Tuesday Morning, January 27, 2026

PCSI

Room Ballroom South - Session PCSI-TuM2

Atomic Layer Deposition

Moderator: Jessica Hilton, SPECS-TII, Inc.

11:00am PCSI-TuM2-31 UPGRADED: In vacuo LEIS and XPS Studies on Reaction Mechanisms in ALD and ALE Processes, Mykhailo Chundak, Heta-Elisa Nieminen, Marko Vehkamäki, Matti Putkonen, Mikko Ritala, University of Helsinki. Finland

Atomic layer deposition (ALD) and atomic layer etching (ALE) are becoming increasingly important methods in advanced semiconductor manufacturing. With their rising utilization, there is a growing need for better understanding of chemical reactions and film growth mechanisms in these processes.

To study the films growth in detail under *in vacuo* conditions we utilize the cluster tool setup at the HelsinkiALD laboratory (Fig. 1). The system integrates a flow-type ALD reactor with low-energy ion scattering (LEIS), X-ray photoelectron spectroscopy (XPS) and temperature programmed desorption (TPD) spectroscopy [1]. This unique configuration allows us to analyze surface reaction intermediates formed during the cycle-by-cycle growth/etching of the films, without exposing the samples to the air. In addition, the ALD reactor is equipped with a quartz crystal microbalance (QCM) providing in situ monitoring mass changes and the film growth rates. LEIS and XPS allow us to also examine film closure, substrate-film interactions and area-selective growth.

Here we present the results focused on the growth of high-K oxides. The main emphasis will be on ALD of HfO_2 and ZrO_2 thin films (HZO) using $CpHf(NMe_2)_3$ and $CpZr(NMe_2)_3$ in combination with ozone on TiN substrates. The results of HZO growth, as measured by LEIS after varying number of ALD cycles (Fig. 2) will be demonstrated.

We also study the ALD processes of platinum and ruthenium thin films using trimethyl(methylcyclopentadienyl) platinum(IV) (MeCpPtMe $_3$) and bis(cyclopentadienyl) ruthenium(II) (RuCp $_2$) as precursors together with O $_2$ as the co-reactant. We explore the underlying mechanisms of noble metal ALD processes, revealing the role of adventitious airborne hydrocarbons in directing the selectivity of these processes.

11:20am PCSI-TuM2-35 X-ray Photoemission Spectroscopy for Non-Destructive Analysis of Si Trench Bottoms, Shiika Murase, Tomoki Higashi, Taizo Kawashima, Kouji Inagaki, Kenta Arima, The University of Osaka, Japan

Three-dimensional (3D) structures with high aspect ratios (ARs) have become standard in highly integrated semiconductor devices [1,2]. Ensuring high yield requires stringent cleanliness; however, non-destructive evaluation of cleaning in 3D structures remains limited, despite extensive studies on flat surfaces. To address this issue,we aim to develop a novel non-destructive method for evaluating cleaning performance at the bottoms of 3D nanostructures. Specifically, we apply angle-resolved X-ray photoemission spectroscopy (AR-XPS) to 3D structures such as deep trenches, embedding heterogeneous "landmark" elements selectively embedded at the bottoms as vertical markers.

In this talk, we examine the feasibility of the proposed method by obtaining XPS spectra of Si trenches with different ARs (1–7). To this end, Si trench structures were fabricated with gold (Au) selectively embedded at the bottoms using a wet etching process known as metal-assisted chemical etching (MACE) [3, 4]. AR-XPS measurements of these structures revealed a strong take-off angle (TOA) dependence of the Au 4f signal, particularly at higher ARs. This indicates that the embedded Au serves as an effective marker for aligning the sample and detector axes. AR-XPS was also conducted after removing Au from the trench bottoms. The resulting Si 2p spectrum exhibits a clear component corresponding to bulk Si(Fig. 1b), clearly distinguishable from that of Au-embedded samples (Fig. 1a), indicating that the signal originates from the trench bottoms. In other words, Fig. 1 demonstrates that MACE-fabricated Si trenches possess chemically distinct surface conditions at the top and bottom, enabling separation in Si2p XPS spectra without additional surface treatments [5]. The proposed method is expected to be used in evaluating wet and dry cleaning processes at the bottoms of high-aspect-ratio structures.

