aluminum, the standard p-dopant for SiC, while also requiring substrate heating up to temperatures between 500-1100 K during the entire process.

Our study aims to evaluate a novel method of dopant implantation, adapting an innovative plasma torch device to perform both thermal diffusion and ionic implantation concurrently by using accelerated ions within a thermal plasma discharge. The main source of ion energy are Lorentz electromagnetic forces, which also increase the plasma plume's temperature via magnetic self-confinement, a process which has been experimentally shown to reach temperatures to extremes of 4000 K in the original device.

This plasma torch, which originally operated at atmospheric pressure, was fitted with a fused-quartz high-vacuum (10-5 Torr) chamber to reduce the beam's temperature while also boosting ion energies by increasing their mean free path. A silicon carbide wafer coated on one side with aluminum will be placed perpendicularly to the plasma flight path, where nitrogen ions (n-type SiC dopant) will bombard the wafer, simultaneously heating it while pushing accelerated dopants into the crystal lattice, a novel hybrid method which combines the best aspects of the two existing alternatives, conceivably doping the uncoated side to an n-type semiconductor while the coated to a p-type, creating a standard diode junction, which will be tested to determine the quality of this new processing method.

PS-ThP-34 Machine-Learning-Assisted Investigation of CF_3–X (X=H, F, I) Plasma Kinetics In Semiconductor Manufacturing for Etch Effectiveness and Environmental Sustainability, ***Chi-Yun Lin***, *Jane Chang,* UCLA

Hydrofluorocarbons (HFCs) gases are commonly used in semiconductor manufacturing to etch silicon dioxide, an essential insulator in integrated circuits, either from chamber wall deposits or patterned features. CHF_3 plasma is utilized for its high etch rate (ER), comparable to CF_4, and favorable anisotropic etching characteristics, though its high global

warming potential (GWP100) of 12400 and long atmospheric lifetime (LT) of 222 have prompted its phasedown by the EPA. CF_3I has a lower atmospheric lifetime (<0.005) and GWP100 (<1), which are 4-5 orders of magnitude smaller than those of HFCs, making it a promising alternative gas.

This work investigates CF_3X-based plasmas (where X = H, I) in etching SiO_2 with a focus on machine learning to extract meaningful kinetic parameters for modeling. $CHF_3/O_2/Ar$ plasma was first used to evaluate the reduce and abate strategies. O_2 serves a dual role: process-gas additive to reduce the usage of CHF3 for improving SiO2 etching and abatement reactant for reducing high-GWP fluorocarbon emissions. The experimental and modeled SiO2 etch rate increased with measured emission of SiF_4 (kg-CO_2e) and the modeled ratio of fluorine flux to oxygen flux (Γ_F/Γ_O), reaching above 150 nm/min under selected conditions. The corresponding downstream composition was converted to $MMTCO_2e$ for CHF_3, CF_4, and C_2F_6. After introducing O2 to downstream abatement, the modeled $MMTCO_2e$ decreased by approximately a few orders of magnitude relative to the untreated emission.

$CF_3I/O_2/Ar$ was evaluated as a lower-GWP alternative. A differentiable surface-kinetic model was developed to infer the unknown iodine adsorption and abstraction probabilities, using experimental SiO2 etch rates as the ground truth, while modeled ion fluxes and etch rates served as known inputs. Descriptor information from CF_3X (X = F, Cl, Br, and I), including C–X bond dissociation energy, Si–X bond strength, and electronegativity, was used to define physically reasonable bounds for the unknown iodine-related surface kinetics. Automatic differentiation through the ODE solver reduced the average absolute percent error from 23% for the initial assumption to 12.5% after applying new surface kinetic by AI/ML inference. As the SiO_2 etch rate increases from 50–80 nm/min to above 100–130 nm/min, the corresponding measured and modeled emission for CF_3I and CF_4 decreases by an order of magnitude in $MMTCO_2e$.

Overall, selected $CF_3I/O_2/Ar$ operating conditions showed the SiO_2 etch rate increased by approximately 70% while the estimated emission impact reduce by an order of magnitude, indicating that higher etch performance can be achieved with lower greenhouse-gas-equivalent emissions.

