Live Session
Room Live - Session LI-WeA1

Wednesday Afternoon Live Session I: Controlling Matter at the Ultimate Limits

Moderators: Eric Joseph, IBM T.J. Watson Research Center, Arthur Utz, Tufts University

12:50pm **LI-WeA1-1 Welcome and Opening Remarks*, Eric Joseph,*** IBM T. J. Watson Research Center

Welcome to the AVS 67 Virtual Symposium! We hope you will enjoy the event!

12:55pm **LI-WeA1-2 The Development of Atomic Layer Processes for Scaling & Future Device Architectures*, Rudy Wojtecki,*** International Business Machines (IBM) - Almaden Research Center **INVITED**

A major aspect governing progress in electronic technologies is the ability to control or guide the deposition or subtraction of thin films.As the semiconductor community continues scaling, interfaces and surfaces become increasingly important. Traditional deposition and subtraction methods then may not be sufficient in future technology nodes as they may damage or amorphize surfaces to an otherwise crystalline and risk device performance or yield.Atomic layer processes present methods to preserve these interfaces by taking advantage of surface reactivities to either add or subtract a material one atomic layer at a time.Furthermore, these offer the opportunity to more broadly extend fabrication capabilities that may enable integration schemes for alternative computing architectures such as neuromorphic type devices.Within this space area selective depositions (ASD) offer a powerful tool to direct film growth from a chemically distinct surface in a self-aligned process with the potential to relax down-stream processing such as overlay requirements. There are many examples for the integration of these techniques to encapsulate and inhibit the oxidation of a metal or introduce surface topography from an underlying pre-pattern, for instance. Guiding this deposition is particularly challenging as it requires the careful interplay between deposition precursors and inhibiting (or activating) layers. Achieving this control, through judicious design and engineering of a surface affords exquisite control over the film characteristics such as composition and thickness.The development of processes that extend these capabilities will be discussed that include strategies to enable ASD with surface topography using an area selective polymerization that provides control over inhibitor thickness which acts as an effective inhibiting material.In addition, the combination of ASD with a patternable organic monolayer will be discussed that provides a versatile additive lithography platform, where a broad range of desired feature geometries can be readily generated.In the pursuit of methods to broaden the application of ASD processes fundamental insights to desirable material characteristics for these processes are useful parameters to consider in future ASD processes such as supramolecular interactions between inhibitors and chemical crosslinking.

1:15pm **LI-WeA1-6 Recent Innovations in Tof-Sims and Their Industrial Applications*, Julia Zakel,*** IONTOF GmbH, Germany **INVITED**

Time-of-flight secondary ion mass spectrometry (TOF-SIMS) is known to be an extremely surface sensitive analytical technique. It provides detailed elemental and molecular information about surfaces, thin layers, interfaces, and full three-dimensional analysis of the sample.In our contribution we will provide an overview on recent advances in TOF-SIMS instrumentation and data evaluation that are extending existing applications or even make new applications accessible. Among the discussed improvements are key values that are inherent for a dedicated TOF-SIMS instrument as mass resolution and lateral resolution, as well as improvements that are based on the integration of additional analytical components or due to the combination with complementary techniques.The latest technology step now pushes the standard lateral resolution of dedicated TOF-SIMS instruments to the sub 50 nm region. Best achieved values are even in the 20 nm range and therefore not far away from the physical limit given by the size of the sputter cascade. While new ion sources expanded the usability of SIMS instruments, SIMS analyzers lacked the required mass resolution and mass accuracy, required for the thorough investigation of molecular materials. One major challenge is based on the enormous number of molecules in the mass range of interest. An important step in order to reduce the number of interpretation possibilities is to improve the mass resolution and the mass accuracy. State-of-the-art TOF-SIMS instruments are reaching a mass resolution in the range of 30.000 and a mass accuracy in the range of few ppm. This improves the analytical possibilities compared to the previous instrument generation and reduces the complexity of data evaluation and interpretation.MS/MS capabilities are required in order to further increase identification possibilities. In this respect it is also of high importance to generate the MS/MS spectra at high mass resolution and high mass accuracy. We will discuss an MS/MS approach that is fully integrated into a TOF analyzer. The benefit of this approach is that it can easily be integrated in the given analysis scheme and data format.While the discussed performance represents the limit attainable with recent TOF-SIMS instruments, further improvement is achieved by combining an Orbitrap™-based mass analyzer with a high-end TOF-SIMS system (Hybrid SIMS). The instrument provides highest mass resolution (> 240,000) and highest mass accuracy (< 1ppm) with high lateral resolution cluster SIMS imaging. We will present data acquired on a Hybrid SIMS instrument demonstrating fast and robust identification of main constituents in unknown samples.

1:35pm **LI-WeA1-10 Microscopic Visualization of Electron Correlations in TMD Moiré Superlattices*, Shaowei Li,*** University of California at San Diego **INVITED**

Van der Waals heterostructures of atomically thin layered materials provide an exciting new platform to design and fabricate novel electronic and optical devices. Through the precise control of the stacking order and the twist angle between two adjacent layers, the moiré superlattice can lead to tunable narrow electronic minibands. With the unique ability to image the structural and electronic properties of low-dimensional materials at the atomic-scale, scanning tunneling microscopy and spectroscopy provide an opportunity to study the strongly correlated physics with real-space visibility. In this talk, I will present the real-space visualization of the localized correlated electron states in the closely aligned WS_2/WSe_2. These correlated states have shown the promise of exotic electron transfer properties such as charge order states, electron transfer insulator, Mott insulator, and superconductivity.

