

MEMS and NEMS Technical Group

Room 302 - Session MN+AS+NS+QS+SE-MoM

Dynamics and Engineering of MEMS/NEMS

Moderators: Jürgen Brugger, EPFL, Switzerland, Eva Weig, University of Munich, Germany

9:00am **MN+AS+NS+QS+SE-MoM-3 MEMS-Based Surface Nanoengineering Using Thermal AFM Probes: 30 Years and Counting, Jürgen Brugger**, École Polytechnique Fédérale de Lausanne, Switzerland **INVITED**

Soon after the first publication in 1985 of the atomic force microscope (AFM) attempts were made to extend AFM-based surface probing from microscopy to lithography [reviewed in 1]. The potential applications in writing and reading for data storage in the early years served as technology driver and showed remarkable performances [2]. One of the variants of AFM-based writing (and reading) operates a heated nano-tip to perform thermally induced phase changes of materials. The three-fold combination of nano-scale heat localization (30 nm scale), high temperature (~ 500 °C) and particularly fast heating/cooling cycles (10E-6 s) is unique and opens new opportunities for surface engineering and material conversion using heat. In the meantime, nano-tips and cantilevers were further perfected as nanotools to locally induce phase changes in materials for a wide range of exploratory studies. Today, thermal scanning probe lithography (t-SPL) has matured into turn-key systems that can be compared to some extent to electron beam lithography, but without the use of charged particles and without the need for development. The full grasp of potential applications in R&D and production is still growing as the technique is still emerging.

In this talk, we will give first some background how heated AFM probes were initially designed and fabricated that led to today's advanced thermo-mechanical probe design of micro-cantilevers and nano-tips. The paper will then review some main achievements up to date [3] and then present recent results on t-SPL utilized for 2D materials by our own work [4, 5], and will conclude with some outlook on further challenges in hot-tip nanoengineering.

References:

- [1] R. Garcia, et al. *Nature Nanotechnology* (2014)
- [2] H. J. Mamin et al. *Applied Physics Letters* (1992)
- [3] S. T. Howell et al. *Microsystems & Nanoengineering* (2020)
- [4] X. Liu et al. *Advanced Materials* (2020)
- [5] X. Liu et al. *Nano Letters* (2020)

10:40am **MN+AS+NS+QS+SE-MoM-8 Atomically-Thin MoS₂ Nanoelectromechanical Resonators**, R. Yang, Shanghai Jiao Tong University, China; **Jaesung Lee**, University of Texas at El Paso **INVITED**

With the development of the Internet of Things (IoT), new sensors and signal processing elements that consume *near-zero* power to operate on resonance, have high tunability and small form factor are necessary. The ultralow mass and large resonance tunability make resonant 2D nanoelectromechanical systems (NEMS) suitable for ultrasensitive mass, force and biomolecular sensing, radio-frequency (RF) front end, and strain-tunable devices. Further, molybdenum disulfide (MoS₂) resonators only require picowatt level of power for sustaining the strong and stable resonance operations due to their ultralight weight. This opens an opportunity to explore new sensors and signal processing elements for IoT applications that really require near-zero power to operate on resonance, and at the same time, have wide dynamic ranges and tuning ranges. In this talk, we summarize our most recent advances in 2D MoS₂ NEMS resonators.

11:20am **MN+AS+NS+QS+SE-MoM-10 Can a Single Nanomechanical Mode Generate a Frequency Comb?**, **Eva Weig**, Technical University of Munich, Germany **INVITED**

Doubly-clamped nanostring resonators excel as high Q nanomechanical systems enabling room temperature quality factors of several 100,000 in the 10 MHz eigenfrequency range. Dielectric transduction via electrically induced gradient fields provides an integrated control scheme while retaining the large mechanical quality factor [1]. Dielectrically controlled nanostrings are an ideal testbed to explore a variety of dynamical phenomena ranging from multimode coupling to coherent control [2]. Here I will focus on the nonlinear dynamics of a single, resonantly driven mode. The broken time reversal symmetry gives rise to the squeezing of the

string's fluctuations. As a result of the high mechanical Q factor, the squeezing ratio is directly accessible from a spectral measurement [3]. It is encoded in the intensities of the two spectral peaks arising from the slow dynamics of the system in the rotating frame. For stronger driving, an onset of self-sustained oscillation is observed which leads to the generation of a nanomechanical frequency comb. The effect is a consequence of a resonantly induced negative effective friction force induced by the drive. This is the first observation of a frequency comb arising solely from a single mode and a single, resonant drive tone [4].

- [1] Q. P. Unterreithmeier et al., *Nature* 458, 1001 (2009)
- [2] T. Faust et al., *Nature Physics* 9, 485 (2013)
- [3] J. Huber et al., *Phys. Rev. X* 10, 021066 (2020)
- [4] J. Ochs et al., in preparation

MEMS and NEMS Technical Group Room 302 - Session MN+2D-MoA

Emerging Materials and Structures for MEMS/NEMS Devices

Moderators: Azadeh Ansari, Georgia Institute of Technology, Yanan Wang, University of Nebraska - Lincoln

1:40pm **MN+2D-MoA-1 Phononic Crystals based on Two-Dimensional Materials**, Yanan Wang, University of Nebraska - Lincoln **INVITED**

Thanks to the ultimate thinness, excellent elastic properties, and unparalleled advantages in device integration, two-dimensional (2D) materials have emerged as compelling candidates for enabling high frequency nano-/microelectromechanical systems (NEMS/MEMS). This talk will discuss the further exploration of 2D materials in phononic devices, such as quasi-1D phononic waveguides and tunable phononic crystal lattices, emphasizing their potential applications in quantum information processing and quantum sensing systems.

2:20pm **MN+2D-MoA-3 Scaling Acoustics into mm-Wave: Higher-Order Lamb Mode Devices in Piezoelectric Thin Films**, Ruochen Lu, J. Kramer, S. Cho, O. Barrera, The University of Texas at Austin **INVITED**

The evolving wireless communication moves to higher frequency bands with broader bandwidth for faster data rate. New types of front-end elements are required to perform the signal processing at the new bands. Acoustic devices are among the processing candidates, thanks to their compact footprints and low loss. However, it has been a long-standing challenge to scale piezoelectric resonators beyond 6 GHz without significantly losing quality factor (Q) and electromechanical coupling (k^2).

Until now, three approaches have been investigated, including reduced wavelength, higher-order modes, and multi-layer periodically poled piezoelectric films (P3F) structures. The first method requires small feature sizes, e.g., the electrode pitch width of laterally vibrating devices or the thickness of film bulk acoustic wave resonators (FBARs). The direct scaling inevitably leads to fabrication challenges and more importantly, severely reduced Q from the electrical resistance and acoustic damping. The second approach utilizes the additional thickness component in higher-order Lamb modes to relax the lateral feature size requirement. However, sub-400 nm piezoelectric thin films are needed if operated at the first-order thickness mode, e.g., first-order antisymmetric (A1) mode, inducing limited Q below 500 from the surface damages during the implementation. Alternatively, one can operate at higher frequencies using increased thickness mode order acoustic modes, e.g., second-order antisymmetric (A2) mode. Nevertheless, further increasing the mode order in the thickness direction without modifying the transducer configuration leads to reduced k^2 , as the generated charge tends to cancel out, limiting the applications.

Recently, we proposed the P3F platforms using thin-film lithium niobate (LiNbO₃) to address the challenge. By stacking transferred thin-film LiNbO₃ with alternating orientations in the thickness direction, we can achieve remarkable frequency scaling without losing k^2 or relying on thinner films. Complementary oriented bi-layer acoustic resonator (COBAR) following thickness-shear modes have been demonstrated. We will report COBARs leveraging the thickness-extensional (TE) modes at 15.8 GHz using sixth-order antisymmetric (A6) mode COBAR with a high loaded Q of 720. The measured loaded Q and $f \cdot Q$ product (1.14×10^{13}) are among the highest for piezoelectric acoustic resonators beyond 6 GHz.

3:00pm **MN+2D-MoA-5 AlScN Piezoelectric Metamaterials for Next Generation RF Systems**, C. Cassella, Dan Zhao, Northeastern University **INVITED**

In the last two decades, microacoustic resonators (μ ARs) have played a key role in integrated 1G-to-4G radios, providing the technological means to achieve compact radio frequency (RF) filters with low loss and moderate fractional bandwidths (BW < 4%). More specifically, Aluminum Nitride (AlN) based filters have populated the front-end of most commercial mobile transceivers due to the good dielectric, piezoelectric and thermal properties exhibited by AlN thin-films and because their fabrication process is compatible with the one used for any Complementary Metal Oxide Semiconductor (CMOS) integrated circuits (ICs). Nevertheless, the rapid growth of 5G and the abrupt technological leap expected with the development of sixth-generation (6G) communication systems are expected to severely complicate the design of future radio front-ends by demanding Super-High-Frequency (SHF) filtering components with much

larger fractional bandwidths than achievable today. Even more, the recent invention of on-chip nonreciprocal components, like the circulators and isolators recently built in slightly different CMOS technologies, has provided concrete means to double the spectral efficiency of current radios by enabling the adoption of full-duplex communication schemes. Nevertheless, for such schemes to be really usable in both military and commercial wireless systems, self-interference cancellation networks including wideband, low-loss and large group delay lines are needed. Yet, the current on-chip delay lines that are also manufacturable through CMOS processes, which rely on the piezoelectric excitation of Surface Acoustic Waves (SAWs) or Lamb Waves in piezoelectric thin films, have their bandwidth and insertion-loss severely limited by the relatively low electromechanical coupling coefficient exhibited by their input and output transducers. As a result, these components are hardly usable to form the delay lines forming any desired self-interference cancellation networks. In order to overcome these challenges, only recently, new classes of microacoustic resonators and delay lines exploiting the high piezoelectric coefficient of Aluminum Scandium Nitride (AlScN) thin films and the exotic dispersive features of acoustic metamaterials have been emerging. These devices rely on forests of locally resonant piezoelectric rods to generate unique modal distributions, as well as unconventional wave propagation features that cannot be found in conventional SAW and Lamb wave counterparts. In this talk, the design, fabrication and performance of the first microacoustic metamaterials based resonators and delay lines will be showcased.

4:00pm **MN+2D-MoA-8 Fabrication, Actuation and Control of 3D-Printed Microscale Robots**, Azadeh Ansari, The Georgia Institute of Technology **INVITED**

This talk covers the fabrication methods of micro scale robots using two photon lithography nanoscale 3D printing of various micro robot designs for biomedical applications. The polymer-based 3D printed robots are integrated with piezoelectric actuators, or magnetic thin films/cubes. Tiny polymer legs/bristles and contacts are designed for precise robot motion control. Furthermore, the microbots are equipped with various mechanical add-ons such as micro-tips/needles for penetration into soft tissues, micromanipulators, micro-drillers, and pH sensitive drug delivery units.

4:40pm **MN+2D-MoA-10 Fabrication of Resistor-based Zinc Devices using Selective Chemical Deoxidation of Screen Printed Zinc Inks by Inkjet Printing**, A. Radwan¹, Case Western Reserve University; Y. Sui, University of Colorado at Boulder; Christian Zorman, Case Western Reserve University

Zinc (Zn) is a common metal that harmlessly decomposes in the environment and thus is considered a leading metal for use in environmentally-friendly electronics. Zn readily oxidizes under ambient conditions forming a thin, electrically-insulating zinc-oxide (ZnO) layer on the surface of Zn particles. Fortunately, conductive Zn structures can be formed by etching the ZnO layer using aqueous solutions of acetic acid dispensed by drop casting. Although drop-casting is simple to implement, dispensing extremely small volumes is difficult. As such, drop casting is limited to producing structures with high conductivity (i.e., electrodes) but is not suitable to produce structures with tunable resistivity. Although designed to dispense inks, inkjet printers are precision liquid dispensing systems capable of depositing picoliter droplets at designated locations. Therefore, it is feasible to use an inkjet printer as an acetic acid dispenser to form Zn structures by selective etching of Zn-based inks. Unlike drop casting, this reactive inkjet printing (RIJ) process enables the resistivity of Zn structures to be tuned by controlling the amount of acetic acid dispensed. Moreover, inkjet printing offers precision lateral control of the dispensing process which could enable the fabrication of both conductive and resistive structures in the same Zn layer.