11:25am PCSI-TuM2-36 Interface Energy Barrier Inhomogeneity of Pt/4H-SiC Junction Probed with Planar Ballistic Electron Emission Spectroscopy, Jiwan Kim, Jaehyeong Jo, Jungjae Park, Hyunjae Park, Eunseok Hyun, Jisang Lee, Sejin Oh, Kibog Park, Ulsan National Institute of Science and Technology, Republic of Korea

The inhomogeneity of the interfacial energy barrier is associated with crystallographic variations of the interface, which is inevitable in heterojunctions. The ballistic electron emission microscopy/spectroscopy (BEEM/BEES) has been commonly used to observe the local variation of interfacial energy barrier with high spatial resolution (1-10 nm) [1]. However, the tip-related issues [2, 3] and long scanning time make it difficult to investigate the large area reliably. Here, we suggest an experimental methodology utilizing the device version of BEES to estimate the inhomogeneity of interfacial energy barrier with single spectral measurements covering the entire junction area. Our approach (i) relies on the Bell-Kaiser theory [1] for a 'point' BEEM response, (ii) treats the tunnel junction as an ensemble of virtual BEEM tips, and (iii) models the secondderivative spectrum (SDS) of the 'lumped' BEEM response using a known statistical nature of interfacial barriers [4]. For the case of simple two distinct Schottky barriers (SBs), the working principle of 'planar BEES' is illustrated in Fig. 1. To validate our methodology, we apply it to Pt/4H-SiC junction, adopting the Gaussian distribution of interfacial barriers. In its SDS (see Fig. 2), we observe two peaks at 1.60 V and 1.74 V corresponding to two lowest conduction band minima of 4H-SiC located at the M point of the Brillouin zone [5] and the standard deviation of SB is obtained to be 156.7 meV. Our methodology can be used broadly for other heterojunctions as long as the inhomogeneous interface possesses the Gaussian nature.

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- [2] M. Prietsch and R. Ludeke, Phys. Rev. Lett. 66, 2511 (1991).
- [3] J. P. Pelz and R. H. Koch, Phys. Rev. B 41, 1212 (1990).
- [4] R. T. Tung, Phys. Rev. B 45, 13509 (1992).
- [5] B. Kaczer, H.-J. Im, J. P. Pelz, J. Chen, and W. J. Choyke, Phys. Rev. B 57, 4027 (1998).

*Author for correspondence:kibogpark@unist.ac.kr NRF-2023R1A2C1006519, RS-2023-00227854

11:30am PCSI-TuM2-37 Mineral Interface Doping: A Safer Alternative to Doping Silicon Substrates with Phosphorus/Arsenic Without Hazardous Chemicals, Roman Konoplev-Esgenburg, KIT, Germany

This work explores Mineral Interface Doping (MID): a safer alternative that offers a simple, reproducible, and industry-relevant approach to doping without hazardous chemicals. MID is an incipient method based on the deposition of a mineral containing the dopant of interest on a silicon wafer, followed by a rapid thermal annealing (RTA) step. MID can utilize a variety of minerals, that effectively form metal silicates in contact with silicon oxide. For this specific application, a mineral should consist of three components: a metal ion (K+, Mg2+, Ce3+, ...), element that can be a source of electrons or holes in silicon bulk (such as P, As, B, etc) and oxygen/chlorine components. The proposed method uses ultra-thin films of minerals, for example Hydroxyapatite (Ca₅(PO₄)₃OH), Struvite (MgNH₄PO₄*6H₂O), Cerium Orthophosphate (CePO₄), and Monopotassium Phosphate (KH₂PO₄), applied via the Tethering by aggregation and growth (T-BAG) process and activated by RTA. Infrared and Electrochemical Impedance Spectroscopy analyses confirm that phosphorus diffuses through native silicon oxide and into the silicon, altering its electrical properties. To further explain and investigate experimental doping processes using thin films of P-containing minerals, mineral interfaces were modelled and DFT calculations were performed. The Nudged Elastic Bands method provides us with the mechanism of phosphorus transport. Our findings reveal that the required doping temperature decreases with the charge density of metal ions, however there is a required minimum temperature to achieve diffusion of phosphorus into the silicon bulk. Finally, the metal silicates are removed post-doping using non-toxic acids, thus making the process broadly applicable.

