Atomic Scale Processing Mini-Symposium
Room Ballroom A - Session AP+EL+PS+TF-ThP

Atomic Scale Processing Mini-Symposium Poster Session

AP+EL+PS+TF-ThP-1 Design of Gas Flow Field for a Slip Flow ALD Processing Chamber, ***Kyung-Hoon Yoo***, Korea Institute of Industrial Technology, Republic of Korea*; Geun-Soo Song,* The KUMYOUNG Inc., Republic of Korea*; Chun-Sik Kim,* TNG Co., Republic of Korea*; Jun-Young Hwang, Sang-Ho Lee, Jeong-Jin Kang, Shin-Ae Song, Kyung-Tae Kang,* Korea Institute of Industrial Technology, Republic of Korea*; Hyeong-Cheol Lee,* Hanyang University, Republic of Korea*; Kun-Hyung Lee,* SAMSUNG DISPLAY, Republic of Korea

As semiconductor feature sizes reach the nanometer scale, ALD processing equipment has become indispensable for atomic-layer control. However, conventional ALD processes face significant challenges regarding economic and environmental feasibility due to the excessive consumption of precursors and energy.[1,2] To address these issues, it is essential to establish sustainable manufacturing technologies through the development of high-efficiency ALD processing chambers. In the present study, we propose a slipflow based ALD chamber designed to optimize the process space and minimize resource waste. The nitrogen flow fields within the chamber were numerically investigated using Computational Fluid Dynamics (CFD) for process gap sizes of 1, 10, and 100 mm at 400 °C. Under an inlet static pressure of 1 Torr and a mass flow rate of 4.233×10^{-5} kg/s, the Knudsen number (Kn) and flow Reynolds number (Re) were evaluated as 0.0137 and 0.822, respectively for the 10 mm gap. These values confirm that the flow resides within the slip flow regime, where rarefaction effects at the surface wall become significant. Accordingly, the steady-state compressible laminar flow field was simulated by solving the continuity, momentum, and energy equations.[3,4]

Acknowledgment

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AP+EL+PS+TF-ThP-2 Nucleation and Evolution of Dislocations and Extended Faults in Complex Perovskite Oxides, ***Rishi Raj***[1], *K. Andre Mkhoyan,* University of Minnesota, USA

The stoichiometric flexibility of a perovskite oxide (ABO_3) results in several unique properties due to the presence of three elements in the crystal structure. This allows it to host a variety of defects across all dimensions. 1D primitive edge dislocations with varying terminations, screw dislocations as well as 2D structural faults like Ruddlesden-Popper, elastic distortions, and BO_3 octahedral tilts are commonly observed and studied. Even though structure and electronic properties of some of these defects have been reported, the nucleation and growth of such defects and dislocations is still unclear. Analytical STEM study of perovskite oxide thin films of $BaSnO_3$ and $SrSnO_3$ show the existence of two kinds of edge dislocations: single ([001]/(100)-type) and dissociated ([001]/(110)-type) edge dislocation each with two half planes missing. Six different types of such dislocations are possible and observed due to the terminations of the perovskite half planes. Similarly, 2D Ruddlesden-Popper faults are also observed to result from missing planes of atoms, suggesting a correlation with 1D dislocations. Apart from such conventional topological defects, complex perovskite oxides also showcase several line defects and dislocations with reconstructed cores. This suggests we can selectively populate the material with defects by altering the terminations of crystal half planes. Strain tuning during growth by swapping substrates or decorating the surface morphology can effectively allow termination control. This would allow certain defect and dislocation structures to be more favorable than others. By establishing this correlation between 1D and 2D faults, this work provides a potential pathway to transition from passive extended defect management to intentional, termination-controlled defect engineering.

AP+EL+PS+TF-ThP-5 Oxidation-Assisted SF_6 Remote Plasma Etching for Surface Roughness Reduction of TiN, ***Min Kyun Sohn***, *Subin Heo, Seong Hyun Lee, Sun Kyu Jung, Jeong Woo Park, Dongwoo Suh,* Electronics and Telecommunications Research Institute, Republic of Korea

Titanium nitride (TiN) is widely used as a conductive diffusion barrier and work-function metal in advanced semiconductor devices. As device dimensions continue to scale down, controlling not only the etch amount but also the post-etch surface morphology becomes increasingly important, because nanoscale roughness can directly affect electrical reliability, interface quality, and subsequent film deposition. In the present study, we investigate the effect of SF_6 remote plasma-based etching on the surface morphology of TiN thin films, with particular emphasis on the role of a pre-oxidation step.