In this paper, a selective RIJ method to dispense an etching agent on screen printed Zn structures with a high degree of volumetric and spatial control is described. This RIJ process is used in conjunction with screen printing to precisely control the amount of acetic acid deposited on the surface of printed Zn structures. The number of print passes and drop spacing are utilized to precisely regulate the exposure of the Zn structures to acetic acid thus enabling unparalleled control of the etching process. The screen printing and RIJ processes are performed at room temperature, making them compatible with temperature sensitive substrates including many that are attractive for flexible, implantable and biodegradable electronics. The substrate only needs to be inert to acetic acid. This study specifically focuses on the formation of Zn structures with tunable resistivity and

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explores the relationships between key printing parameters and electrical resistivity of the resulting Zn structures. As process demonstrators, microheaters and RC filters are fabricated and characterized.

5:00pm **MN+2D-MoA-11 Mechanically Tunable One-Dimensional Photonic Crystals Fabricated by Two-Photon Polymerization**, *Victoria P. Stinson¹, N. Shuchi, M. McLamb, G. Boreman, T. Hofmann*, University of North Carolina at Charlotte

Photonic crystals have attracted interest in optical applications, due to their highly reflective photonic bandgaps [1-3]. These photonic bandgaps are formed by creating a dielectric periodicity. Depending on the complexity of this periodicity the photonic crystal can be described as being one-, two-, or three-dimensional. In the one-dimensional case, this periodicity is created in a single direction. One-dimensional photonic crystals fabricated by two photon polymerization have demonstrated high-contrast photonic bandgaps in the infrared spectral range [2]. This is achieved by alternating layers of high- and low-density. In order to allow additional spectral filtering of the photonic bandgap, defects have also been implemented into these designs, allowing narrow band transmissions to exist within the otherwise reflective photonic bandgap [3]. While the spectral position of these features can be easily designed for a desired range, there are currently few methods for manipulating these features post-fabrication. Introducing mechanically sensitive flexures as low-density layers into these one-dimensional photonic crystals could fill this gap. Opto-mechanical devices fabricated by two-photon polymerization is an emerging field which has applications in areas such as MEMS and microrobotics [4]. The ability to control the spectral response via an external mechanical stimuli opens the door for more complex and adaptable sensing and filtering bandgap devices. The use of two-photon polymerization in the development of these devices allows for three-dimensional design freedom with efficient fabrication times. In this study we report on the use of sub-wavelength mechanical flexures in the low-density layers of one-dimensional photonic crystals fabricated by two-photon polymerization. Upon compression the change in thickness of these low-density layers will result in an overall spectral shift of the photonic bandgap. The degree of spectral shifting, as well as an analysis of the mechanical properties of one-dimensional photonic crystals with flexures are presented and discussed.

[1] H. Shen, Z. Wang, Y. Wu, B. Yang, *RSC Adv.* **6**, 4505-4520 (2016).

[2] Y. Li, D. Fullager, S. Park, D. Childers, R. Fesperman, G. Boreman, T. Hofmann, *Opt. Lett.* **43**, 4711-4714 (2018).

[3] V.P. Stinson, S. Park, M. McLamb, G. Boreman, T. Hofmann, *Optics* **2**, 284-291 (2021).

[4] Z. Lao, N. Xia, S. Wang, T. Xu, L. Zhang, *Micromachines* **12**, 465 (2021).

MEMS and NEMS Technical Group Room Ballroom A - Session MN-TuP

MEMS and NEMS Poster Session

MN-TuP-1 Nanoelectromechanical Resonators Based on Mechanically Anisotropic 2D Material, *Bo Xu¹, F. Xiao, J. Zhu, Y. Liang, C. Jiao, J. Li, Q. Deng, S. Wu, T. Wen, S. Pei, J. Xia, Z. Wang*, University of Electronic Science and Technology of China

The rich properties of atomic layer crystals enable researchers to design and fabricate micro/ nanoelectromechanical devices and systems towards signal processing and sensing applications. In particular, mechanical properties of two-dimensional (2D) materials play an increasingly important role in designing devices with predictable responses in order to achieve desired device performance, such as frequency and mode sequence in 2D nanoelectromechanical systems (NEMS) resonators.

Rhenium disulfide (ReS₂) crystal is a 2D semiconductor with weak interlayer coupling which can lead to relatively low Young's modulus ($E_{yz}=0.4$ GPa) along the out-of-plane direction of the layered crystal. Interestingly, it exhibits strong in-plane anisotropy. However, its mechanical anisotropy has not been experimentally demonstrated yet. Here, we experimentally demonstrate ReS₂ nanomechanical resonators, and elucidate their mechanical anisotropy using multi-mode spectromicroscopy measurements.

ReS₂ nanomechanical resonators are fabricated by mechanically exfoliating MoS₂ crystal onto Si/SiO₂ substrates with pre-patterned cavities and electrode. We measure the multi-modal resonance response using a customized scheme that incorporates electrical driving and optical detection. For each resonance peak, by using XY stage and spectromicroscopy measurement scheme, we can visualize the mode shape. We then perform extensive calculations to fit to the experimental results. Specifically, we sweep the input parameters (E_{yx} and E_{xy}) in an FEM model for an anisotropic circular drumhead resonator, and pinpoint the optimal input parameters by minimizing the collective difference between measurement and calculation for all modes.

The thickness t and diameter d of the ReS₂ resonator are $t=106$ nm and $d=10$ μ m. The frequency response of first six vibrational modes are shown in the Figure, respectively. Using the spectromicroscopy technique [8], the mechanical vibration modes shapes are visualized. We then run numerical simulations (using both mechanically anisotropic and isotropic models) to predict multimode response and mode shape of the ReS₂ resonator, and optimize the input Young's moduli to achieve the best agreement between measurement and simulation results. We find that the best result is produced by the mechanically anisotropic model, with $E_{yx}=191$ GPa and $E_{xy}=134$ GPa for our ReS₂ device. We thus quantitatively determine the mechanical anisotropy in ReS₂.

In summary, we clearly prove that ReS₂ is mechanically anisotropic, and successfully obtain its Young's moduli.

Figures and Refs in PDF.

MN-TuP-2 Frequency Scaling in Electrically Tunable WSe₂ Nanomechanical Resonators, *Jiankai Zhu², B. Xu, F. Xiao, Y. Liang, C. Jiao, J. Li, Q. Deng, S. Wu, T. Wen, S. Pei, J. Xia, Z. Wang*, University of Electronic Science and Technology of China

Nanomechanical resonators based on atomic layers of tungsten diselenide (WSe₂) show good promises for ultralow-power signal processing and novel sensing functions. However, frequency scaling in WSe₂ NEMS resonators remains yet to be explored, which impedes the realization of 2D circuits involving WSe₂ resonators at large scale. Here, we elucidate frequency scaling law in such 2D semiconducting resonators, and determine that the Young's modulus of WSe₂ is 130GPa. Further, by operating devices from the appropriate mechanical region, we demonstrate a broad frequency tuning range (up to 230%) with just 10V gate voltage, representing some of the highest gate tuning efficiency in 2D NEMS resonators reported to date.

We fabricate a total of 26 circular drumhead WSe₂ resonators of different diameters using mechanical exfoliation and dry transfer technique, with device thickness ranging from single layer to 127 layers. We measure the resonant response of WSe₂ resonators using a custom-built 2D resonator measurement system based on laser interferometry, in which the device's

vibratory motion is transduced into optical signal and detected by a photodetector.

From measured data of all the devices, we determine that the Young's modulus E_r of WSe₂ is 130GPa, in good agreement with theoretical predictions and nanoindentation measurements, as well as the pre-tension to be 0.05-0.4N/m, in good agreement with other measurements.

We further analyze the frequency scaling and elastic transition of WSe₂ resonators. From the experimental data, we clearly observe the elastic transition from the "membrane" limit (left end) to "plate" limit (right end) in different devices, allowing us to fully explore resonant characteristics by leveraging the unique mechanical responses from each specific region. For example, we observe that devices with lower pre-tension see a greater relative change of total tension, and thus exhibit larger relative frequency shifts. We therefore choose the 8 μ m-diameter, 18.4 nm-thickness device to demonstrate efficient gate tuning. This NEMS resonator exhibits clear and consistent gate tuning of frequency under three measurement schemes: electrical excitation, optothermal excitation, and thermomechanical resonance. We achieve an excellent tuning range $\Delta f/f_0$ reaching 230%, comparable to the best performance found in NEMS resonators, as well as a gate tuning efficiency of 23%V⁻¹, the highest among 2D NEMS resonators reported to date. Our results offer important design guidelines for frequency tunable NEMS resonators based on these emerging 2D materials.

Fig & Ref in PDF

MN-TuP-3 Strain-Modulated Dissipation and Signal Transduction in Two-Dimensional Molybdenum Disulfide Nanoelectromechanical Resonators, *Pengcheng Zhang³, Y. Rui*, Shanghai Jiao Tong University, China

Resonant nanoelectromechanical systems (NEMS) based on two-dimensional (2D) materials such as molybdenum disulfide (MoS₂) are interesting for highly sensitive mass, force, photon, or inertial transducers, as well as for fundamental research approaching the quantum limit, by leveraging the mechanical degree of freedom in these atomically thin materials. For these mechanical resonators, the quality factor (Q) and signal transduction are essential, yet the mechanism for energy dissipation and accurate signal transduction model in 2D NEMS resonators have not been fully explored. Here, we present the accurate strain-modulated dissipation model and equivalent circuit model focusing on NEMS resonators based on a 2D semiconductor: MoS₂. We further show that for doubly-clamped resonators, the Q increases with larger DC gate voltage, while fully-clamped drumhead resonators show the opposite trend. Using DC gate voltages, we can tune the Q by $\Delta Q/Q = 120\%$ for fully-clamped resonators, and by $\Delta Q/Q = 229\%$ for doubly-clamped resonators. We develop the strain-modulated dissipation model for these 2D NEMS resonators, which is verified against our measurement data for a fully clamped resonator and a doubly clamped resonator. We find that static tensile strain decreases dissipation while vibration-induced strain increases dissipation, and the actual dependence of Q on DC gate voltage depends on the competition between these two effects, which is related to the device boundary condition. Furthermore, we find that strain also tunes the mobility and carrier density of MoS₂, and develop a strain-modulated equivalent circuit model for 2D MoS₂ NEMS resonators, to show the enhancement of signal transduction efficiency due to the strain effect. Such strain dependence is useful for optimizing the resonance linewidth and signal transduction efficiency in 2D NEMS resonators towards low-power, ultrasensitive, and frequency-selective devices for sensing and signal processing.

MN-TuP-4 Titania Nanotube Array Electrochemical Characterization and Integration Into a Mechanically-Adaptive Neural Interface, *D. Sacco, H. Wang, T. Stegall, A. Menon, Y. Yang, J. Capadona*, Case Western Reserve University; *H. Amani Hamedani, Allison Hess-Dunning*, Louis Stokes Cleveland VA Medical Center

Optimizing the functional performance and lifetime of implanted biosensor technologies requires close integration and interaction at the biotic-abiotic interface. Devices that penetrate into tissue (e.g., intracortical neural interfaces) evoke biologically-mediated responses that isolate the device from the tissue and inhibit biosensing capabilities. Two materials strategies used to promote device integration with local tissue are 1) mechanically-compliant structural materials that reflect the mechanical properties of biological tissues, and 2) nanostructured materials that reflect the scales at which cells and proteins interact. Functional devices for biosensing are typically heterogeneous systems comprised of multiple materials that each

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serve a purpose (e.g., structural vs. functional, conductive vs. insulating), suggesting that multiple strategies are needed within the same implanted device to improve integration with tissue.