- [1] Thissen, P.; Longo, R. C., Mineral Interface Doping: Hydroxyapatite Deposited on Silicon to Trigger the Electronic Properties, Advanced Materials Interfaces 2024 11 (31), 2400061.
- [2] Konoplev-Esgenburg, R.; Koenig, M.; Welle, A.; Bogner, A.; Longo, R.; Thissen, P., The Role of Metal-Ion Charge in Mineral Interface Doping, ACS Appl. Mater. Interfaces 2025, XXXX, XXX, XXX-XXX

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11:35am PCSI-TuM2-38 Porous W2N Fibrous-Nanograins and TiN Nanopyramids Framework for High Energy Density Flexible Asymmetric Supercapacitors, *Rajesh Kumar*, *Bhanu Ranjan*, *Davinder Kaur*, Indian Institute of Technology Roorkee, India

Enhancing the energy density of flexible asymmetric supercapacitors (ASCs) necessitates developing and implementing high-performance anode materials for technological developments in wearable energy storage systems. Tungsten nitride (W2N) offers enormous potential as an anode material for ASCs, ascribed to its substantial specific capacitance, massive electrical conductivity, and extended negative potential window. In this work, we fabricated a durable coin cell and flexible ASC utilizing W₂N/SSM fibrous-nanograins anode and TiN/SSM nanopyramids cathode deposited over flexible stainless steel mesh (SSM) substrate by the DC magnetron sputtering technique. The W2N/SSM//TiN/SSM ASC device demonstrates a high areal capacitance of 21.3 mF.cm⁻² operating across a wide and stable electrochemical voltage window of 1.3 V with outstanding cycling robustness demonstrating 89.09% retention over 8000 charge-discharge cycles. Notably, the ASC achieved a high energy density of 34.33 mWh.cm⁻³ and a high power density of 17.32 W.cm⁻³. The persistent electrochemical performance of ASC is mainly attributed to the dominance of surfacecontrolled capacitive and pseudocapacitive charge storage kinetics of W₂N/SSM for Na⁺ions comprehensively examined employing 3D Bode and Dunn's techniques. The flexible ASC shows remarkable mechanical stability of 92.36% up to 500 bending cycles. This study establishes W2N nanograin's potential as a high-energy anode material, revealing the capability to increase the effectiveness of ASC for portable and miniaturized energy storage devices.

11:40am PCSI-TuM2-39 Magnetocrystalline Anisotropy as a Design Principle in PtPdFe Intermetallic Alloys for Fuel Cell Electrocatalysis, *Muhammad Irfansyah Maulana*, *DongHyun Lee, Jong-Sung Yu*, DGIST, Republic of Korea

Ordered Pt-based intermetallic alloys are emerging as efficient oxygen reduction reaction (ORR) electrocatalysts in hydrogen fuel cells, outperforming their disordered counterparts. However, the intrinsic role of atomic ordering in governing ORR catalytic performance remains unclear. In this work, we report ferromagnetic PtPdFe ternary intermetallics with structurally ordered tetragonal L10 and cubic L12 phases (Figure 1a), each featuring distinct crystal structures and atomic arrangements. Our study highlights magnetocrystalline anisotropy as a key structure-dependent descriptor that governs ORR activity in these alloys. Electrochemical halfand single-cell tests reveal that L1₀-PtPdFe magnetic intermetallic catalysts (MICs) deliver higher ORR activity than their L12 counterparts (Figure 1b). Combined experimental and theoretical analyses attribute this enhancement to the unique tetragonal $L1_0$ structure, where strong 5d-3dorbital interactions along the c-axis induce ferromagnetic ordering and elevate magnetocrystalline anisotropy energy, thereby accelerating ORR kinetics. Furthermore, membrane electrode assemblies fabricated by L1₀-PtPdFe cathode MICs sustain fuel cell performance beyond the 2025 US Department of Energy stability targets under H2-O2, H2-air, and H2-N2 conditions. These findings establish a new design principle for Pt-based intermetallic catalysts, demonstrating that magnetic anisotropy arising from ferromagnetic ordering can be strategically harnessed to optimize fuel cell performance.