Three TiN surface conditions were compared: as-deposited TiN, TiN exposed to SF_6 radicals only, and oxidized TiN followed by SF_6 radical exposure. The etch per cycle (EPC) increased from 0.16 Å/cycle for the SF_6-only process to 0.38 Å/cycle for the oxidation-assisted SF_6 radical process, indicating that surface oxidation enhanced the fluorine-radical-driven removal of TiN. Atomic force microscopy measurements showed that the as-deposited TiN exhibited an RMS roughness of 1.313 nm, which modestly decreased to 1.117 nm after direct SF_6 radical exposure. In contrast, when the TiN surface was oxidized prior to SF_6 radical exposure, the RMS roughness further decreased to 0.850 nm, corresponding to an approximately 35% reduction compared with the as-deposited TiN surface, demonstrating a clear surface-smoothing behavior.

This difference suggests that the oxidation step plays a critical role in modifying the TiN surface before fluorine-radical exposure. The smoothing behavior is attributed to the formation of a TiO_x or TiO_xN_y surface layer during oxidation, followed by its conversion into volatile TiF_x species during SF_6 radical exposure. The higher EPC and lower RMS roughness obtained after oxidation-assisted SF6 exposure suggest that the modified surface layer can be removed more efficiently and uniformly than the native TiN surface. This oxidation-assisted pathway provides a chemically controlled route for reducing TiN surface roughness without relying on ion-driven physical sputtering.

These results indicate that surface pre-oxidation can be an effective strategy for controlling the morphology of TiN during radical-based etching. The proposed oxidation-assisted SF_6 radical process offers a potential strategy for morphology-controlled TiN etching in nanoscale device integration.

AP+EL+PS+TF-ThP-6 Development of in-Situ Laser Diagnostics Measurements of CH_3 Radical Concentrations for Study of Thin Film Depositions Using Organo-Metallic Precursors, ***Mruthunjaya Uddi***, Advanced Cooling Technologies Inc.*; Prawal Agarwal, Devon Jensen,* ACT*; Anatoli Morozov,* Princeton University*; Arthur Dogariu,* Texas A&M University

Many environmentally friendly non-halogen precursors contain CH3 structure component. Plasma chemical vapor deposition of pure metallic thin films using these precursors is challenging and requires better understanding of the gas phase and surface reaction mechanisms. We present a novel, time and spatially resolved, in-situ femtosecond laser diagnostics method to measure CH3 radicals in a non-equilibrium plasma environment. The CH3 radicals are predissociated to CH2 and H radicals using a 275 nm femtosecond laser pulse, followed by a 205 nm probe beam to measure the H radical concentrations. A single femtosecond laser is used to generate the required 275 nm and 205 nm beams. Measuring and knowing the dissociation cross section of CH3 radical by 275 nm pump beam, allows the quantification of CH3 radical concentrations with spatial and time resolution.

AP+EL+PS+TF-ThP-7 Hybrid Electrospun ZnO Nanofiber and ALD ZnO Electron Transport Layers for Near-Infrared Organic Photodiodes, ***Anna Leonard***, *Neha Chaturvedi, Veena Misra,* North Carolina State University

Organic photodiodes (OPDs) require efficient electron transport layers (ETLs) to achieve charge-selective extraction while minimizing recombination and dark current impacts. In this work, hybrid ZnO ETLs consisting of electrospun ZnO nanofibers and atomic layer deposited (ALD) ZnO were investigated for integration into near-infrared OPDs with a PTB7-Th:IEICO-4F active layer. The inclusion of the electrospun ZnO nanofibers

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increases the interfacial area between the ETL and active layer and provides enhanced electron transport pathways while the ALD ZnO layer provides film continuity and assists in passivating traps to mitigate defect states introduced by the nanofibers.