Our team has augmented our previous mechanically-adaptive, polymer nanocomposite (NC) neural interfaces with nanostructured titania nanotube arrays (TNAs) as the sensing electrode material. TNAs are vertically-oriented, highly-organized arrays of nanoscale-diameter open-ended tubes that form from titanium in an electrochemical anodization process and have previously been shown to promote tissue integration. Implementing this dual-faceted approach to improving neural interfaces required 1) that the TNAs have a sufficiently low electrode-electrolyte impedance of $<20 \Omega\text{-cm}^2$ at 1 kHz to facilitate sensing, and 2) a fabrication process to produce a functional device that incorporates TNA microelectrodes into the soft NC substrate. Electrochemical impedance spectroscopy was used to characterize a series of as-anodized and post-treated TNAs. The impedance magnitude and variability across a sample were heavily influenced by the processing conditions, with annealing at 450°C yielding the lowest impedance. Plasma-based surface modification lowered the impedance of samples by up to 83%, thereby bringing them into an acceptable impedance range. An inverted microfabrication process for integrating TNA microelectrodes into the NC structure was developed using a combination of photolithography and laser micromachining to produce a functional device with six layers in a four-photomask process. We expect that the improvements in integration with biological systems afforded by the combined tissue response mitigation strategies will enable the long-term, high-quality performance needed for advancing neuroscience and clinical brain-machine interfaces.

MN-TuP-5 One-Dimensional Photonic Crystals with Narrow-Band Defect Modes Fabricated by Direct Laser Writing, Victoria P. Stinson, M. McLamb, T. Hofmann, University of North Carolina at Charlotte

The ability of two-photon polymerization to fabricate high contrast one-dimensional photonic crystals for the infrared spectral range has been demonstrated [1]. In general, photonic crystals induce a reflective photonic bandgap where transmission is forbidden. This is achieved by creating a dielectric periodicity in one-, two-, or three-dimensions [2]. One-dimensional photonic crystals create a dielectric periodicity in a single direction. These photonic crystals can be easily tuned to the desired spectral range by altering the geometrical structure. The introduction of defects which disrupt the dielectric periodicity of these one-dimensional photonic crystals can induce narrow band transparencies within the photonic bandgap. This spectral effect has recently been demonstrated in one-dimensional photonic crystals fabricated by two-photon polymerization [3]. Photonic crystals with defects show an increased sensitivity to layer thickness non-uniformity. For this presentation we will further analyze the sensitivity these photonic crystals have to this important fabrication parameter and discuss potential applications.

[1] Y. Li, D. Fullager, S. Park, D. Childers, R. Fesperman, G. Boreman, T. Hofmann, *Opt. Lett.* **43**, 4711-4714 (2018).

[2] A.H. Aly, H.A. Elsayed, *Physica B* **407**, 120-125 (2012).

[3] V.P. Stinson, S. Park, M. McLamb, G. Boreman, T. Hofmann, *Optics* **2**, 284-291 (2021).

MN-TuP-6 Ultra-High-Quality-Factor Membrane Resonators for Gas Pressure Sensing, Christoph Reinhardt, Deutsches Elektronen-Synchrotron (DESY), Germany; H. Masalehdan, University of Hamburg, Germany

Nanomechanical resonators are chip scale implementations of a mechanical oscillator, which are of both practical and fundamental interest. In many applications, such as force sensing and quantum control of mechanical oscillators, it is typically advantageous to create lightweight, compliant mechanical elements with high quality factors Q . Recent years have seen a rapid development of devices with ever higher Q values, with current records approaching $Q \sim 10^{10}$ at room temperature. As a result, these devices become increasingly sensitive to smallest changes in certain environmental parameters, such as the pressure of the surrounding gas. In this work, we demonstrate the practical use of a mm-scale nanomechanical trampoline resonator with intrinsic resonance frequencies $f \sim 100$ kHz and $Q \sim 10^7$ for gas pressure sensing. To this end, we place the trampoline inside an ultra-high-vacuum chamber and interferometrically measure

resonance frequency and quality factor of its fundamental out-of-plane mode as a function of gas pressure, using air and helium. In the pressure (p) range from 10^{-6} mbar to 10^3 mbar (i.e., ambient pressure), the quality factor continuously decreases from 10^7 to 15 (30) for air (helium). At ~ 10 mbar we observe a change from a $Q \sim p^{-1}$ to a $Q \sim (1 + \alpha \sqrt{p})^{-1}$ dependency, with fit parameter α , related to a transition from the free molecular to the viscous flow regime. This transition is accompanied by the onset of a decrease in the trampoline's resonance frequency towards higher pressures. Leading to a 10 % (3 %) reduction at ambient air (helium) pressure. We find excellent agreement within ~ 10 % between the measured data and a model, covering the investigated pressure range. Based on additional measurements for higher-order modes, we argue, that the estimated deviation might be mainly limited by a commercial reference pressure gauge. In this regard, we discuss prospects for nanomechanical-resonator-based pressure sensing with a precision on the order of few percent and the inherent benefit of self-calibration. In addition, we highlight the possibility for extending the measurement range with optimized devices by more than two orders of magnitude towards both lower and higher pressure ranges.

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MN-TuP-7 The Effect of Laser Processing on Drug-Loaded Polymers for Microfabricated Neural Interfaces, Natalie Mueller, M. Ya Mungu Ocoko, D. Chirra, P. Dernelle, A. Hermoso, J. Capadona, A. Hess-Dunning, Case Western Reserve University

Drug-loaded polymers can be used in a multitude of biomedical applications, including drug-eluting, polymer-based intracortical microelectrodes to mitigate the neuroinflammatory response (Fig. 1). While these devices have shown promising results in reducing neuroinflammation around the microelectrode implant site, fabrication processes can affect the therapeutic efficacy of the drug. In our device, we load a polymer (polyvinyl acetate) substrate with the antioxidant/anti-inflammatory natural product, resveratrol. Resveratrol undergoes transformation from its more therapeutic isomer trans-resveratrol to its less potent form cis-resveratrol when exposed to heat and UV light. During our microfabrication process to integrate functional recording electrodes (Fig. 2), the resveratrol-loaded polymer substrate is exposed to both heat and UV light, particularly during the laser-micromachining step to create individual devices. We hypothesized that a higher power and laser path density would facilitate the conversion of trans-resveratrol to cis-resveratrol. Trans- to cis- conversion can be detected through a decrease in the absorbance peak in UV-vis spectrophotometry, as cis-resveratrol has a lower absorbance wavelength (287 nm) than trans-resveratrol (306-317 nm).

To test the effect of laser-micromachining on the resveratrol-loaded polymer devices, we first cut unloaded and resveratrol-loaded polymer substrates with 6 different combinations of laser power and geometry (Fig. 3). The cut devices were then incubated in 1X PBS, in which the hydrated state of the polymer allows the loaded resveratrol to elute from the sample to determine resveratrol release rate. The incubation solution was measured using UV-vis spectrophotometry at set time points (Fig. 4). The resveratrol release profile suggests that resveratrol-loaded polymer samples with a higher laser path density release more resveratrol (Fig. 5). Laser power did not strongly impact the peak absorbance or wavelength at peak absorbance. However, higher laser power corresponds to a less precise cut and increased damage to the resveratrol-loaded polymer substrate (Fig. 6). Samples with a higher laser path density (100 μm -wide serpentine, 200 μm -wide serpentine) have a lower wavelength at peak absorbance compared to samples with a lower laser path density (rectangular, 1000 μm -wide serpentine), which could be attributed to changes in the polymer, resveratrol form, or both. Together, these results inform the loading parameters for resveratrol-loaded polymer substrates, the fabrication process parameters to optimize active molecule release, and interpretation of the histology data from *in vivo* studies.

MN-TuP-8 Pressure Control During Bronze Infiltration of Binder-Jet Printed Stainless-Steel to Create Metal Microchannels, H. Davis, J. Harkness, I. Kohls, N. Crane, B. Jensen, R. Vanfleet, Robert C. Davis, Brigham Young University

Additive manufacturing (AM) of metal microscale channels could enable microfluidic applications requiring higher temperature and higher thermal

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conductivity materials. Combining these thermal properties with AM's ability to form small-scale complex flow paths could create functional structures like microscale gas chromatography columns or heat exchangers. We are developing processes to fabricate sealed metal microchannels using bronze infiltration of binder-jet printed stainless-steel parts. In this approach, bronze infiltrant must fill the porous material produced by binder jetting without filling the formed microchannels. This was achieved using pressure control reservoirs, wherein the powder filled reservoirs (pore size $\sim 60 \mu\text{m}$) are used to control infiltrant pressure. With pressure control, the infiltrant selectively filled the small pores between particles in the printed part (pore size $\sim 3 \mu\text{m}$) while leaving formed microchannels (200 to $900 \mu\text{m}$) empty.

Quantum Information Science Focus Topic Room 302 - Session QS+EM+MN+NS-WeA

Systems and Devices for Quantum Information

Moderators: Megan Ivory, Sandia National Laboratories, Dave Pappas, Rigetti Computing

2:20pm **QS+EM+MN+NS-WeA-1 Photonics-Integrated Microfabricated Surface Traps for Trapped Ion Applications, Megan Ivory, W. Setzer, N. Karl, J. Schultz, J. Kwon, M. Revella, R. Kay, M. Gehl, H. McGuinness, Sandia National Laboratories** **INVITED**

Some of the more advanced quantum systems for applications spanning clocks, sensors, and computers are based on the control and manipulation of atoms. While these atomic systems have led to promising results in laboratory systems, the transition of these devices from the laboratory to the field remains a challenge. Recently, advances in compact vacuum technology, microfabricated surface traps, and integrated photonics are paving the way toward deployable solutions. Here, I discuss ongoing efforts at Sandia National Laboratories to leverage microfabricated surface traps for low size, weight, and power (SWaP) deployable trapped-ion systems, and the unique systematics presented by these integration efforts. In particular, I present initial demonstrations of trapped ions utilizing multilayered waveguides for UV and visible/IR light and single photon avalanche detectors integrated with microfabricated surface traps. I also present characterization of heating rates and frequency shifts in these integrated devices, and an outlook for further reducing SWaP via compact vacuum systems.

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3:00pm **QS+EM+MN+NS-WeA-3 Toward Heterogeneous Quantum Networks: Interfacing Trapped Ion, Superconducting, and Integrated Photonic Qubits, Kathy-Anne Soderberg, A. Paul, Air Force Research Laboratory; N. Barton, A. Brownell, Murray Associates; D. Campbell, Air Force Research Laboratory; C. Craft, Technergetics; M. Fanto, D. Hucul, Air Force Research Laboratory; A. Klug, Griffiss Institute; M. LaHaye, Air Force Research Laboratory; M. Macalik, Booz Allen Hamilton; K. Scalzi, Technergetics; J. Schneeloch, Air Force Research Laboratory; M. Senatore, Griffiss Institute; E. Sheridan, National Academies of Sciences, Engineering, and Medicine; D. Sica, Griffiss Institute; A. Smith, Z. Smith, C. Tison, Air Force Research Laboratory; C. Woodford, Griffiss Institute** **INVITED**

Effective and efficient ways to connect disparate qubit technologies is an outstanding challenge in quantum information science. However, the ability to interface different qubit modalities will have far-reaching implications for quantum computing and quantum networking. Here we present plans and progress toward interfacing trapped ion, superconducting, and integrated photonic qubits for the purpose of entanglement distribution in a quantum network. We will also discuss how this work connects to the AFRL distributed quantum networking testbed.

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4:20pm **QS+EM+MN+NS-WeA-7 Superconductor/Semiconductor Heterostructures for Quantum Computing Applications, Chris Palmström, University of California, Santa Barbara** **INVITED**

Superconductor/semiconductor heterostructures have potential for quantum computing applications. Coupling superconductivity to near surface quantum wells (QW) and nanowires of high spin-orbit semiconductors have allowed the observation of zero bias peaks, which can be a signature of, but not proof of, Majorana Zero Modes, a key ingredient for topological computing. These results of induced superconductivity pave the way for lithographically defined complex superconductor/semiconductor nanostructured networks necessary for quantum computation.

Our efforts have focused on developing high mobility of near surface quantum wells of the high spin-orbit semiconductors InAs, InSb and InAs_{1-y}Sb_y. Rather than relying on post growth lithography and top down etching to form semiconductor nanostructures, we have investigated the development of shadow superconductor growth on atomic hydrogen cleaned MOVPE-grown vapor-liquid-solid InSb nanostructures and in-

vacuum chemical and molecular beam epitaxy selective area grown InAs nanostructures. We have identified Sn as an alternative for Al for use as superconductor contacts to InSb vapor-liquid-solid nanowires, demonstrating a hard superconducting gap, with superconductivity persisting in magnetic field up to 4 Tesla. Further, a small island of Sn-InSb exhibits the two-electron charging effect, a clear indication of a supercurrent.