2:05pm **LI-WeA1-16 Characterizing Unconventional Strain and Bending in 2D Materials and Heterostructures with Aberration-Corrected STEM*, Pinshane Huang*,** University of Illinois at Urbana-Champaign, USA*; E. Han, J. Yu, C. Lee,* University of Illinois at Urbana Champaign*; D. Luo,* University of Illinois at Urbana Champaign*; A. Khan,* University of Illinois at Urbana Champaign*; T. Santos,* University of Illinois at Urbana Champaign*; S. Kang, W. Zhu, N. Sobh, A. Schleife, B. Clark, E. Ertekin, A. van der Zande,* University of Illinois at Urbana Champaign **INVITED**

The properties of 2D materials can be strongly impacted by the presence of defects, strain, and out-of-plane bending.In this talk, we discuss our development of techniques that use aberration-corrected scanning transmission electron microscopy (STEM) to measure the unconventional strain and bending of 2D materials and heterostructures with unprecedented precision.

First, we will discuss our studies of defect-induced strain in 2D materials. High-precision characterization of defects in 2D materials remains challenging because they are irradiation sensitive, making it difficult to achieve high resolution and signal-to-noise structural data without modifying the intrinsic structure. Here, we apply deep learning techniques based on convolutional neural networks to process large volumes of atomic-resolution images of the 2D transition metal dichalcogenide $WSe_{2-x}Te_{x}$. By class-averaging hundreds of nominally identical defects, we measure the local picometer-scale strain fields around single vacancies with 0.2 picometer precision, and we observe previously-unseen radial strain oscillations [1].

Second, we will discuss bending in 2D materials and heterostructures.Understanding the bending of two-dimensional materials and heterostructures is crucial for the development of next-generation electronics including deformable electronics, and nanoelectromechanical systems. Here, we show that electron microscopy can provide a powerful platform for measuring the bending of 2D materials. We use aberration-corrected STEM to image graphene and 2D heterostructures draped over atomically sharp hexagonal boron nitride steps. This approach enables atomic-resolution studies of their bending conformation, producing insight into both the bending stiffness and mechanisms of bending. We find that the bending stiffness of multilayer 2D materials is a strong function of bending angle, tuning by almost 400% for trilayer graphene [2]. This unusual behavior results from the atomic-scale bending mechanism in 2D multilayers, which is dominated by interlayer shear and slip. In combination with density functional theory (DFT) and continuum mechanics modeling, we derive a unifying model for bending in 2D materials and their heterostructures. Our findings have profound implications on 2D heterostructures, where we demonstrate that the bending stiffness can be controlled by tailoring the interfacial interactions between individual atomic layers of 2D materials.

[1] Lee, C.-H. *et al.* Deep Learning Enabled Strain Mapping of Single-Atom Defects in 2D Transition Metal Dichalcogenides with Sub-picometer Precision. *Nano Lett.* (2020). doi:10.1021/acs.nanolett.0c00269

[2] Han, E. *et al.* Ultrasoft slip-mediated bending in few-layer graphene. *Nat. Mater.* **19**, 305–309 (2020).

2:25pm **LI-WeA1-20 Chemistry in Confined Spaces: 2D-Porous Silicates on Metal Supports***, **J. Anibal Boscoboinik**,* Brookhaven National Laboratory **INVITED**

Confinement effects can give rise to interesting properties in the chemistry and physics of small molecules. In this talk, we will explore 2D-porous silicates on a metal support. These can trap noble gases (Ar, Kr, and Xe) at elevated temperatures (>300 K) within the silicate structure and at the interface with the metal. They can also affect chemical reactions taking place on the metal surface, and the case of water formation from H_2 and chemisorbed O will be used to illustrate this effect.

2:45pm **LI-WeA1-24 Basic Science Needs for Transforming Manufacturing Through Atomically Precise Manufacturing***, **Cynthia Jenks**, H. Lee,* Oak Ridge National Laboratory*; J. Lewis,* Harvard University **INVITED**

In March of 2020, the Department of Energy, Office of Science, Basic Energy Sciences, ran a workshop aimed at providing strategic research directions that could ultimately transform manufacturing as we know it through a better understanding of fundamental science. The attendees at this workshop on Basic Research Needs for Transformative Manufacturing developed five priority research directions to revolutionize manufacturing. These directions include the following: (1) achieve precise, scalable synthesis and processing of atomic-scale building blocks for components and systems; (2) integrate multiscale models and tools to enable adaptive control of manufacturing processes; (3) unravel the fundamentals of manufacturing processes through innovations in operando characterization; (4) direct atom and energy flow to realize sustainable manufacturing; and (5) co-design materials, processes, and products to revolutionize manufacturing. This talk with provide an overview of these five areas with a particular emphasis on the priority research direction on atomically precise manufacturing. Atomically precise materials and molecules would lead to unparalleled structures and functions that, at the moment, are unattainable. There are several scientific questions to consider to achieve precision manufacturing of materials and molecules. W*hat are the mechanisms needed for manufacturing multiscale, atomically and molecularly precise materials? How can basic research uncover structure-function relationships across multiple scales in components and systems? How can chemical processes readily be scaled from laboratory results?*

3:05pm **LI-WeA1-28 Closing Remarks and Thank You's***, **Art Utz**,* Tufts University

Thank you for attending today's session! Remember to check out the AVS 67 On Demand Sessions which are available in the mobile app and online scheduler until 11/30/21 and then in the AVS Technical Library for all Platinum Members. We will see you at AVS 68 in Pittsburgh, PA, November 6-11, 2022!

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