Three ETL architectures were investigated: ZnO fibers beneath ALD ZnO, ZnO fibers above ALD ZnO, and ALD ZnO control devices. ZnO nanofibers were fabricated through electrospinning of a zinc acetate dihydrate/polyvinylpyrrolidone (PVP) solution followed by calcination to oxidize the fibers and remove excess PVP. Device performance was evaluated through dark current density vs. voltage (J_{Dark}-V) and external quantum efficiency (EQE) measurements. Devices utilizing hybrid nanofiber/ALD ZnO ETLs exhibited reduced initial dark current compared to control devices indicating suppression of leakage pathways and trap-assisted recombination. Enhanced EQE response was observed in devices with fibers deposited above the ALD ZnO layer, suggesting improved interface quality and charge extraction.

These results demonstrate that combining electrospun ZnO nanostructures with ALD ZnO provides a promising method to engineer ETLs for high-performance OPDs and other optoelectronic devices.

AP+EL+PS+TF-ThP-8 Site-Specific and Temperature-Dependent Hydration of Faceted Hematite, ***Asare Dua***, Illinois Institute of Technology*; Luke Pretzie,* Purdue University*; Ashley Bielinski,* Argonne National Laboratory*; Yue Li,* Argonne National Lab*; Valentine Novosad, Cong Liu, Alex Martinson,* Argonne National Laboratory*; Adam Hock,* Illinois Institute of Technology

Alpha hematite (α-Fe_2O_3) is an abundant metal oxide whose surfaces and interfaces control key processes in catalysis, sensing, and photoelectrochemistry. While the more stable α-Fe_2O_3 (001) surface is well studied, less stable facets such as (012) and (104) which are more relevant in the aforementioned applications due to higher surface activity remain least studied. Surface sites of α-Fe_2O_3 (012) and (104), as well as their distinct stability were identified through temperature-dependent hydration by combining in situ infrared reflection absorption spectroscopy (IRAS) with density functional theory (DFT) vibrational analysis. For α-Fe_2O_3 (012), we found sites that promoted the dissociative and molecular adsorption of D_2O. Dissociatively adsorbed D_2O were either terminal or bridging. In both cases the hydroxyls were either isolated or interacting with nearby species. Protons of bridging hydroxyls (μ3a-OD (isolated); μ3b-OD (interacting with nearby hydroxyls)) are bound to triply coordinated surface oxygens while terminal hydroxyls (μ1a-OD (interacting with nearby hydroxyls)) were bound to octahedral surface Fe atoms (Fe_{oct}^{3+}). Similar to dissociatively adsorbed D_2O, molecularly adsorbed D_2O was either isolated (D_2Oa) or interacting with nearby hydroxyls (D_2Ob). α-Fe_2O_3 (104) on the other hand exhibited an isolated doubly coordinated bridging hydroxyl (μ2a-OD) and an interacting bridging species (μ2b-OD) rather than triply coordinated bridging hydroxyls. This preference is backed by our DFT calculations which shows triply coordinated bridging hydroxyls were highly unstable on α-Fe_2O_3 (104). Results from IRAS showed two isolated terminal hydroxyls, μ1a-OD and μ1b-OD, were present on the surface of α-Fe_2O_3 (104). This indicates two types of undercoordinated surface atoms existed with the first being undercoordinated tetrahedral Fe atoms (Fe_{tet}^{3+}) since they're the surface atoms of α-Fe_2O_3 (104), while the second is from the second layer of Fe atoms which have octahedral geometry. The undercoordination of Fe_{oct}^{3+} atoms however suggests oxygen vacancies (V_o) were present and some of these might migrate from surface to the second lattice of α-Fe_2O_3 (104). Our temperature dependent studies support this hypothesis since the population of μ1a-OD, μ1b-OD, and μ2a-OD increased with increasing temperature when under vacuum (0.8 torr). The distinct local environments of the sites on α-Fe_2O_3 (012) and α-Fe_2O_3 (104) and changes in properties with respect to temperature revealed through this work provide a fundamental tool that may be used to engineer the surface of alpha hematite through site- or facet-selective atomic layer deposition.