In more conventional superconductor qubits, a dramatic size reduction of the superconducting transmon devices is predicted by the development of merged element transmon devices based on superconductor/semiconductor/superconductor heterostructures. These superconductor/semiconductor/superconductor heterostructures also allow for selective control of conductance modes in planar lateral multi-terminal Josephson Junctions

In this presentation, progress in developing superconductor/semiconductor heterostructures for quantum computing applications will be presented. This will include progress in in-situ patterning and selective area growth, multi-terminal Josephson Junctions and the recent progress towards developing a Si fin based merged element transmon – the FinMET.

5:00pm **QS+EM+MN+NS-WeA-9 High Throughput Measurements of III-V Semiconductor Materials Stack of 2DEG-Based Tunable Couplers, Nicholas Materise, Colorado School of Mines; J. Pitten, University of Colorado at Boulder; W. Strickland, New York University; A. McFadden, National Institute for Science and Technology (NIST); J. Shabani, New York University; E. Kapit, Colorado School of Mines; C. McRae, University of Colorado at Boulder**

Recent success in integrating cryogenic semiconductor classical systems with superconducting quantum systems promises to reduce the room temperature classical signal processing bottleneck. Incorporating semiconductor quantum devices with superconducting ones as tunable couplers and hybrid quantum systems requires quantitative estimates of the loss introduced by those devices. We report loss measurements of the III-V semiconductor stack used in 2DEG-based gatemon qubits and couplers using a superconducting microwave cavity. Extending the high throughput, low-cost substrate measurement method to thin films grown by molecular beam epitaxy, we can investigate surface roughness losses, bulk losses, and interface losses in a single microwave package. As with our previous measurements of substrates, we perform comparison studies with CPW resonators to validate our approach.

5:20pm **QS+EM+MN+NS-WeA-10 Strong Coupling between a Superconducting Microwave Resonator and Low-Damping Magnons Using Vanadium Tetracyanoethylene Thin Films, Q. Xu, H. Cheung, Cornell University; D. Cormode, H. Yusuf, The Ohio State University; Y. Shi, University of Iowa; M. Chilcote, Cornell University; M. Flatté, University of Iowa; E. Johnston-Halperin, The Ohio State University; G. D. Fuchs, Cornell University** **INVITED**

Hybrid quantum systems – in which excitations with distinct origin are hybridized through a resonant interaction – are attractive for quantum technologies because they enable tunability and the ability to combine desirable properties of each excitation. Here we study the hybrid excitation of a superconducting microwave resonator mode and a ferromagnetic resonance mode of vanadium tetracyanoethylene (V[TCNE]_x) thin films. Our work addresses a key challenge for hybrid superconducting resonator-magnon devices: the integration of a low damping thin-film material with microfabricated superconducting circuits. V[TCNE]_x is a molecular-based ferrimagnet with exceptionally low magnetic damping – as low as 5×10^{-5} at room temperature. The ability to grow thin films of this material at low temperature via chemical vapor deposition and pattern it via lift-off processing enables the fabrication of integrated quantum magnon devices using this material. We couple a V[TCNE]_x magnon mode to the mode of a thin-film Nb lumped-element LC resonator and demonstrate strong coupling, characterized by cooperativities in above 10^2 . Characterization of this hybrid resonator-magnon system in both the frequency domain and the time domain reveals hybridization between resonator photons and magnons. This work demonstrates a pathway for scalable and integrated quantum magnonic technologies.

6:00pm **QS+EM+MN+NS-WeA-12 Role of Point Defect Disorder on the Extraordinary Magnetotransport Properties of Epitaxial Cd₃As₂, Jocienne Nelson, A. Rice, C. Brooks, I. Leahy, G. Teeter, M. van Schilfgaarde, S. Lany, B. Fluegel, M. Lee, K. Alberi, NREL**

Three-dimensional topological semimetals host extremely large electron mobilities and magnetoresistances making them promising for a wide

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range of applications including in optoelectronic devices, renewable energy, and quantum information. However, the extent to which disorder influences the properties of topological semimetals remains an open question and is relevant to both the understanding of topological states and the use of topological materials in practical applications. As a particular example, epilayers of the prototypical Dirac semimetal Cd₃As₂ exhibit high electron mobilities despite a having very high dislocation densities.^{1,2}

Native point defects are inevitable in crystalline materials and introduce long and short-range disorder potentials that will impact carrier transport behavior. To understand their role in topological semimetals, we use molecular beam epitaxy to achieve unmatched and systematic control of point defect concentrations in Cd₃As₂. By reducing the concentration of scattering point defects, we increased the mobility from 5000 to 18,000 cm²/Vs and the magnetoresistance from 200% to 1000%. We find good agreement with the guiding center diffusion model, which indicates point defects are essential to the large linear magnetoresistance in topological semimetals.³ However, the degree of linear magnetoresistance, is found to correlate inversely with measures of disorder. Our results demonstrate the importance of engineering high quality material with dilute concentrations of point defects to optimize the magnetoresistance properties in topological semimetals.⁴

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[1] J. N. Nelson, A. D. Rice, C. Brooks, I. A. Leahy, G. Teeter, M. Van Schilfgaarde, S. Lany, B. Fluegel, M. Lee, K. Alberi *arXiv:2206.10023* (2022).

Advanced Surface Engineering Division Room 317 - Session SE+MN+PS+TF-WeA

Vapor Deposition Technologies and New Trends in Surface Engineering

Moderators: Jianliang Lin, Southwest Research Institute, Filippo Mangolini, The University of Texas at Austin

2:20pm SE+MN+PS+TF-WeA-1 Breaking the Back-Attraction by Bipolar HiPIMS Bursts, *Rajesh Ganesan*, University of Illinois at Urbana-Champaign
INVITED

Limiting the back-attraction of ions is crucial to increase the deposition rate in HiPIMS processing. Back-attraction can be considerably limited by bipolar plasma bursts in which a positive voltage pulse is applied instantaneously after the negative voltage pulse. Energy-resolved mass spectroscopy confirms that, in addition to the increased flux, the energy of the target metal ions travelling from the target to the substrate is also increased, as a function of positive pulse length. Amorphous carbon coatings have been deposited by bipolar HiPIMS (BiPIMS) as a case study. The increased energy of the depositing flux led to a higher density of the carbon coatings and a significant reduction in the incorporation of the sputter gas atom, argon, was observed in the coatings. Langmuir probe measurements suggest the optimum plasma density window to minimize arc generation and reduce the probability of generated arcs moving away from the target racetrack, which results in smoother coatings. BiPIMS voltage pulses of optimized length and magnitude help to coat high quality amorphous carbon coatings with excellent machining functionalities.

3:00pm SE+MN+PS+TF-WeA-3 Experimental and Theoretical Study of the Thermal Shock Behavior of MAX Phase Thin Films, *Matej Fekete*, C. Azina, P. Ondračka, L. Löfler, D. Bogdanovski, RWTH Aachen University, Germany; D. Primetzhofer, Uppsala University, Sweden; M. Hans, J. Schneider, RWTH Aachen University, Germany

Components subjected to rapid temperature changes are prone to thermal shock, which may result in damage or catastrophic failure. Thus, thermal shock resistance is one of the performance-defining properties for an application where extreme temperature gradients are required. The thermal shock resistance can be described by the thermal shock parameter (R_T), which depends on the flexural strength, thermal conductivity, Poisson's ratio, linear coefficient of thermal expansion, and elastic modulus. In this study, these thermomechanical properties of Ti₃AlC₂ and Cr₂AlC MAX phase coatings are investigated by both experiment and theory. The R_T of Ti₃AlC₂ obtained through quantum mechanical predictions

is in good agreement with the experimentally obtained R_T . However, for Cr₂AlC, the theoretical predictions result in approximately two times larger R_T than experiments. This difference may be caused by omitted spin-polarization in the calculation of the electronic part of the thermal conductivity. Correlating the studied MAX phase thin films, both experiments and theory indicate superior fracture behavior of Ti₃AlC₂ in comparison to Cr₂AlC. This is attributed primarily to the higher thermal conductivity of Ti₃AlC₂.

4:20pm SE+MN+PS+TF-WeA-7 Combinatorial Application of Advanced Characterization Methods to Illuminate the Role of Interfaces in Multilayer Coatings, *Nina Schalk*, C. Kainz, F. Frank, Montanuniversität Leoben, Austria; C. Czettl, M. Pohler, CERATIZIT Austria GmbH, Austria; M. Tkadletz, Montanuniversität Leoben, Austria
INVITED

The microstructural characterization of multilayer coatings and their interfaces is challenging, especially if the layer thicknesses are only in the nm range. Within this talk, two model coatings are used to evaluate the suitability of several characterization methods for the investigation of their microstructure and interfaces on different length scales. The fine grained cathodic arc evaporated ZrN/TiAlN and the rather coarse grained chemical vapor deposited TiCN/TiC multilayer model coatings exhibit different bilayer thicknesses and layer thickness ratios and thus allow also insight into the effect of the layer thickness on coherency, grain size and strain state. Starting with methods such as scanning electron microscopy and laboratory X-ray diffraction, an overview of the coating structure and information on the average strain/stress state can be obtained. Depending on the grain size and individual layer thickness, high resolution electron backscatter diffraction allows a more detailed insight into the microstructure and strain state of individual layers. In addition, information about gradients of strain/stress across the coating thickness is accessible by cross-sectional X-ray nanodiffraction. However, for a detailed investigation of the interfaces, the application of high resolution methods such as transmission electron microscopy and atom probe tomography is indispensable, providing information about lattice misfits and related strain evolution in the layers as well as on the sharpness of the interfaces in terms of elemental distribution down to the atomic scale. The present talk highlights that for the characterization of the different multilayer systems the combinatorial application of different characterization methods is possible and reasonable.

5:00pm SE+MN+PS+TF-WeA-9 Influence of Al-Content on Structure, Mechanical Properties and Thermal Stability of Reactively Sputtered AlTaTiVZr High-Entropy Nitride Coatings, *Alexander Kirnbauer*¹, TU Wien, Austria; S. Kolozsvári, Plansee Composite Materials GmbH, Germany; P. Mayrhofer, TU Wien, Austria

In the field of materials research, a novel alloying concept, so-called high-entropy alloys (HEAs), has gained particular attention within the last decade. These alloys contain 5 or more elements in equiatomic or near-equiatomic composition. Properties, like hardness, strength, and toughness can be attributed to the specific elemental distribution and are often superior to those of conventional alloys. In parallel to HEAs also high-entropy ceramics (HECs) moved into the focus of research. These consist of a solid solution of 5 or more binary nitrides, carbides, oxides, or borides. Within this work, we investigate the structure and, mechanical properties of thin films based on the high-entropy concept, with particular emphasis on the thermal stability, dependent on the Al content in AlTaTiVZr thin films.

Therefore, AlTaTiVZr nitride coatings were reactively sputtered in a lab-scale sputter deposition facility using a single powder-metallurgically produced composite target and Al cubes placed along the racetrack to increase the Al content within the coatings. The coatings in as-deposited state show a fine-columnar growth and crystallise in a single-phase face-centred cubic (fcc) structure. The hardness of our coatings in as-deposited state is ~32.8 GPa and relatively independent on the Al-content. We studied the influence of the Al content on the thermal stability by investigating the structural evolution of our coatings by DSC and powder X-ray diffraction, as well as nanoindentation upon vacuum annealing. The study reveals a distinct influence of the Al-content on the decomposition of the solid solution into an fcc-matrix and Al-rich domains.

¹ 2021 ASED Young Investigator Awardee

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5:20pm **SE+MN+PS+TF-WeA-10 Ternary Transition Metal Diborides – Future Defect Engineered Protective Coating Materials?**, A. Hirle, L. Zauner, C. Fuger, A. Bahr, R. Hahn, T. Wojcik, T. Glechner, Christian Doppler Laboratory for Surface Engineering of high-performance Components, TU Wien, Austria; J. Ramm, O. Hunold, Oerlikon Balzers, Oerlikon Surface Solutions AG, Liechtenstein; P. Polcik, Plansee Composite Materials GmbH, Germany; **Helmut Riedl**, TU Wien, Austria

In the progression of novel protective thin film materials, the attention for transition metal diborides (TMB₂) substantially increased during the last years. The unique strength of their hybridized covalent bonds combined with their hexagonal close-packed (hcp) structures is a big advantage and limiting factor at the same time. The related brittleness, variety of crystal structures, and stoichiometries depict significant challenges for a broad usage of these structurally imperfect coating materials. Furthermore, the formation of non-adherent and volatile oxide scales is also a major limiting factor.