PS-ThP-35 Advanced Waveform-Modulated Pulsed Biasing for Seam Suppression in Dielectric Gap-Fill Processes, ***Yejin Shin***, *Tae Cho,* WONIK IPS Co., Ltd., Republic of Korea*; Junghoon Kim,* WONIK IPS Co., Ltd.*; Hyun-Jong Woo, TaeIn Kim, YongBaek Jeon, TaeJoon Kim, Gyu-Tai Kim, Dongll Choi, Eun Sun Jung,* WONIK IPS Co., Ltd., Republic of Korea

Advanced waveform-modulated pulsed biasing techniques were investigated for surface treatment and profile modification during dielectric gap-fill processes. The primary advantage of this approach is the precise control of ion energy, enabling optimization of the biasing effect while minimizing plasma-induced surface damage. Dielectric films are commonly deposited using CVD or ALD processes; however, as next-generation memory devices adopt increasingly high-aspect-ratio structures, the risk of seam formation in gap-filled features has increased significantly.

Various approaches have been explored to suppress seam formation, including post-deposition densification treatments and profile-shaping processes designed to prevent premature pinch-off near the trench opening. These plasma-assisted surface modification processes require carefully controlled ion bombardment to regenerate the surface and reshape deposited materials.

To independently control ion energy and ion flux, dual-frequency plasma excitation using low- and high-frequency sources has been widely adopted. However, achieving independent controllability remains highly challenging, particularly in capacitively coupled plasma (CCP) reactors commonly used for dielectric deposition systems. To minimize coupling between the two frequencies, the lower-frequency source is typically selected in the range of several kilohertz to a few megahertz. Although this approach improves the controllability of ion energy and ion flux, the low-frequency bias often produces excessively energetic ion bombardment, resulting in undesirable sputtering or excessive surface treatment.

In this study, a waveform-modulated pulsed biasing technique was developed to maintain sufficiently high ion energy while minimizing perturbation of ion flux. By tailoring pulse-shape parameters, precise control of ion bombardment characteristics was achieved. To implement this technique in a PEALD system developed at Wonik IPS, several chamber components were newly designed, including a ground-layer-embedded high-temperature heater pedestal and a broadband RF notch filter. Initial experimental studies demonstrated effective reshaping behavior of the filled dielectric layer, indicating the strong potential of advanced pulse waveform modulation for future seam-suppression and gap-fill optimization processes.

PS-ThP-36 Wafer Edge Yield Improvement through SOH Mask Tilt Optimization by Edge Insert Ring Height Adjustment, ***Junhyuk Choi,*** Samsung Electronics, Republic of Korea

All values except radius are normalized to arbitrary units (a.u.) for confidentiality.

As DRAM design rules shrink, the impact of wafer edge yield on overall profitability has significantly increased. However, in the Spin-On Hard mask (SOH) etch process, edge yield degradation was observed as the accumulated Radio Frequency (RF) time increased. Specifically, the extreme edge (E1) Bit-Line Bridge Disturb (BBD)—a defect associated with the outermost chips—deteriorated over time (Fig. 1). Notably, standard mass production monitoring metrics, such as Non-Pattern Wafer Etch Rate (NPW ER), top edge Critical Dimension (CD), and Virtual Metrology (VM), did not exhibit meaningful correlations with this yield loss.

To investigate the root cause, non-destructive Slope CD (SCD) metrology was employed to measure the mask left-right tilt at nine different radii (Fig. 2). The analysis confirmed a clear correlation between RF time, SCD values, and E1 BBD (Fig. 3). The identified mechanism is that as RF time accumulates, the edge ring is eroded, which alters the edge plasma sheath characteristics. This modification shifts the ion incident angle distribution, inducing a subtle tilt in the SOH mask profile at the wafer edge. When this non-uniform profile is transferred to the subsequent bit line, it results in E1 BBD defects. The analysis indicated that this degradation was most pronounced before the Actinium (a mechanical ring-lift technology for sheath control) compensation function initiated at RF time 4.

To address the mask tilt and resulting defects caused by plasma sheath distortion, the edge insert ring height was optimized. Reducing the ring height shifts the edge plasma sheath curvature area outward, thereby minimizing the sputtering variance caused by ion incident angles (Fig. 4). Based on a measured etch rate of 1.22 and considerations for measurement and process tolerances, the ring height was reduced from 2.1 to 1.6. Additionally, the Actinium application point was advanced from RF time 4 to 0 to proactively compensate for ring erosion from the start of the process.

The implementation of the 1.6 ring, combined with the adjusted Actinium timing, significantly reduced the correlation between SCD and RF time, demonstrating enhanced mask profile stability against RF time accumulation (Fig. 5). Consequently, the E1 BBD defect rate improved by approximately 3.66 over the RF time 0–4 range (Table 1). This study presents a practical, cost-effective, and data-driven edge ring optimization methodology applicable to high-volume manufacturing lines.

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