AP+EL+PS+TF-ThP-9 Impact of TiN Metal Gate Deposition Process on Oxygen-Vacancy-Related Defects and Electrical Characteristics of HfO2-Based Gate Stacks, *Sangho Lee, Seonghwan Shin,* ***Seong Hyun Lee****, Gustavo Panama, Sun Kyu Jung, Minkyun Sohn, Min-A Park, Dongwoo Suh,* Electronics and Telecommunications Research Institute (ETRI), Republic of Korea

Hafnium-oxide-based high-k/metal gate (HKMG) stacks are a cornerstone of advanced CMOS technology. The electrical quality of the high-k dielectric is determined not only by its intrinsic film properties but also by interfacial reactions and defect formation induced during the overlying metal gate deposition. In particular, the TiN capping process, whether by sputtering or plasma-enhanced atomic layer deposition (ALD), can strongly modulate sub-oxide formation and oxygen-vacancy-related defects in the underlying HfO_2. In this study, we investigate how the TiN deposition method and ALD plasma power affect the chemical and electrical characteristics of HfO_2-based MOS capacitors.

TiN electrodes were formed on HfO_2 (4 nm) / chemical oxide SiO_2 (1 nm) / Si stacks by sputtering (7.2 kW) and by plasma-enhanced ALD at 150, 225, and 300 W, using p+ Si substrates for C–V analysis and n++ Si substrates for leakage-current evaluation. X-ray photoelectron spectroscopy revealed that the fraction of sub-stoichiometric HfO_x (Hf_2O_3-like) states increases with ALD plasma power, which is attributed to surface damage from accelerated Ar ions and highly reactive $TiCl_4$-derived radicals, indicating an elevated oxygen vacancy concentration in the HfO_2 film.

These chemical trends were directly reflected in the electrical behavior. Leakage conduction was governed by trap-assisted tunneling (TAT), and model fitting yielded trap energy levels consistent with the oxygen vacancy level of HfO_2. The sputtered sample exhibited the highest leakage current and trap density, while the trap density decreased monotonically with decreasing ALD plasma power. Furthermore, the interface trap density extracted by the conductance method (1 kHz–1 MHz) decreased from ~1.8 × 10^{12} $cm^{-2}eV^{-1}$ for the sputtered sample to ~9.4 × 10^{10} $cm^{-2}eV^{-1}$ for the 150 W ALD TiN sample, a reduction of more than 19 times. This suggests that oxygen vacancy formation is not confined to the HfO_2 layer but also couples to the SiO_2 interlayer through oxygen scavenging reactions, degrading the Si/SiO_2 interface quality.

These results demonstrate that gate-stack engineering must extend beyond the dielectric itself, since the metal capping process directly governs the defect landscape of the underlying insulators. The proposed power-controlled ALD TiN deposition offers a damage-minimized metallization route potentially applicable to aggressively scaled gate-all-around (GAA) HKMG technologies.

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AP+EL+PS+TF-ThP-10 Understanding the Influence of Plasma Surface Interactions using MOS Capacitors, ***Emily Frederick***[1], University of Central Florida*; John Murphy, Glenn Jernigan, David Boris, Scott Walton,* U.S. Naval Research Laboratory

Plasma-surface interactions are fundamental to atomic layer processing, driving the structural and chemical changes that enable the growth of high-quality materials or the removal of functionalized layers. However, the effects of these interactions are not limited to the surface. While the penetration depth of charged and reactive neutral species is minimal, photon penetration can be much greater, and the overall energy deposition can extend well into the material. As films are grown or etched by atomic layer processes, and devices continue to shrink, it becomes increasingly critical to understand and quantify the impact and depth of changes plasma exposure has on the compositional and electronic properties of thin films, and as a result, functionality of the resulting structures and devices.

In this work, we discuss the influence of plasma exposure on Al_2O_3 films grown by thermal atomic layer deposition (ALD) on p-type silicon substrates. This is accomplished by "interrupting" the growth of the oxide layer with a brief exposure to an argon plasma before resuming growth.Through varying both the depth and duration of this plasma interrupt, we systematically probe the impact plasma treatments have on the capacitance-voltage (CV) characteristics of metal-oxide-semiconductor (MOS) capacitors. When the plasma interrupt is near the oxide-semiconductor interface, we see a pronounced shift in the flatband voltage and a corresponding increase in hysteresis, indicating an increase in trapped charges and a greater density of mobile charge or defect states in the oxide. X-ray photoelectron spectroscopy (XPS) analysis was also done to reveal chemical changes induced in the Al_2O_3 by plasma exposure, thus linking these electrical signatures to underlying compositional changes.

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