Within this study, we want to address these specific challenges on various ternary model systems within group IV to VI transition metal diborides (e.g. TM_{1-x}X_yB_{2+z} prototypes). As structural defects play a major role for the phase formation of the two characteristic hexagonal structure types (α -AlB₂ vs. ω -W₂B_{5-x}-prototype), the target composition and ionization degree within the plasma, has been systematically correlated with the deposition parameters for non-reactive DCMS and HiPIMS depositions. In addition, different alloying concepts for enhancing the ductile character – by microstructural design of imperfect grain boundary structures [1, 2] – as well as oxidation resistance – up to 1200 °C through Si alloying [3] – of these superhard ternary diborides will be discussed in detail. To describe all these relations comprehensively, we correlated the synthesis parameters with structural and morphological evolution using XRD, HR-TEM, APT, as well as micro-mechanical testing methods. Furthermore, specific aspects have also been described by atomistic modelling (DFT).

Keywords :Ternary Borides; Protective Coatings; Defect Engineering; High Temperature Oxidation;

[1] T. Glechner, H.G. Oemer, T. Wojcik, M. Weiss, A. Limbeck, J. Ramm, P. Polcik, H. Riedl, Influence of Si on the oxidation behavior of TM-Si-B_{2+z} coatings (TM = Ti, Cr, Hf, Ta, W), *Surf. Coat. Technol.* 434 (2022) 128178.

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5:40pm **SE+MN+PS+TF-WeA-11 Influence of Interplay of Substrate Template Effects and Bias Voltage on the Microstructure of Cathodic Arc Evaporated Fcc-Ti_{0.5}Al_{0.5}N Coatings**, **Michael Tkadletz**, N. Schalk, H. Waldl, Montanuniversität Leoben, Austria; B. Sartory, J. Wosik, Materials Center Leoben Forschung GmbH, Austria; C. Czettl, M. Pohler, CERATIZIT Austria GmbH, Austria

Ever since the implementation of hard coatings as wear protection for cutting tools, their microstructural design has been of major interest. While the effect of the deposition parameters, such as the applied bias voltage or the substrate temperature, on the microstructure are frequently investigated and rather well understood, commonly less attention is paid to the used cemented carbide substrates. Yet properties like their phase composition and carbide grain size significantly influence the resulting coating microstructure. Thus, within this work substrate template effects are studied on fcc-Ti_{0.5}Al_{0.5}N coatings grown by cathodic arc evaporation onto cemented carbide substrates with different WC grain sizes. A systematic variation of the bias voltage resulted in coarse, intermediate and fine grained coating microstructures, which revealed substrate template-based coating growth at low bias voltages and bias dominated coating growth at high bias voltages. In addition, a strong influence of the applied bias voltage on the resulting preferred orientation of the deposited coatings was observed, providing the basis to tailor the texture to 100, 110 or 111. Elaborate X-ray diffraction and electron microscopy studies contributed to gain further understanding of the substrate template effects and revealed that implementation of a suitable baselayer offers the possibility to effectively prevent any influence of the used substrate on the microstructural evolution of the coating. Supplementary micromechanical experiments illuminated the impact of microstructure, template and non-template based coating growth on the obtained mechanical properties. The obtained results set the fundament to implement tailored microstructures with designed gradients of crystallite size, preferred orientation and consequently mechanical properties, which, as required, either utilize substrate template effects or avoid them.

6:00pm **SE+MN+PS+TF-WeA-12 Super Hard High Temperature TaC-Based Superlattice Protective Coatings Prepared by Magnetron Sputtering**, **Barbara Schmid**, TU Wien, Austria; S. Kolozsvari, Plansee Composite Materials GmbH, Germany; P. Mayrhofer, TU Wien, Austria

Transition metal carbides belong to ultra-high temperature ceramics (UHTC) and are particularly valued for their high thermal and mechanical stability as well as melting points of even above 4000 °C. Therefore, those materials are especially interesting for the application as protective coatings. However, a considerable limitation of these materials is their high inherent brittleness. Inspired by the success of nanolayered superlattice architecture—shown to enhance both hardness and toughness of transition metal nitrides like TiN/CrN or TiN/WN—we developed superlattice films based on TaC. These combinations are motivated by ab initio density functional theory calculations exhibiting large and small shear modulus and lattice parameter misfits. Our coatings are prepared via non-reactive DC and pulsed DC magnetron sputtering using binary carbide compound targets. In our study, we want to compare TaC-based superlattice systems and investigate the influence of the superlattice architecture on material characteristics like mechanical, thermal and electrical properties. Apart from nanoindentation and micromechanical cantilever testing for hardness and fracture toughness, material stability at elevated temperatures as well as thermoelectrical properties are being characterized.

Electronic Materials and Photonics Division Room 304 - Session EM+MN+TF-ThM

Wide and Ultra Wide Band Gap Materials and Devices

Moderators: Erica Douglas, Sandia National Laboratories, **Rehan Kapadia**, University of Southern California, **Rachael Myers-Ward**, U.S. Naval Research Laboratory

8:00am **EM+MN+TF-ThM-1 What Can We Do With Ga₂O₃?**, **Man Hoi Wong**, University of Massachusetts Lowell **INVITED**

The past few decades have witnessed technological innovations driven by physical electronics solutions embodying novel materials and device concepts that fundamentally change our lives today. Ultrawide-bandgap semiconductors represent a new area of intensive research covering a wide spectrum of materials, physics, devices, and applications. As the critical electric field of avalanche breakdown increases super-linearly with increasing bandgap energy, ultrawide-bandgap semiconductors can address critical needs across many areas including energy-efficient power switching, radio-frequency power, and electronics in harsh thermal or radiation environments. I will illustrate efforts to pursue these visions with Gallium Oxide (Ga₂O₃) devices, which have been making rapid strides thanks to ongoing breakthroughs in crystal growth and device processing technologies. Demonstrations of multi-kilovolt breakdown, normally-off operation, vertical device concepts, and heterostructures have positioned Ga₂O₃ devices as relevant contenders for practical applications. In this talk, the achievements on various types of Ga₂O₃ power switches and rectifiers will be reviewed. Materials science pertinent to the implementation of those device concepts will be highlighted. Several approaches to address challenges related to field management and doping will be discussed, using our recent work on enhancement-mode Ga₂O₃ power transistors as an illustration. We are also developing a novel Ga₂O₃ ultrahigh-speed transistor concept that harnesses quasi-ballistic transport effects through heterojunction engineering to reduce carrier transit delay. Such a device can simultaneously serve as an effective spectroscopy tool for studying hot-carrier dynamics in Ga₂O₃. This as well as other types of Ga₂O₃ quantum devices have seen scant experimental and theoretical developments to date and represent a fertile ground for research.

8:40am **EM+MN+TF-ThM-3 Controlled Growth of Epitaxial Ga₂O₃ Polymorphs for Ultra-Wide Bandgap Semiconductor Devices**, **Lisa Porter**, **K. Jiang**, **J. Tang**, **M. Cabral**, **R. Davis**, Carnegie Mellon University, USA

Gallium oxide (Ga₂O₃) is attracting increased interest for electronics that can operate in extreme conditions, such as high power, high temperature and high radiation fluxes. This ultra-wide bandgap semiconductor has an interesting feature in that it exists in different phases, or polymorphs. β-Ga₂O₃ is thermodynamically stable at atmospheric conditions up to its melting point and is therefore the phase produced in melt-grown, single-crystal substrates. Epitaxial films of the other metastable polymorphs, however, are also of interest because they possess unique properties – such as high spontaneous polarization, ferroelectricity, or ferromagnetism – that could lead to new types of heterostructure devices. In this presentation we will summarize our results on the growth of epitaxial films of phase-pure vs. mixed-phase ε(κ), β, and γ-Ga₂O₃ using metal-organic chemical vapor deposition. We will focus on variables (temperature, triethylgallium (TEG) flow rate, and type of substrate) that have led to optimum control over the resulting polymorph and its microstructure, as characterized using x-ray diffraction (XRD), scanning electron microscopy, and high-resolution transmission electron microscopy (TEM). For example, for growth on (0001) sapphire substrates the phase composition of a 700-nm-thick epitaxial layer – from nominally 100% ε(κ) to 100% β-Ga₂O₃ – can be controlled by varying the substrate temperature (470 °C to 570 °C) and TEG flow rate (0.29 sccm to 2.1 sccm). We also show that nominally single-phase γ-Ga₂O₃ and β-Ga₂O₃ epitaxial films are produced under the same growth conditions (in the same growth run) by employing different substrates. High-resolution TEM and XRD ω-2θ and phi-scans suggest that the γ-Ga₂O₃ films are single crystal.

9:00am **EM+MN+TF-ThM-4 Plasma Enhanced-ALD Amorphous Gallium-Oxide Channel Thin Film Transistors for Back-End-of-Line Integration**, **Charlotte Van Dijk**, Helmholtz-Zentrum -Berlin für Materialien und Energy, Germany; **F. Maudet**, Helmholtz-Zentrum-Berlin für Materialien und Energy, Germany; **S. Banerjee**, **V. Deshpande**, **C. Dubourdieu**, Helmholtz-Zentrum Berlin für Materialien und Energy, Germany

Amorphous metal oxide semiconductors exhibit promising properties such as high mobility at low deposition temperatures (< 400°C) and hence are widely investigated as channel materials for thin film transistors (TFT). The low processing temperature also enables their integration on the back-end-of-line (BEOL) of Si CMOS circuits for More-than-Moore applications. While amorphous Indium Gallium Zinc Oxide (IGZO) and Indium Zinc Oxide (IZO) are the most studied amorphous metal oxides for TFT applications, amorphous gallium oxide (a-GaO_x) is interesting due to its ultrawide bandgap (~4.9 eV) combined with the ability to control the carrier density by varying the oxygen content in it [1]. Thus, a-GaO_x has potential for high voltage TFT, sensing, and memristive device applications. There have been few reports of a-GaO_x TFTs with pulsed laser deposition or solution processing, yet a detailed study of TFTs featuring ALD based a-GaO_x channel has not been reported up to now.

Here TFTs with a-GaO_x channel deposited with plasma-enhanced atomic layer deposition (PE-ALD) are discussed. PE-ALD allows for relatively low deposition temperatures (~ 250°C), uniform and conformal films. We recently showed that the current through the a-GaO_x layer can be increased with shorter O₂ plasma exposure times during PE-ALD as it increases the number of sub bandgap defects in the oxide [2]. We present a detailed study of a-GaO_x back-gated TFTs deposited with short (1s) O₂ plasma times to obtain a conductive channel. We discuss the main device characteristics such as subthreshold slope (SS), threshold voltage and ON current and their dependence on the a-GaO_x channel length and thickness (22, 50, 75 nm) with 20 nm ALD Al₂O₃ as gate oxide. Transistors with SS < 150 mV/dec and an ON/OFF ratio of 10⁵ have been shown for a channel length of 6 μm. Impact of encapsulation of the GaO_x channel with in situ ALD-grown Al₂O₃ and ex situ PECVD-grown SiO₂ on the hysteresis in the transfer characteristics (drain current as a function of gate voltage) of the devices is investigated. A reduction of the hysteresis is achieved after in situ encapsulation of the devices with 2 nm Al₂O₃. Finally, the effect of post-metal annealing on the device performance is discussed.

