PCSI
Room Ballroom South - Session PCSI-TuM2

Atomic Layer Deposition
Moderator: Jessica Hilton, SPECS-TII, Inc.

11:00am **PCSI-TuM2-31 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.

11:05am **PCSI-TuM2-32 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 second-derivative 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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[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).

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11:10am **PCSI-TuM2-33 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 (W_2N) 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 W_2N/SSM fibrous-nanograins anode and TiN/SSM nanopyramids cathode deposited over flexible stainless steel mesh (SSM) substrate by the DC magnetron sputtering technique. The W_2N/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 surface-controlled capacitive and pseudocapacitive charge storage kinetics of W_2N/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 W_2N 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.

11:15am **PCSI-TuM2-34 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 $L1_0$ and cubic $L1_2$ 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 half- and single-cell tests reveal that $L1_0$-PtPdFe magnetic intermetallic catalysts (MICs) deliver higher ORR activity than their $L1_2$ counterparts (Figure 1b). Combined experimental and theoretical analyses attribute this enhancement to the unique tetragonal $L1_0$ structure, where strong 5d–3d orbital interactions along the c-axis induce ferromagnetic ordering and elevate magnetocrystalline anisotropy energy, thereby accelerating ORR kinetics. Furthermore, membrane electrode assemblies fabricated by $L1_0$-PtPdFe cathode MICs sustain fuel cell performance beyond the 2025 US Department of Energy stability targets under H_2–O_2, H_2–air, and H_2–N_2 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.

11:20am **PCSI-TuM2-35 Orientated Deposition of Li_2S for Fast-Charging Lithium-Sulfur Batteries**, ***Jeong-Hoon Yu***, *Donghyun Lee, Jong-Sung Yu,* DGIST, Republic of Korea

Precipitation/dissolution of insulating Li_2S 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 Li_2S 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 nitrogen-doped 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 Li_2S nanocrystalline between (002)-dominated graphitic layers. Our approach directs an alternative Li_2S 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

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

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11:25am **PCSI-TuM2-36 Platforms 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.

11:30am **PCSI-TuM2-37 Substrate-Strain-Controlled Molecular Beam Epitaxial Growth and Scanning Tunneling Microscopy of Antiperovskite Mn_3GaN**, ***Ali Abbas,*** Ohio University*; Juan Carlos Moreno Hernandez,* Universidad Autonoma de Puebla, Mexico*; Ashok Shrestha,* Ohio University*; Daniel Russell, Fengyuan Yang,* Ohio State University*; Kai Sun,* Michigan State University*; Arthur R. Smith,* Ohio University

This study investigates the epitaxial growth, structural characterization, and theoretical modeling of thin-film antiperovskite Mn_3GaN, a chiral antiferromagnetic material with a kagomespin lattice grown on MgO (001) substrates via nitrogen plasma-assisted molecular beam epitaxy (MBE). The resulting films exhibit a homogeneous composition with atomically smooth surfaces and sharp interfaces, characterized by minimal in-plane tensile strain and out-of-plane compressive strain. First-principles calculations are employed to determine the energetically favorable configurations of both the MGN surface and the MGN /MgO heterostructure, and STM images reveal an atomically smooth surface with atomic-height steps [1].

The results show that the MnGa layer along the (001) direction is energetically favorable [1]. This layer is ferromagnetic in-plane, whereas in the (111) plane, all Mn3Ga layers have chiral antiferromagnetic spin structure, making these very interesting from the spin perspective. In principle, this spin structure is accessible via spin-polarized STM, which is currently our aim. Furthermore, measurements at low temperatures can be accomplished using our new variable-temperature STM system, which enables better tip stability and lower noise. Since the Neel temperature of Mn3GaN is 298 K, by investigating this system using spin-polarized STM tips at cryogenic temperatures, it is possible to resolve the temperature-dependent spin structure, and even the Neel transition.

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