11:45am PCSI-TuM2-40 Orientated Deposition of Li₂S for Fast-Charging Lithium-Sulfur Batteries, *Jeong-Hoon Yu*, *Donghyun Lee*, *Jong-Sung Yu*, DGIST. Republic of Korea

Precipitation/dissolution of insulating Li₂S has long been recognized as the rate-determining step in lithium-sulfur (Li-S) batteries, which dramatically undermines sulfur utilization at elevated charging rates. Herein, we present an orientated Li₂S deposition strategy to achieve extreme fast charging (XFC, ≤15 min) through synergistic control of porosity, electronic conductivity, and anchoring sites of electrode substrate [1]. Via magnesiothermic reduction of a zeolitic imidazolate framework, a nitrogendoped and hierarchical porous carbon with highly graphitic phase was developed. This design effectively reduces interfacial resistance and ensures efficient sequestration of polysulfides during deposition, leading to (110)-preferred growth of Li₂S nanocrystalline between (002)-dominated graphitic layers. Our approach directs an alternative Li₂S deposition pathway to the commonly reported lateral growth and 3D thickening growth mode, ameliorating the electrode passivation. Therefore, a Li-S cell capable of charging/discharging at 5 C (12 min) while maintaining excellent cycling stability (82% capacity retention) for 1000 cycles is demonstrated. Even under high S loading (8.3 mg cm⁻²) and low electrolyte/sulfur ratio (3.8

 $\mu L\ mg^{-1}),$ the sulfur cathode still delivers a high areal capacity of >7 mAh cm^{-2} for 80 cycles.

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11:50am PCSI-TuM2-41 Long-Term Cycling of Ultrathin Li Metal Anode via Interfacial Design Using Silver Trifluoromethanesulfonate as an Additive, Jong Hun Sung, Jong-Sung Yu, DGIST, Republic of Korea

The use of ultrathin lithium (Li) metal anode in Li metal batteries (LMBs) has the potential to significantly improve the energy density in comparison to the conventional LMBs. However, they possess several challenges such as intrinsic dendrite growth and dead Li, leading to poor cyclability and coulombic efficiency (CE). In addition, the ultrathin Li metal can cause much faster degradation of performances than thicker one owing to the exhaustion of Li resource with less compensation. To address these problems, silver trifluoromethanesulfonate (AgCF₃SO₃, AgTFMS) is proposed as a functional electrolyte additive in carbonate-based electrolyte to buffer the dendritic Li growth and to provide enhanced cyclability.[1] Interestingly, Ag metal derived from the AgTFMS exhibits lithiophilic properties through an alloying reaction with Li. Furthermore, the CF3 functional group of AgTFMS generates a physically stable LiF-rich solidelectrolyte interphase (SEI), which further suppresses the Li dendrite growth. An LiNi_{0.8}Mn_{0.1}Co_{0.1}O₂ (NMC811) full-cell comprising the ultrathin Li metal anode (20 μ m) with AgTFMS additive reveals an excellent capacity retention of up to 88.2% over 200 cycles, as well as outstanding rate capability under harsh practical conditions. As a result, the AgTFMS additive can pave a new dimension for the design of high energy density LMBs using the ultrathin Li metal anode.

11:55am PCSI-TuM2-42 PPlatforms for Boundary-Controlled Synthesis of Screw Dislocations in Single-Crystalline Semiconductors, Zachary Handoklow, University of New Mexico

We present our efforts on the fabrication of materials platforms to investigate boundary-controlled synthesis of screw dislocations. Our developed structures are based on twisted bicrystals formed by single-crystalline nanomembranes of various thicknesses bonded onto a bulk crystal of the same chemical and physical structure.

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