- [1] J. Kim et al. "Conversion of an ultra-wide bandgap amorphous oxide insulator to a semiconductor", *NPG Asia Materials* 9, e359 (2017)
[2] H. Kröncke et al., "Effect of O₂ plasma exposure time during atomic layer deposition of amorphous gallium oxide." *Journal of Vacuum Science & Technology A* 39, 052408 (2021)

9:20am **EM+MN+TF-ThM-5 Interface Trap State Analysis of ALD-deposited Gate Dielectrics on Gallium Nitride using a Modified C-ψ_s Procedure**, **Brian Rummel**, **L. Yates**, **C. Glaser**, **A. Binder**, **J. Steinfeldt**, **T. Smith**, **P. Sharps**, Sandia National Laboratories; **J. Cooper**, Sonrisa Research; **R. Kaplar**, Sandia National Laboratories

The large breakdown electric field strength and high electron saturation velocity of gallium nitride (GaN) make it an attractive semiconductor for high-power and high-frequency applications. GaN-based power systems greatly exceed the power density capabilities of silicon-based systems and currently rival silicon-carbide-based (SiC) systems. However, GaN has been observed to have large interface trap densities at the gate dielectric/semiconductor interface, which inhibits channel mobility in contemporary MIS devices. In addition, typical gate dielectrics are usually deposited by atomic layer deposition (ALD) rather than being thermally grown due to a lack of a high-quality native oxide for GaN. ALD-deposited dielectrics are often associated with a higher concentration of charged oxide defects that promote significant gate leakage currents and induce large shifts in threshold voltages.

Mitigating these defects in wide band gap devices requires reliable characterization techniques suitable for large-scale device fabrication processes. Typical techniques used to characterize the density of interface states for gate dielectrics, such as the high-low method, require unconventionally large probing frequencies to account for fast trap states associated with wide-bandgap materials. The C-ψ_s technique is a quasi-static capacitance-voltage characterization method known for accurately determining surface potentials in MISCAP structures and has been rigorously demonstrated for SiC-based systems. For GaN systems, trap states located at the insulator/GaN interface or within the ALD-deposited

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dielectric may lead to dynamic charge/discharge processes that are less prevalent in SiC MIS structures with thermally grown oxides and thereby alter the C- ψ _S analysis. In this work, we successfully adapt the C- ψ _S analytical procedure to GaN-based MIS structures by imposing sensible mathematical conditions and accurately measure interface state densities and oxide charges for ALD-deposited gate dielectrics on n-GaN substrates. A range of post-deposition annealing temperatures is investigated to probe how processing conditions may alter defect states associated with alumina or silicon dioxide gate dielectrics. This work highlights recent progress in our endeavor to fabricate robust GaN-based high-power devices and establish reliable wide-bandgap device characterization procedures.

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9:40am **EM+MN+TF-ThM-6 Characterization of Intervalence Band (IVB) Transitions in Boron-Doped Diamond, Souvik Bhattacharya**, University of Illinois at Urbana Champaign; J. Boyd, Case Western Reserve University; A. Hossein, S. Reichardt, University of Luxembourg; N. Maccaferri, Umea University, Sweden; O. Shenderova, Adamas Nanotechnologies Inc.; L. Wirtz, University of Luxembourg; M. Sankaran, University of Illinois at Urbana Champaign; G. Strangi, Case Western Reserve University

Heavily-doped semiconductors are a special class of materials distinct from both their metal and semiconductor counterparts that can exhibit greatly enhanced electrical conductivity¹ and tunable localized surface plasmon resonances (LSPR)²⁻³. For example, boron-doped diamond is a wide band-gap, p-type semiconductor which has elicited interest for quantum computing⁴ and superconductivity⁵. Here, we characterized boron-doped diamond (BDD) powders by valence electron-energy loss spectroscopy (VEELS) using a scanning transmission electron microscope to reveal potentially new electronic transitions within the valence band. The diamond samples were synthesized commercially by high-pressure-high-temperature (HPHT) methods and obtained from Adamas Nanotechnologies. Basic materials characterization such as high-resolution transmission electron microscopy (HR-TEM), core-EELS and micro-Raman spectroscopy were conducted to assess the structure and crystallinity. The boron doping level was determined to be ca. 800 pm by modelling the Fano line shape and shifts of the zone center peak at 1332 cm⁻¹. The majority of our study then focused on the low-loss region of EELS (i.e., VEELS) where we observed an intense and relatively broad signal on the shoulder of the zero-loss peak (ZLP) that was completely absent in a similarly synthesized undoped (intrinsic) diamond sample. The feature was found to vary spatially within the body of each particle and inferred to correlate with the distribution of boron atoms along the diamond crystal planes. Ab-initio calculations were carried out in support of the experiments to calculate the loss function from the dielectric function. We find that intervalence band transitions of valence band electrons can lead to the observed VEELS features, and that these transitions can couple to form a "plasmon-like" excitation.

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Quantum Information Science Focus Topic Room 302 - Session QS+AP+EM+MN+NS+SS-ThM

Systems and Devices for Quantum Computing

Moderators: Vivekananda Adiga, IBM, T.J. Watson Research Center, **Kathy-Anne Soderberg**, Air Force Research Laboratory

8:00am **QS+AP+EM+MN+NS+SS-ThM-1 Effects of Environmental Radioactivity on Superconducting Qubits, L. Cardani, Ambra Mariani**, Istituto Nazionale di Fisica Nucleare, Italy **INVITED**

Environmental radioactivity was recently discovered as a potential limit for superconducting quantum bits.

We review recent works proving that ionizing radiation lowers the coherence of single qubits and induces correlated errors in qubits arrays. We also present preliminary studies showing that operating qubits in a low-radioactivity environment improves their performance. These results fuelled the interest of several European and US groups in further investigating and mitigating radioactivity for next-generation quantum processors.

Using radioactivity measurements and simulations, we estimated the separate contribution of "far" radioactive sources (cosmic rays and laboratory radioactivity) and close materials contamination (chip holder, magnetic shield, ...) on a typical chip, focussing on a qubit prototype developed within the SQMS center. We present such contributions and discuss the possibility of mitigating them in "standard" qubit laboratories or, eventually, in deep underground facilities.

8:40am **QS+AP+EM+MN+NS+SS-ThM-3 Dynamics of a Dispersively Coupled Transmon in the Presence of Noise from the Control Line, Antti Vaaranta**, Bluefors Oy, Finland; M. Cattaneo, University of Helsinki, Italy; R. Lake, Bluefors Oy

In this talk we present theoretical results from a complete description of transmon qubit dynamics in the presence of noise introduced by an impedance-matched resistor (50 Ohm) that is embedded in the qubit control line, acting as a noise source [1]. We derive a model to calculate the qubit decoherence rate due to the noise emanating from this noise source [2]. The resistor is treated, using the Caldeira-Leggett model, as an infinite collection of harmonic LC-oscillators making it a bosonic bath [3]. To obtain the qubit time evolution affected by this remote bath, we start with the microscopic derivation of the Lindblad master equation using the dispersive Jaynes-Cummings Hamiltonian with added inductive coupling to the bath. To solve the resulting master equation, we transform it into a block diagonal form by exploiting its underlying symmetries following Ref. 4. The block diagonalization method reveals that the long time decoherence rate is given by the slowest decaying eigenmode of the Liouvillian superoperator. Moreover, when the readout resonator is in the equilibrium thermal state, the rate of exponential decoherence of the qubit is almost exactly exponential for all times with the predicted rate given by the slowest decaying eigenmode. We also study how the decoherence rate depends on the temperature of the noise source and explore the strong and weak dispersive coupling regimes. The model captures the often used dispersive strong limit approximation of the qubit decoherence rate being linearly proportional to the number of thermal photons in the readout resonator. However, in the dispersive weak limit we predict remarkably better decoherence rates. The model parameters are completely determined by the values of the circuit components, allowing for the exact study of the dynamics on the level of each individual circuit element.

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9:00am **QS+AP+EM+MN+NS+SS-ThM-4 Accurate Microwave Characterization for Superconducting Quantum Technology, Slawomir Simbierowicz**, Bluefors Oy, Finland

Recent breakthroughs in quantum technology have highlighted a need for methods for accurate characterization of cryogenic microwave devices at millikelvin temperatures. In this two-part talk, I will highlight recent progress on microwave measurements at the quantum device reference

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plane including: (1) system noise characterization of amplifier chains, and (2) calibrated S-parameters of qubit drive line components. In the first part, I will discuss an impedance-matched variable temperature noise source which can be installed in a coaxial line of a cryostat. Using the method of hot/cold source with many input noise temperature points, the system noise temperatures of qubit readout amplifier cascades can be determined. I present measurement results in terms of added noise in Kelvins or photons from a four-wave (4WM) mixing traveling wave parametric amplifier (TWPA) [1], a Josephson parametric amplifier [2], 3WM TWPA, and high electron mobility transistor amplifiers [1]. In the second part of the talk, I will present measurements of the 1-port S-parameters of qubit drive line components using a data-based short-open-load calibration at a temperature of 30 mK [3]. The measurement enables us to model systematic errors in qubit state preparation due to non-idealities in qubit control lines such as impedance mismatch. We model the results using a master equation simulation of all XY gates performed on a single qubit. Our work directly addresses the gap between electrical engineering parameters of individual measurement components and performance of the quantum device itself.

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9:20am **QS+AP+EM+MN+NS+SS-ThM-5 Improving Qubit Performance Through Engineering of the Substrate-Josephson Junction Interface**, **Cameron Kopas**, H. Cansizoglu, R. Cochrane, B. Ercan, Rigetti Computing; D. Goronzy, C. Torres-Castaneda, Northwestern University; J. Oh, Ames Laboratory; A. Murthy, Fermi Lab; E. Lachman, Rigetti Computing; A. Romanenko, A. Grassellino, Fermi Lab; M. Kramer, L. Zhou, Ames Laboratory; M. Bedzyk, Northwestern University; J. Mutus, Rigetti Computing; M. Hersam, Northwestern University; K. Yadavalli, Rigetti Computing

INVITED

The performance of a superconducting qubit is often limited by dissipation and two-level systems (TLS) losses. The dominant sources of these losses are believed to come from interfaces and surfaces, likely as a result of fabrication processes, materials, or atmospheric exposure. We show that certain chemical surface treatments can be used to modify the silicon surface before Josephson junction deposition, reducing the number of strongly-coupled TLS, and improving T₁. While identifying specific microscopic sources for loss and TLS is still an open question, targeted characterization of test structures will show which physical changes correlate with performance improvements. We report chemical, structural, and low-temperature microwave characterization of superconducting qubits and films fabricated with different Si surface treatments.

11:00am **QS+AP+EM+MN+NS+SS-ThM-10 Design and Optimal Control of Superconducting Qubits to Achieve Quantum Speed Limits**, **Meenakshi Singh**, Colorado School of Mines, USA

INVITED

Fast two-qubit entangling gates are essential for quantum computers with finite coherence times. The finite interaction strength between qubits introduces a theoretical speed limit on the speed of these two-qubit entangling gates. This speed limit has been analytically found only for a two-qubit system under the assumption of negligible single qubit gate times. Here, we demonstrate such a speed limit experimentally using optimal control on two superconducting transmon qubits with a fixed capacitive coupling and finite single qubit gate times. Furthermore, we investigate the effect of additional couplings on the speed limit, both through introduction of an ancillary qubit as well as through utilization of higher transmon energy states. Finally, we discuss the generalization to many qubit systems where properly leveraging all available couplings can provide dramatic speedups.

11:40am **QS+AP+EM+MN+NS+SS-ThM-12 Atomic Scale Processing for Quantum Computing**, **Harm Knoops**, Oxford Instruments Plasma Technology, Netherlands

INVITED

With the increasing technological readiness of quantum technology (QT) the field has to start focussing on scalable fabrication methods for

quantum bits (qubits) and quantum circuits. This contribution will focus on the enabling role atomic scale processing (ASP) methods such as atomic layer deposition (ALD) and atomic layer etching could play in scaling of QT. The main focus will relate to superconducting qubits and processing of superconducting nanolayers.

Superconducting nanolayers (metals, metal-nitrides) are required for various roles in QT including use in resonators, single-photon detectors, and interconnects.¹ The electrical contacts needed to control the qubits will require non-planar connectivity using superconducting interconnects.² Adequate routes for fabrication of planar superconducting layers exist, but for 3D interconnects or through-silicon vias (TSVs), the excellent conformality of ALD nanolayers could be essential. Although for resonators conformality is not a challenge, ALD's thickness control and uniformity should allow high-quality resonators with low spread in properties. For these superconducting nanolayers, metal-nitride compounds have been identified as particularly promising since they exhibit limited surface oxidation (compared to pure metals such as Nb), combined with relatively high critical temperature (T_c) for superconductivity (e.g., as compared to Al). Despite the challenges that the synthesis of high-quality nitrides pose, plasma ALD has demonstrated the capability to deposit high-quality nitrides (e.g., low O content, high electrical conductivity).³ Furthermore, substrate-biased plasma-ALD offers unique opportunities to obtain and tune high-quality nitrides.⁴ For removal of surface oxides or smoothing of resonator surfaces and interfaces, approaches combining ALD and ALE could be of interest.⁵ Both ALD and ALE are envisaged to be key tools to allow scaling of these devices and advance the QT field.

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Quantum Information Science Focus Topic Room 302 - Session QS+EM+MN+NS-ThA

The Quantum Metrology Revolution

Moderator: Dave Pappas, Rigetti Computing

2:20pm QS+EM+MN+NS-ThA-1 Magnetic Textures in Quantum Materials Revealed by SQUID-on-tip Microscopy, *Ella Lachman*, Rigetti Computing INVITED

Quantum materials are rapidly emerging as the basis for possible novel computation devices. However, fully understanding the interplay between magnetic and electronic excitations prevents us from realizing their full potential. In my talk, I will present the nano-SQUID-on-tip device and the scanning microscope built around it. Originally built to study superconducting vortex dynamics, this microscope has unprecedented magnetic sensitivity and spatial resolution.

I will show how expanding the microscope's range and realizing the microscopic magnetic textures in quantum materials is crucial to the understanding of transport phenomena on the macro scale. This will be demonstrated with two examples from two different types of materials. First, I will show how scanning nanoSQUID-on-tip magnetic imaging of magnetically doped topological insulators reveals the underlying fragility of the Quantum Anomalous Hall effect at elevated temperatures. Then, I will show how with a combination of transport, magnetization, and magnetic imaging of the Weyl semimetal $\text{Co}_3\text{Sn}_2\text{S}_2$, we find that the dynamics of domain walls are responsible for the anomalous transport behavior in the material.

These examples show that better understanding of the microscopic magnetism in these systems reveal new phenomena and deepen our understanding of the interplay between magnetic textures and electronic properties.

3:00pm QS+EM+MN+NS-ThA-3 Quantum-Based Measurements for Pressure and Vacuum and the NIST on a Chip Program, *Jay Hendricks, B. Goldstein*, NIST

The world of pressure and vacuum measurements and standards is currently undergoing a revolution in both measurement traceability, "the fundamental philosophy behind a measurement chain back to primary units", and measurement technology, the "how a measurement is made". This keynote presentation covers a bit of metrology history of how we got to where we are today and gives a forward-looking vision for the future. The role of NIST as a National Metrology institute is described along with an explanation of how and why our world-wide standards changed on May 20th, 2019. The NIST on a Chip program (NOAC) is introduced which seeks to utilize fundamental physics and laws of nature to develop quantum-based sensors and standards that one day may be miniaturized to the chip scale. The technical core of the lecture will be a deeper dive into new research on measurement methods for pressure, the Fixed Length Optical Cavity (FLOC) and for vacuum, the Cold Atom Vacuum Standard (CAVS). What is exciting about these new measurement approaches is that they are both primary (relying on fundamental physics), are quantum-based and use photons for the measurement readout which is key for taking advantage of the fast-growing field of photonics. The FLOC will enable the elimination of mercury barometers pressure standards worldwide and the CAVS will be first primary standard for making vacuum measurements below 1.3×10^{-5} Pa.

3:20pm QS+EM+MN+NS-ThA-4 Materials and Devices for Efficient Quantum Memories and Sensors, *Lee Bassett*, University of Pennsylvania INVITED

Certain point defects in semiconductors exhibit quantum-mechanical features comparable to isolated atoms or molecules, in a solid-state materials platform amenable to nanofabrication, heterointegration with other materials and classical devices, and large-scale system engineering. Well-known quantum point defects such as the diamond nitrogen-vacancy center are leading candidates as robust quantum memories, versatile quantum sensors, and efficient light-matter interfaces. Meanwhile it is increasingly clear that alternative materials and defect systems offer potential advantages and new capabilities for quantum science [1]. However, millions of potential defects exist, and their identification is often tedious and challenging. This talk will introduce the opportunities and challenges of identifying point defects, including several new approaches to

efficiently predict, characterize, and engineer their properties for quantum science and technology.

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Advanced Surface Engineering Division

Room 317 - Session SE+AS+MN+SS-ThA

Mechanical and Tribological Properties of Thin Films and Coatings

Moderators: *Jyh-Wei Lee*, Ming Chi University of Technology, Taiwan , *Filippo Mangolini*, The University of Texas at Austin

3:00pm SE+AS+MN+SS-ThA-3 Differential Impact of Scale Dependent Roughness on Lubricant Infused Surfaces, *Robert Chrostowski, B. Fang, J. Smith, F. Mangolini*, University of Texas at Austin

Lubricant Infused Surfaces (LIS), which consist of an engineered surface texture with an absorbed lubricant, have recently emerged as an innovative approach for achieving pressure-stable omniphobicity and for improving tribological performance in the presence of external contaminants. The design of successful LIS heavily relies on the effect of surface texture, which is quantified using a single dimensionless parameter, namely the ratio of the true surface area to the nominal surface area. Previous published studies have thus focused on the evaluation and optimization of microscale patterned morphologies with simple geometries (for which the ratio of the true surface area to the nominal surface area can be determined analytically), such as ordered arrays of pillars. Texture, however, is defined both by these larger-scale structures, and by smaller sub-micron scale asperities called roughness. Roughness can exhibit scale-dependent fractal self-similarity, and the absolute finest scales of roughness can have outsize impact on the quantitative value of the area ratio. Despite the scientific relevance of previous studies on fractal surfaces and the effect of roughness on contact mechanics, our understanding of the effect of surface roughness on the retention of a lubricant is elusive.

Here, we evaluate the lubricant infusion behavior of two different fluorinated polymer lubricants of substantially different molecular size, but similar surface chemistry, on fractal nano-rough boehmitized aluminum surfaces. Power spectral density (PSD) analysis of atomic force microscopy (AFM) topography maps is used to estimate the area ratio for each surface at the length scale of the radius of gyration of the different lubricants. The area ratio values computed from the PSD are then related to true area value that matches predicted spin-coating curves to observed gravimetric ones. The experimental results demonstrate, for the first time, the impact of fractal roughness on the shear-retention of LIS.

The outcomes of this work, providing evidence that different molecular length fluids could experience different quantitative magnitudes of roughness on the same, significantly contribute to our understanding of the impact of scale-dependent roughness on the retention of liquids on engineered surface textures, while enhancing the scalability of LIS systems and their cost-effective implementation in several technological applications.

3:20pm SE+AS+MN+SS-ThA-4 Imperfectly Perfect Coatings for Rolling Bearing Applications, *Esteban Broitman*, SKF B.V. - Research and Technology Development, Netherlands INVITED

Machines with rotating components usually rely on bearings to reduce friction in moving its parts around a fixed axis. The increasing demand for more precise bearings to lower power consumption and heat generation, while simultaneously support increasing applied loads and/or higher speeds, has given place to the use of surface engineering processes.

In the case of bearings, it is widely accepted the advantages of using coatings as the surface process to improve its performance. During the last three decades, advanced coatings have enjoyed a growing interest in several industrial applications because they can be engineered to provide different properties like electrical insulation, low friction, and resistance to corrosion, plastic deformation, etc.

In this talk I will compare the structural, mechanical and tribological properties of two coatings that are used nowadays to improve the

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performance of rolling bearings made of standard bearing steel: they provide lower friction, resistance to surface initiated rolling contact fatigue, and decreased wear: NoWear® (a carbon-based nanostructured coating made by plasma-assisted chemical vapor deposition PACVD) of about 3 μm -thick, and Black Oxide (an iron oxide film made by a chemical conversion method) of about 1 μm -thick. Being coatings produced by different techniques, both have a common feature: they are “*imperfectly perfect coatings*.” Scanning electron microscopy, X-ray photoelectron spectroscopy, and nanoindentation measurements show that, from the microstructural point of view, these coatings are full of “*imperfect*” features, like cracks, voids, porous, columns, and other naughty irregularities. The different mechanisms contributing to the positive tribological behavior of each coating under lubricated conditions will be discussed. I will demonstrate that these coatings, taking advantage of their own different “*imperfect*” features, behave “*perfectly*” from the tribological point of view, and therefore can successfully be used to extend maintenance and life expectancy of specialized rolling bearings.

4:00pm **SE+AS+MN+SS-ThA-6 Tribological Behavior of WC/WCN/CNx Thin Films Deposited by HIPIMS**, Luis Flores-Cova, O. Jimenez, M. Flores, Universidad de Guadalajara, Mexico

Coatings and thin films are used to protect against wear in many applications. If that coating also shows a low coefficient of friction, it brings better benefits, therefore, the research on coatings with these properties is of great interest. In this respect, carbon containing, or carbon-based coatings are the most popular. 52100 alloy used in wear environments has its own disadvantages. Consequently, many coating systems have been deposited on this alloy to improve its wear resistance. In this study, a multilayer coating with carbon content (WC/WCN/CNx) was deposited by High Power Impulse Magnetron Sputtering (HiPIMS) on AISI 52100 alloy. No external heating was applied during the deposition, energetic tungsten ions increase adatoms mobility that enhance adhesion. The thickness and the growth morphology of the films were studied from FE-SEM cross-sectional images. The chemical composition was analyzed by XPS. The structure of the coatings was analyzed by XRD technique. The mechanical properties (hardness and Elastic Modulus) were studied through nanoindentation techniques. The adhesion of coatings to the substrate was measured by means of scratch tests. Wear tests were performed using a tribometer with a pin on disc configuration, using a 10 mm diameter 52100 ball. The wear tracks were analyzed by SEM and the wear volume was obtained by optical profilometry. The coating showed a coefficient of friction lower than 0.3 and the wear rate was reduced 100 times relative to the substrate.

Electronic Materials and Photonics Division

Room 304 - Session EM1+MN+NS-FrM

Piezoelectric, Ferroelectric, and Multiferroic Devices & Microelectronics

Moderators: M. David Henry, Sandia National Labs, Stephen McDonnell, University of Virginia

8:20am EM1+MN+NS-FrM-1 Piezoelectric Adjustable X-ray Optics, Susan Trolrier-McKinstry, Penn State University **INVITED**

Next generation X-ray observatories require lightweight, high throughput optics that maintain a < 0.5 arcsecond resolution. Thin adjustable X-ray mirrors can correct deformations generated from fabrication errors, gravity release, mounting stresses, and thermal variations, maintaining the high angular resolution (< 0.5 arcsecond) and large effective area ($> 2 \text{ m}^2$) required for future X-ray missions. This paper describes fabrication of adjustable mirrors for the Lynx X-ray observatory mission concept. Prototype X-ray mirrors were built on either a $400 \mu\text{m}$ thick curved Corning EAGLE XG[®] glass substrate or on polished Si. In both cases, a Cr/Ir X-ray mirror coating was deposited on the front (concave) side, and an array of $1.5 \mu\text{m}$ thick radio frequency (RF) sputtered $\text{Pb}_{0.995}(\text{Zr}_{0.52}\text{Ti}_{0.48})_{0.99}\text{Nb}_{0.01}\text{O}_3$ (PZT) piezoelectric thin film actuators on the back (convex) side to enable correction of figure errors. A two-layer metal routing scheme with a polymeric insulator was used to independently address 288 actuators on the mirror. The two-layer metal allows narrow kerfs between actuators and increased actuator density. A chrome-iridium layer was deposited on the concave side to function as the X-ray reflective coating for the films deposited on the convex side. Anisotropic conductive film was used to bond thin flexible copper cables to flat edges of the mirror to interface with external control electronics. Improved stress balancing process was achieved using compressively stressed SiO_2 films deposited on the convex side of the mirror to balance the tensile integrated stress of the actuator array while also matching the film thickness distribution. Finite element methods were used to assess the impact of film thickness distributions on the convex and concave substrate surfaces. The resulting models show peak-to-valley figure errors of 105 nm , well within the $1 \mu\text{m}$ peak-to-valley dynamic range of the piezoelectric adjusters. In contrast, when stress compensation was done with an iridium mirror film deposited on the front side, the mismatched thickness distribution results in peak-to-valley figure errors over $3 \mu\text{m}$.

9:00am EM1+MN+NS-FrM-3 Oxide and Nitride Ferroelectric Wurtzite Crystals, Jon-Paul Maria, Penn State University

In the past three years, the demonstration of ferroelectricity in wurtzite-based crystals introduced exciting opportunities to explore and discover new structure-property relationships in novel formulation spaces, and to investigate new integration and device implementations given new process compatibilities. The seminal discovery of ferroelectric $\text{Al}_{1-x}\text{Sc}_x\text{N}$ by Fichtner *et al.* initiated this excitement and was followed by comparable observations of polarization reversal in the structurally similar $\text{Al}_{1-x}\text{B}_x\text{N}^2$ and the $\text{Zn}_{1-x}\text{Mg}_x\text{O}^3$ systems.

In this presentation our group will present recent results that demonstrate the structure-process-property relationships in the B-substituted AlN and Mg-substituted ZnO nitride and oxide systems. The B-substituted materials exhibit square hysteresis loops with polarization values between $150 \mu\text{C}/\text{cm}^2$ and $120 \mu\text{C}/\text{cm}^2$ when boron concentrations range between 2% and 15% respectively. Coercive field values fall with additional boron, from $5.5 \text{ MV}/\text{cm}$ to about $5 \text{ MV}/\text{cm}$ at B saturation. Bandgap values are approximately 5 eV or above in all cases. Material can be prepared between $100 \text{ }^\circ\text{C}$ and $350 \text{ }^\circ\text{C}$ with very little difference in electrical properties. W bottom and top electrodes are used in all cases. Capacitors can be prepared down to 50 nm thick before leakage current becomes problematic during low frequency hysteresis measurements. First principles calculations that rationalize the unit cell volume, bond angle distribution, and remanent polarization will be presented.

Comparable results are found in the $\text{Zn}_{1-x}\text{Mg}_x\text{O}$ system. Between 25% and 35% Mg substitution, square hysteresis loops with remanent polarization values above $100 \mu\text{C}/\text{cm}^2$ are readily achieved. Transmission measurements show bandgap values between 4.0 eV and 4.2 eV in this range. In comparison to AlBN, coercive field values for ZMO are as low as $1.7 \text{ MV}/\text{cm}$. As is the case with AlBN and AlScN, sustaining high insulation resistance to arbitrarily low thickness is challenging, the current thinness limit for low-leakage switching is $\sim 125 \text{ nm}$. SHG analysis will also be

presented for the ZMO system – preliminary measurements suggest values comparable to ferroelectric niobates.

9:20am EM1+MN+NS-FrM-4 Development and Processing of $\text{Al}_{1-x}\text{Sc}_x\text{N}$ ($x < 0.40$) Films for Resonator and Filter Applications, Giovanni Esteves, S. Yen, T. Young, Sandia National Laboratories; Z. Tang, The University of Pennsylvania; E. Schmidt, L. Gastian, M. Henry, T. Bauer, C. Nordquist, Sandia National Laboratories; R. Olsson, The University of Pennsylvania

As the development of aluminum scandium nitride ($\text{Al}_{1-x}\text{Sc}_x\text{N}/\text{AlScN}$) films continues to be pushed towards higher Sc content, fabricated devices yield insight into the challenges associated with processing while demonstrating increased electromechanical coupling coefficients (k_t^2) over AlN. The addition of Sc into AlN presents film development and fabrication challenges that increase with higher Sc content such as the reduction of abnormal grains (AG), higher compressive stress, and etching. The development of $\text{Al}_{0.6}\text{Sc}_{0.4}\text{N}$ films using a single-alloyed target poses a significant challenge in terms of managing stress and the density of AG. Compressive stress help in reducing the amount of AG density through tuning the Ar/N_2 flow and pressure, but the magnitude of stress needed to achieve a low density of AG exceed -600 MPa . The use of certain metal templates aid in reducing AG density but are not sufficient to achieve AG-free films. Etching AlScN leads to long etch times due to slow etch rates of $25 \text{ nm}/\text{min}$ and result in sidewall angles of $\sim 74^\circ$. Nevertheless, AlScN lamb wave resonators (LWR) have been fabricated to demonstrate k_t^2 over 10%. Additionally, LWR with varying k_t^2 were interconnected to fabricate ladder filter configurations to determine that amount of bandwidth increase that can be achieved over AlN. Though AlScN demonstrates higher k_t^2 , that lead to higher bandwidth, pushing this current technology to achieve more desirable metrics requires more stringent process quality.

SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

9:40am EM1+MN+NS-FrM-5 Formation of Aluminum Scandium Nitride Microelectromechanical Systems Via Etching in Aqueous Potassium Hydroxide (KOH), Zichen Tang, M. D'Agati, R. Beaucejour, S. Sofronici, J. Zheng, K. Kaylan, University of Pennsylvania; G. Esteves, Sandia National Laboratories; R. Olsson, University of Pennsylvania

We report on the etch rate of sputter deposited piezoelectric and ferroelectric Aluminum Scandium Nitride ($\text{Al}_{1-x}\text{Sc}_x\text{N}$) thin films in aqueous potassium hydroxide (KOH). Specifically, we report on the vertical etch rate, lateral etch rate, and sidewall angle as a function of the scandium alloying ratio (x), temperature, and KOH concentration. As the scandium alloying ratio is increased, the vertical etch rate in 30% KOH at $45 \text{ }^\circ\text{C}$ is reduced from $> 100 \text{ nm}/\text{s}$ for AlN to $< 4 \text{ nm}/\text{s}$ for $\text{Al}_{64}\text{Sc}_{36}\text{N}$. The lateral etch rate, however, follows a very different trend, arriving at a minimum values of $0.05 \text{ nm}/\text{sec}$ for $\text{Al}_{88}\text{Sc}_{12}\text{N}$. This is in contrast to the much higher lateral etch rates observed for both AlN and $\text{Al}_{64}\text{Sc}_{36}\text{N}$ of $2 \text{ nm}/\text{s}$. These trends in vertical and lateral etch rate are shown to hold for KOH concentrations from 10 to 30% and etch temperatures from 45 to $65 \text{ }^\circ\text{C}$. We show that the etched sidewall angle can be predicted from a combination of the crystal structure and the vertical and lateral etch rates. We report a technique that utilizes the crystal structure and the vertical and lateral etch rates to form vertical (i.e. 90°) sidewalls solely from aqueous KOH etching. The ability to control the sidewall angle is vitally important in the formation of microelectromechanical systems (MEMS). We report on several piezoelectric MEMS devices fabricated utilizing the KOH etching processes. Finally, we report on the etching of AlScN as a function of ferroelectric polarization.

10:00am EM1+MN+NS-FrM-6 Interface Reactions During the Ferroelectric Switching of HfZrO Thin Films on InAs, A. Irish, Y. Liu, R. Atle, A. Persson, R. Yadav, M. Borg, L. Wernersson, Rainer Timm, Lund University, Sweden

Traditional MOSFET-based electronic components have reached severe bottlenecks regarding data handling speed and power dissipation. A very promising alternative approach builds on MOS material stacks with thin ferroelectric oxide films in novel device architectures for e.g. steep-slope transistors, neuromorphic networks, or in-memory computation [1]. Hf_{1-x}Zr_xO₂ (HZO) films grown by atomic layer deposition are widely used in this context, due to their excellent film quality and conformity with existing semiconductor technology. Ferroelectric MOS devices based on III-V semiconductors are especially promising for high-speed applications due to the high charge carrier mobility of e.g. InAs. Furthermore, InAs/HZO/TiN devices have shown an unexpectedly high remanent polarization of the ferroelectric film [2]. In spite of the excellent electrical performance, only little is known about the structure, chemical composition, and switching dynamics of the semiconductor-ferroelectric oxide interface. We have

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previously used X-ray photoemission spectroscopy (XPS) to investigate interfaces of ferroelectric HZO [3], but *in situ* structural characterization obtained during the ferroelectric switching has been lacking until now.

Here, we present operando hard X-ray photoelectron spectroscopy (HAXPES) results from ferroelectric InAs/HZO/TiN MOS devices obtained during electrical biasing and switching. We observe an interface layer consisting of In- and As-oxides at the InAs/HZO interface. As 2p and In 3d core level spectra were obtained after subsequent switching processes of a “positive-up-negative-down” (PUND) series, showing a reproducible increase of the amount of interface oxide upon upward polarization and a decrease upon downward polarization. Thereby, electrical PUND cycles confirm the ferroelectric nature of the MOS device. Such a redox reaction at the semiconductor-oxide interface upon ferroelectric switching has – to our knowledge – not been reported before. Furthermore, we observe that the major fraction of the applied bias does not drop over the 10 nm thin HZO layer, but instead over the thin InAs-oxide interface layer.

These observations are challenging the established understanding of ferroelectric behavior in thin oxide films and are a key to understanding the superior performance of III-V/HZO based devices.

- [1] M. Park et al., MRS Commun. **8**, 795 (2018).
- [2] A. Persson et al., Appl. Phys. Lett. **116**, 062902 (2020).
- [3] R. Athle et al., ACS Appl. Mat. Int. **13**, 11089 (2021).

10:20am **EM1+MN+NS-FrM-7 The Effect of Hf Doping on Piezomagnetic Properties of FeCo for Magnetolectric Heterostructure Devices, Thomas Mion, K. Bussmann, M. Staruch, P. Finkel**, US Naval Research Laboratory

New developments in magnetolectric devices have demonstrated increased energy efficiency and temperature stability with reduced size compared to current technologies. Artificial magnetolectrics, built on the combination of ferromagnetic magnetostrictive materials structurally coupled to piezoelectric and ferroelectric materials, display the ability to control magnetic properties of the ferromagnet with electric voltage across the piezo/ferroelectric layer. The best performance requires the implementation of soft magnetic materials with large magnetostriction and large voltage-induced strain in the piezo/ferroelectric layer. Processing requirements for device fabrication often complicate the realization of these combined qualities as inherent stresses from the deposition technique are often detrimental to the magnetolectric functionality. Solutions to these problems are rarely reported though alloying of FeCo and subsequent metalloid substitutions such as $(\text{Fe}_{0.5}\text{Co}_{0.5})_{1-x}\text{C}_x$, and $(\text{Fe}_{0.5}\text{Co}_{0.5})_{1-x}\text{B}_x$, have proven successful in reducing the coercive field while retaining high magnetostriction and piezomagnetic properties [1,2].

In this work we present the systematic study of sputter-deposited Hf-doped $\text{Fe}_{50}\text{Co}_{50}$ alloy thin films with a focus on the correlation between film stress and magnetic softness and find an inflection point from tensile to compressive stress with increasing Hf composition. Scanning electron microscopy (SEM) and X-ray diffraction (XRD) of the $(\text{Fe}_{0.5}\text{Co}_{0.5})_{1-x}\text{Hf}_x$ system reveal the magnetic softening is also correlated to emergence of an amorphous phase with reduced grain size for these sputter-deposited films. We will show the utilization of this new alloy in a multiferroic MEMS resonator device demonstrating a high magnetolectric response required for magnetic sensors.

- [1] Phys. Rev. Applied 12, 034011 (2019)
- [2] Appl. Phys. Lett. 91, 182504 (2007)

Advanced Surface Engineering Division

Room 317 - Session SE+MN+PS-FrM

Nanostructured and Multifunctional Thin Films and Coatings II

Moderators: Jyh-Wei Lee, Ming Chi University of Technology, Taiwan , Filippo Mangolini, The University of Texas at Austin

8:20am **SE+MN+PS-FrM-1 New Challenges and Opportunities for Hard and Superhard Coatings, Aharon Inspektor**, Carnegie Mellon University **INVITED**

Many hard, superhard and lubricious coatings with superior mechanical properties, thermal stability and chemical resistance are being developed and applied for surface protection in harsh and demanding applications. In this paper we will discuss the status and foreseen trends in PVD hard, superhard and lubricious films.

First, we will review the design of current multifunctional hard coatings and their applications in metal cutting, in automotive and in aerospace

industries. Next, we will examine how the Forth Industrial Revolution, a multi-level connectivity of sensors and systems, with “Smart Manufacturing”, computer controlled automated facility system, will affect future usage of multifunctional coatings. The talk will conclude with a critical discussion of the resultant challenges and opportunities for next generation of hard, superhard and lubricious coatings.

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